**Exploring the activity of vanadium, niobium and tantalum PNP pincer complexes in the hydrogenation of phenyl-substituted C≡N, C=N, C≡C, C=C and C=O functional groups**

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**Table S1**. Relative energies (kJ/mol) of M-PNP (**1M**) and H-M-PNHP (**2M**) isomers in *C*s and *C*1 symmetrical geometries

|  |  |  |  |
| --- | --- | --- | --- |
| M-PNP (**1M**) | | | |
| Symmetry | V | Nb | Ta |
| *C*s | 6.6 | 5.6 | 5.4 |
| *C*1 | 0.0 | 0.0 | 0.0 |
| H-M-PNHP (**2M**) | | | |
|  | V | Nb | Ta |
| *C*s | 0.0 | 0.0 | 0.0 |
| *C*1 | 7.3 | 6.8 | 7.8 |

**Table S2**. Computed bond lengths (Å) of M-PNP (**1M**) and H-M-PNHP (**2M**)

|  |  |  |  |
| --- | --- | --- | --- |
|  | **1V** | **1Nb** | **1Ta** |
| M-N | 1.998 | 2.155 | 2.127 |
| M-P | 2.433 | 2.596 | 2.573 |
| M-L1 | 1.723 | 1.890 | 1.876 |
| M-L2 | 1.737 | 1.890 | 1.877 |
|  | **2V** | **2Nb** | **2Ta** |
| M-N | 2.273 | 2.412 | 2.387 |
| M-P | 2.411 | 2.581 | 2.559 |
| M-L1 | 1.730 | 1.895 | 1.881 |
| M-L2 | 1.742 | 1.912 | 1.893 |
| M-H | 1.750 | 1.928 | 1.912 |
| N-H | 1.017 | 1.018 | 1.018 |

**Table S3**. Natural charge (/e), natural bond orbitals and atomic hybrid contributions for the  and  bonds of M-PNP(**1M**) and H-M-PNHP(**2M**).

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  |  | **1V** | **1Nb** | **1Ta** |
| Natural charge | M | -0.732 | -0.091 | +0.101 |
| N | -0.527 | -0.628 | -0.651 |
| N-M |  | No bond | 17.52%Nb[sp2.11d5.92]  82.48%N[sp1.21] | 16.82%Ta[sp2.25d5.14]  83.18%N[sp1.13] |
|  | 13.90%V[pd1.16]  86.10%N[p] | 11.30%Nb[p1.14d]  88.70%N[p] | 11.20%Ta[p1.17d]  88.80%N[p] |
| M-NO |  | 21.77%V[sp0.91d1.74]  78.23%N[sp0.5] | 18.69%Nb[sp1.86d2.12]  81.31%N[sp0.49] | 19.00%Ta[sp1.81d2.12]  81.00%N[sp0.48] |
|  | 45.74%V[d]  54.26%N[p] | 40.09%Nb[d]  59.91%N[p] | 36.60%Ta[d]  63.40%N[p] |
|  | 43.80%V[pd7.77]  56.20%N[p] |  |  |
|  |  | **2V** | **2Nb** | **2Ta** |
| Natural charge | M | -1.283 | -0.660 | -0.469 |
| HM | -0.080 | -0.195 | -0.205 |
| N | -0.515 | -0.554 | -0.559 |
| HN | +0.401 | +0.406 | +0.405 |
| M-H |  | 39.74%V [sp5.14d2.83]  60.26%H[s] | 37.79%Nb[sp3.86d2.86]  62.21%H[s] | 37.54%Ta[sp3.85d2.67]  62.46%H[s] |
| M-P |  | 27.82%V [sp2.37d2.19]  72.18%P[sp1.63] | 25.59%Nb[sp2.08d1.73]  74.41%P[sp1.61] | 26.62%Ta[sp2.11d1.75]  73.38%P[sp1.57] |
| N-H |  | 70.42%N[sp2.75]  29.58%H[s] | 71.01%N[sp4.47]  28.99%H[s] | 71.00%N[sp4.65]  29.00%H[s] |
| N-M |  | No bond | 10.48%Nb[sp8.13d6.75]  89.52%N[sp2.42] | 10.82%Ta[sp8.28d6.24]  89.18%N[sp2.22] |
| M-NO |  | 21.17% V[sp2.33d2.28]  78.83%N[sp0.46] | 18.97%Nb[sp1.86d2.03]  81.03%N[sp0.45] | 19.46%Ta[sp1.83d2.11]  80.54%N[sp0.45] |
|  | 43.22% V[pd11.48]  56.78%N[p] | 39.18%Nb[pd13.96]  60.82%N[p] | 36.20%Ta[pd15.02]  63.80%N[p] |
|  | 49.05% V[d]  50.95%N[p] |  |  |

**Table S4**. Wiberg bonding indexes (WBI) of M-PNP (**1M**) and H-M-PNHP (**2M**).

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
|  | **1V** | **2V** | **1Nb** | **2Nb** | **1Ta** | **2Ta** |
| M-N | 0.832 | 0.362 | 0.793 | 0.346 | 0.815 | 0.362 |
| M-P | 0.662 | 0.703 | 0.680 | 0.723 | 0.719 | 0.766 |
| M-L1 | 1.635 | 1.630 | 1.593 | 1.605 | 1.602 | 1.610 |
| M-L2 | 1.611 | 1.638 | 1.600 | 1.619 | 1.607 | 1.634 |
| M-H | -- | 0.708 | -- | 0.775 | -- | 0.801 |
| N-H | -- | 0.790 | -- | 0.784 | -- | 0.785 |

**Scheme S1**. Potential energy surface for M-PNP and H-M-PNHP interconversion

28.5/30.4/28.7

**1M**

+

H2



0.0



6.6/5.6/5.4



102.5/94.8/99.4



**Scheme S2**. Potential energy surface of benzonitrile hydrogenation



0.0

103.3/96.5/97.7

88.0/80.6/88.3

92.9/85.6/92.4

-16.8

**1M**

+

H2

+

Ph-CN

**2M**

+

Ph-CN

**1M**

+

PhCH=NH



28.5/30.4/28.7

102.5/94.8/99.4

**Scheme S3**. Potential energy surface of phenylmethanimine hydrogenation

****

128.0/119.6/122.1

**2M**

+

PhCH=NH

**1M**

+

PhCH2NH2

**1M**

+

H2

+

PhCH=NH



28.5/30.4/28.7

0.0

-48.3

102.5/94.8/99.4

**Scheme S4**. Potential energy surface of Ph-CH=N-CH2-Ph hydrogenation



**1M**

+

PhCH2NHCH2Ph

**2M**

+

PhCH=NCH2Ph

**1M**

+

H2

+

PhCH=NCH2Ph



170.0/155.7/159.6

28.5/30.4/28.7

0.0

-34.8



102.5/94.8/99.4

**Scheme S5**. Potential energy surface of Ph-CH=N-Ph hydrogenation



**1M**

+

H2

+

PhCH=NPh

**2M**

+

PhCH=NPh

**1M**

+

PhCH2NHPh

28.5/30.4/28.7

-45.8

160.3/145.2/149.2



102.5/94.8/99.4

0.0



**Scheme S6**. Potential energy surface of phenylacetylene hydrogenation (HM transfer to C-H)



**1M**

+

PhCH=CH2

**2M**

+

Ph-CCH

**1M**

+

H2

+

Ph-CCH

-143.0

113.1/115.2/120.8

28.5/30.4/28.7



0.0

102.5/94.8/99.4



**Scheme S7**. Potential energy surface of phenylacetylene hydrogenation (HM transfer to Ph-C)



**1M**

+

PhCH=CH2

**2M**

+

Ph-CCH

**1M**

+

H2

+

Ph-CCH

144.6/142.0/149.7

146.1/141.5/142.8

136.0/137.8/140.3

0.0



28.5/30.4/28.7

-143.0

102.5/94.8/99.4



**Scheme S8**. Potential energy surface of styrene hydrogenation



-83.0

**1M**

+

PhCH2CH3

102.5/94.8/99.4

**2M**

+

Ph-CH=CH2

**1M**

+

H2

+

Ph-CH=CH2

115.8/111.0/123.9

132.3/132.7/134.6

118.8/114.4/126.1

0.0



28.5/30.4/28.7

**Scheme S9.** Potential energy surface of benzaldehyde hydrogenation



**1M**

+

H2

+

Ph-CH=O

**2M**

+

Ph-CH=O

**1M**

+

PhCH2OH

0.0

53.1/45.1/72.4

91.4/81.2/83.8

57.0/49.2/56.9

-10.2



102.5/94.8/99.4

28.5/30.4/28.7



**Scheme S10.** Potential energy surface of acetophenone hydrogenation



**1M**

+

PhC(H)(OH)CH3

28.5/30.4/28.7

**2M**

+

PhCOCH3

**1M**

+

H2

+

PhCOCH3

0.0

133.3/116.4/118.5



-6.3

102.5/94.8/99.4

**Table S5.** Optimized Cartesian Coordinates

|  |  |
| --- | --- |
| **H2**  H 0.00000000 0.00000000 0.37255500  H 0.00000000 0.00000000 -0.37255500 | **Ph-C≡N**  C -0.60749500 0.00033600 0.00000400  C 0.09003600 -1.21136200 0.00002700  C 1.47583300 -1.20504300 0.00003700  C 2.16954600 -0.00032600 0.00003200  C 0.09054200 1.21164900 -0.00001300  C 1.47637700 1.20466200 0.00000800  H -0.45907500 -2.14500800 0.00002800  H 2.01657100 -2.14429100 0.00003300  H 3.25361100 -0.00056900 0.00003400  H -0.45810200 2.14557100 -0.00005500  H 2.01750100 2.14368500 0.00000700  C -2.03543700 0.00055900 -0.00003100  N -3.18955900 -0.00032000 -0.00006200 |
| **Ph-CH=NH**  N -1.48633800 2.45239400 0.00000000  C -0.29934900 1.99993000 0.00000000  C 0.00000000 0.56097900 0.00000000  C 1.32840000 0.13547800 0.00000000  C 1.63527000 -1.21890600 0.00000000  C 0.61281900 -2.15844200 0.00000000  C -1.02326600 -0.39138800 0.00000000  C -0.71645300 -1.74108700 0.00000000  H 2.12598800 0.87252200 0.00000000  H 2.67066800 -1.54051000 0.00000000  H 0.84880300 -3.21689900 0.00000000  H -2.05050700 -0.04633200 0.00000000  H -1.51358600 -2.47634600 0.00000000  H 0.58655000 2.65029500 0.00000000  H -1.48806500 3.47113900 0.00000000 | **Ph-CH2NH2**  N 1.82388100 2.18399800 0.00000000  C 0.41156000 1.95635900 0.00000000  C 0.00000000 0.50176500 0.00000000  C -1.36708700 0.21011300 0.00000000  C -1.82437700 -1.09732400 0.00000000  C -0.91836300 -2.15355400 0.00000000  C 0.89455400 -0.56301700 0.00000000  C 0.43989800 -1.87951000 0.00000000  H -2.08260600 1.02741900 0.00000000  H -2.89081800 -1.29492400 0.00000000  H -1.27128400 -3.17864700 0.00000000  H 1.96481800 -0.39416400 0.00000000  H 1.15839300 -2.69199600 0.00000000  H -0.06462900 2.42077100 0.87799300  H 2.18197900 3.11743400 0.00000000  H -0.06462900 2.42077100 -0.87799300  H 2.48449500 1.43636400 0.00000000 |
| **Ph-CH=NCH2-Ph**  C -3.82426600 1.51515500 0.18137100  C -2.57639600 0.96228000 0.41238100  C -2.31890600 -0.36555800 0.05905500  C -3.33515900 -1.12240000 -0.52592900  C -4.58655300 -0.56698900 -0.75721100  C -4.83295300 0.75298700 -0.40374000  H -4.01728500 2.54587700 0.45774600  H -1.78172600 1.54123100 0.86737600  H -3.14054200 -2.15432700 -0.80202200  H -5.36854200 -1.16394900 -1.21288900  H -5.80909700 1.19005300 -0.58268100  C -1.00687900 -0.98251200 0.28865300  N -0.02632800 -0.36607700 0.79970800  H -0.92366500 -2.03803000 -0.01731200  C 1.21033800 -1.09188100 0.98403600  H 1.38224700 -1.16727000 2.06618900  H 1.15300400 -2.12124600 0.59718000  C 2.39590400 -0.38763300 0.36298100  C 3.42867200 -1.13135800 -0.20253500  C 2.49748800 1.00237400 0.37491100  C 4.54695700 -0.50324700 -0.73767900  H 3.35759000 -2.21462300 -0.22820200  C 3.61203900 1.63156600 -0.16317700  H 1.68919000 1.58524800 0.79986100  C 4.64212100 0.88191200 -0.71937400  H 5.34118900 -1.09806200 -1.17556800  H 3.67628800 2.71430400 -0.14968000  H 5.51120400 1.37514900 -1.14039900 | **Ph-CH2NHCH2-Ph**  C -3.61290100 1.51458600 0.30367300  C -2.33572200 0.97242600 0.33146100  C -2.09265300 -0.30201800 -0.18277400  C -3.15900900 -1.01847300 -0.72121000  C -4.43870000 -0.47603700 -0.75502400  C -4.66924100 0.79320700 -0.24233900  H -3.78570700 2.50669000 0.70682800  H -1.51228700 1.53019200 0.76256400  H -2.98606600 -2.01421500 -1.11813800  H -5.25647400 -1.04910100 -1.17834400  H -5.66674600 1.21797000 -0.26423900  C -0.70218600 -0.88271200 -0.17561000  N -0.05519100 -0.73673600 1.12078200  H -0.75015000 -1.93432700 -0.50700500  C 1.28238400 -1.30516600 1.17562700  H 1.56408900 -1.37391600 2.23196900  H 1.32622100 -2.33135700 0.77144400  C 2.31027400 -0.46276100 0.45476700  C 3.26748800 -1.05471100 -0.36484800  C 2.34121700 0.92050700 0.62941300  C 4.24059400 -0.28638100 -0.99406800  H 3.24878800 -2.12986900 -0.51665200  C 3.30819700 1.69112200 -0.00058700  H 1.58819200 1.38449000 1.25657100  C 4.26382800 1.08980900 -0.81292100  H 4.97722600 -0.76403600 -1.63093500  H 3.31919900 2.76619200 0.14373200  H 5.01894800 1.69250400 -1.30533400  H -0.08267100 -0.35832300 -0.91240300  H -0.63764400 -1.14613200 1.84111100 |
| **Ph-CH=N-Ph**  C -1.84020900 -0.17298500 0.08590900  C -2.70782800 -1.20193400 0.45927000  C -2.37405300 1.03804200 -0.36762300  C -4.08281500 -1.02852700 0.38315900  H -2.29826800 -2.14361300 0.81189800  C -3.74525100 1.20943600 -0.44163900  H -1.69208800 1.82932100 -0.65529200  C -4.60355200 0.17775600 -0.06698900  H -4.74766800 -1.83336900 0.67573600  H -4.15318900 2.15060800 -0.79333600  H -5.67732100 0.31645900 -0.12758800  C -0.39577800 -0.38749000 0.17550700  H -0.08382600 -1.37908100 0.53302200  N 0.45566100 0.51070700 -0.12049900  C 1.82442000 0.22258700 -0.07055200  C 2.36671300 -0.98261000 -0.53090900  C 2.68601900 1.21186600 0.41297300  C 3.73643500 -1.19966700 -0.47585400  H 1.71474500 -1.73266900 -0.96483500  C 4.05030900 0.98022700 0.48346300  H 2.26006300 2.15265200 0.74147800  C 4.58305600 -0.22573800 0.03897500  H 4.14543100 -2.13321100 -0.84694600  H 4.70525500 1.75056600 0.87558400  H 5.65244400 -0.39839500 0.07961900 | **Ph-CH2NH-Ph**  C 1.88822700 0.37586200 -0.12181200  C 2.74092200 0.98339800 0.79568900  C 2.39045800 -0.64137400 -0.93499700  C 4.07100400 0.59046400 0.89806000  H 2.36081200 1.77299000 1.43624200  C 3.71591000 -1.03843100 -0.83201500  H 1.73186000 -1.12318600 -1.65003200  C 4.56106100 -0.42164700 0.08460600  H 4.72262800 1.07497000 1.61680400  H 4.09368100 -1.82797000 -1.47237400  H 5.59747600 -0.73047800 0.16322900  C 0.44769800 0.80236600 -0.23722200  H 0.25151800 1.13472700 -1.26327800  H 0.26928000 1.66987100 0.41554500  N -0.44066500 -0.29991200 0.07032900  H -0.08071400 -0.94226200 0.75872100  C -1.81722100 -0.16036900 0.06392300  C -2.61566100 -1.17249000 0.62110100  C -2.45665100 0.94418700 -0.51332800  C -3.99518300 -1.08203800 0.59431100  H -2.13778000 -2.03755300 1.07106700  C -3.84414700 1.01835200 -0.53885500  H -1.87501700 1.74989000 -0.94326600  C -4.62644700 0.01374500 0.01122100  H -4.58645700 -1.87845500 1.03355800  H -4.31489900 1.88355700 -0.99359200  H -5.70754900 0.08113300 -0.00902300 |
| **Ph-C≡CH**  C 1.20756500 -0.11893900 0.00000000  C 1.20337600 -1.50521100 0.00000000  C 0.00098200 -2.20244700 0.00000000  C -1.20740000 -0.11991300 0.00000000  C -1.20219000 -1.50587000 0.00000000  H 2.14282100 0.42781700 0.00000000  H 2.14413000 -2.04422200 0.00000000  H 0.00109900 -3.28662700 0.00000000  H -2.14275900 0.42666400 0.00000000  H -2.14230300 -2.04599900 0.00000000  C 0.00000000 0.59071200 0.00000000  C -0.00101500 2.01524300 0.00000000  C -0.00147400 3.21959700 0.00000000  H -0.00204600 4.28333700 0.00000000 | **Ph-CH=CH2**  C -1.77279800 -1.04120100 0.00001700  C -0.40472700 -1.27548200 -0.00000400  C 0.51257000 -0.21944000 -0.00001600  C 0.00911000 1.08711900 -0.00002600  C -1.35555000 1.32319000 -0.00001200  C -2.25459700 0.26064200 0.00002000  H -2.46303900 -1.87758500 0.00003800  H -0.03413100 -2.29578000 -0.00000300  H 0.69156300 1.92924100 -0.00005400  H -1.72356900 2.34341800 -0.00001500  H -3.32226000 0.44927200 0.00003300  C 1.94658200 -0.52730900 -0.00002700  H 2.17846900 -1.59044000 -0.00009200  C 2.96320600 0.33418800 0.00004000  H 2.82251200 1.40940700 0.00011700  H 3.98768000 -0.01777800 0.00002400 |
| **Ph-CH2CH3**  C -1.90813500 -0.99847500 0.00000000  C -1.38090400 0.28369500 0.00000000  C 0.00000000 0.50089500 0.00000000  C 0.83585200 -0.61318800 0.00000000  C 0.31171100 -1.90260000 0.00000000  C -1.06066700 -2.10163000 0.00000000  H -2.98371700 -1.13907800 0.00000000  H -2.05199500 1.13789800 0.00000000  H 1.91161500 -0.48294600 0.00000000  H 0.98406600 -2.75386000 0.00000000  H -1.46920300 -3.10600100 0.00000000  C 0.52153300 1.92052900 0.00000000  H 0.10409600 2.43810100 0.87141800  H 0.10409600 2.43810100 -0.87141800  C 2.03414300 2.08640500 0.00000000  H 2.49069200 1.63394400 -0.88385400  H 2.29846200 3.14610400 0.00000000  H 2.49069200 1.63394400 0.88385400 | **Ph-CH=O**  C -0.28638900 2.01845100 0.00000000  C 0.00000000 0.56986600 0.00000000  C 1.32413400 0.13334600 0.00000000  C 1.61131700 -1.22442400 0.00000000  C 0.57231500 -2.14728100 0.00000000  C -1.04034100 -0.36211000 0.00000000  C -0.75278000 -1.71605600 0.00000000  H 2.12805000 0.86360000 0.00000000  H 2.64069300 -1.56422600 0.00000000  H 0.79404200 -3.20885300 0.00000000  H -2.06251500 -0.00097200 0.00000000  H -1.55771000 -2.44235900 0.00000000  O -1.39111800 2.50699000 0.00000000  H 0.61684900 2.66613300 0.00000000 |
| **Ph-CH2OH**  O 1.89155300 1.98666800 0.00000000  C 0.47652200 1.93999900 0.00000000  H 0.06891700 2.44954500 0.88520800  C 0.00000000 0.51167900 0.00000000  C 0.89131800 -0.55550800 0.00000000  C 0.41892300 -1.86375900 0.00000000  C -0.94524800 -2.11903500 0.00000000  C -1.36992400 0.24962100 0.00000000  C -1.84084900 -1.05504500 0.00000000  H 1.95455900 -0.35252800 0.00000000  H 1.12462800 -2.68749200 0.00000000  H -1.31091100 -3.13983500 0.00000000  H -2.07707600 1.07452900 0.00000000  H -2.90906000 -1.24267300 0.00000000  H 0.06891700 2.44954500 -0.88520800  H 2.16315800 2.90785400 0.00000000 | **Ph-CO-CH3**  C 0.26225100 1.68526600 0.00000000  C 0.00000000 0.21189500 0.00000000  C 1.02711000 -0.73382800 0.00000000  C 0.73357800 -2.09080800 0.00000000  C -0.58918000 -2.51516300 0.00000000  C -1.32662200 -0.22622500 0.00000000  C -1.61944800 -1.57969000 0.00000000  H 2.06318600 -0.41656000 0.00000000  H 1.53793800 -2.81775600 0.00000000  H -0.81823600 -3.57515200 0.00000000  H -2.11312400 0.51918200 0.00000000  H -2.65217800 -1.91012400 0.00000000  O -0.65773900 2.47735400 0.00000000  C 1.69377800 2.16789600 0.00000000  H 2.22969100 1.80485700 0.88110400  H 2.22969100 1.80485700 -0.88110400  H 1.69613900 3.25581300 0.00000000 |
| **Ph-CH(OH)-CH3**  H 1.83460600 -1.28024200 -0.77868900  H 1.86351900 0.85028600 -1.75572000  C 1.65020600 -0.34564300 -0.22923700  C 0.15036700 -0.15452400 -0.13286400  C -0.71205100 -1.23483700 -0.30388600  C -2.08667400 -1.07469900 -0.17765900  C -2.61638600 0.17476300 0.11763700  C -0.39080400 1.09639600 0.16323200  C -1.76410300 1.26058800 0.28400300  H -0.30350100 -2.21197000 -0.54478000  H -2.74466900 -1.92559000 -0.31662000  H -3.68886900 0.30386400 0.21191200  H 0.27395900 1.94460100 0.28532700  H -2.17173100 2.23974800 0.51116600  O 2.28942600 0.73721000 -0.89999800  C 2.30517000 -0.45329400 1.13783000  H 1.88498800 -1.28892300 1.70028500  H 3.38033500 -0.60632600 1.02617600  H 2.14161200 0.46437300 1.70658900 |  |
| **1V-cs**  O 1.01700100 -2.73002700 0.00000000  N 0.71197100 -1.58811800 0.00000000  V 0.22588900 0.07920200 0.00000000  P -0.15300800 0.24061300 2.39772400  P -0.15300800 0.24061300 -2.39772400  C -1.20282300 1.76075500 2.45994700  C -1.20282300 1.76075500 -2.45994700  H -0.50142200 2.59810300 2.51608100  H -0.50142200 2.59810300 -2.51608100  H -1.84547600 1.80339800 3.34381300  H -1.84547600 1.80339800 -3.34381300  C -2.01186700 1.86802500 1.17349500  C -2.01186700 1.86802500 -1.17349500  H -2.27523600 2.92788100 1.02573700  H -2.27523600 2.92788100 -1.02573700  H -2.97705500 1.34895700 1.29359900  H -2.97705500 1.34895700 -1.29359900  N -1.30437900 1.36424300 0.00000000  C 1.29384700 0.69856300 -3.50114400  C 1.29384700 0.69856300 3.50114400  H 1.59565300 1.65280800 -3.05303100  H 1.59565300 1.65280800 3.05303100  C -1.14920300 -1.06078500 -3.31241000  C -1.14920300 -1.06078500 3.31241000  C -2.47282700 -1.31125900 -2.59153400  C -2.47282700 -1.31125900 2.59153400  N 1.85995400 0.62692700 0.00000000  O 2.94990100 1.08105700 0.00000000  H -1.36630500 -0.64274900 4.30185200  H -1.36630500 -0.64274900 -4.30185200  C -0.37606900 -2.36708100 3.48309900  C -0.37606900 -2.36708100 -3.48309900  H 0.50097300 -2.25062300 4.12007900  H 0.50097300 -2.25062300 -4.12007900  H -0.04350700 -2.76629100 2.52271600  H -0.04350700 -2.76629100 -2.52271600  H -1.02154900 -3.11675900 3.95091000  H -1.02154900 -3.11675900 -3.95091000  C 2.48258700 -0.25188400 -3.37123900  C 2.48258700 -0.25188400 3.37123900  H 2.30250000 -1.20372900 -3.87352200  H 2.30250000 -1.20372900 3.87352200  H 2.72064400 -0.45865000 -2.32822200  H 2.72064400 -0.45865000 2.32822200  H 3.36466700 0.19879400 -3.83541200  H 3.36466700 0.19879400 3.83541200  C 0.91706800 0.94708900 -4.95922600  C 0.91706800 0.94708900 4.95922600  H 0.09751000 1.66211300 -5.06196900  H 0.09751000 1.66211300 5.06196900  H 0.62394000 0.02165400 -5.46142400  H 0.62394000 0.02165400 5.46142400  H 1.77604100 1.35120800 -5.50351900  H 1.77604100 1.35120800 5.50351900  H -3.03761200 -2.08868400 -3.11457700  H -3.03761200 -2.08868400 3.11457700  H -2.30483800 -1.65318300 -1.56719200  H -2.30483800 -1.65318300 1.56719200  H -3.09983700 -0.41960300 -2.55094800  H -3.09983700 -0.41960300 2.55094800 | **1V-C1**  C -2.47587700 -0.58297400 1.96073000  H -2.57645300 0.33458300 2.54501500  H -3.33887000 -1.21650000 2.18282900  C -1.16404000 -1.26765300 2.32531400  H -1.04156500 -1.20802800 3.41837900  H -1.23258400 -2.34475600 2.10091500  C 1.17855900 -1.10384100 2.41133700  H 1.36406200 -2.18029900 2.26319000  H 0.99550700 -0.98849700 3.49163400  C 2.43428000 -0.31574500 2.05770100  H 3.34228100 -0.84294200 2.36258700  H 2.41796800 0.64349600 2.57945800  C -3.47916800 1.46153000 0.07287600  H -3.40364500 1.74779200 -0.98141900  C -4.94745300 1.23306500 0.42319600  H -5.06325900 0.88756100 1.45439400  H -5.42883100 0.50600000 -0.23289700  H -5.50241400 2.17177600 0.33158800  C -2.88738700 2.60040800 0.90175400  H -3.42076500 3.53054200 0.68651800  H -1.83221900 2.76070100 0.68078400  H -2.98603000 2.41174200 1.97402500  C -3.37387600 -1.37560900 -0.74370600  H -4.36259700 -1.42079300 -0.27397100  C -3.53425800 -0.98830200 -2.21244400  H -2.56384900 -0.89518500 -2.70387900  H -4.07009400 -0.04513200 -2.33869200  H -4.10187500 -1.76051000 -2.74018900  C -2.71108200 -2.74402900 -0.60301100  H -3.28754100 -3.49358400 -1.15335200  H -2.65563400 -3.07069200 0.43727300  H -1.69904800 -2.73569800 -1.01207500  C 3.45257100 1.59684100 0.03892000  H 4.43007600 1.36712700 0.47719600  C 3.62865500 1.91182000 -1.44653200  H 2.66471200 2.10781600 -1.92070400  H 4.11568200 1.10150900 -1.99250200  H 4.24673400 2.80636400 -1.56627700  C 2.85855900 2.79538100 0.77609000  H 3.50736800 3.66599100 0.64195600  H 2.76246600 2.62468200 1.84990400  H 1.87378600 3.05176100 0.38225100  C 3.36797200 -1.29015100 -0.59415300  H 3.23522000 -1.07086500 -1.65881600  C 2.73455500 -2.65382400 -0.32028600  H 3.17167900 -3.40760200 -0.98105900  H 1.65655600 -2.64335600 -0.48796200  H 2.91727900 -2.97545700 0.70810600  C 4.85975100 -1.30565400 -0.27264700  H 5.03986300 -1.46477400 0.79432900  H 5.36423200 -0.38369600 -0.56575900  H 5.34565000 -2.12741200 -0.80766600  N -0.05912600 1.65690300 -0.98130300  N -0.00191600 -0.67950700 1.66095000  O -0.10615200 2.70781600 -1.51932900  P -2.40353800 -0.07216100 0.18700300  P 2.39013400 0.06928200 0.25331300  V -0.00105900 0.12366900 -0.17314400  N 0.08673200 -0.66828000 -1.70435700  O 0.17005000 -1.23734800 -2.73634700 |
| **2V-cs**  O -2.41325000 1.89079000 0.00000000  N -1.46550500 1.17411700 0.00000000  V -0.00288700 0.22727500 0.00000000  H 1.39330700 -0.82755200 0.00000000  P 0.10645900 -0.34121200 -2.34078800  P 0.10645900 -0.34121200 2.34078800  C -0.86311900 -1.94365800 -2.43619000  C -0.86311900 -1.94365800 2.43619000  H -0.14032100 -2.76581800 -2.42518800  H -0.14032100 -2.76581800 2.42518800  H -1.42860000 -2.02780500 -3.36651900  H -1.42860000 -2.02780500 3.36651900  C -1.78862400 -2.05925500 -1.23285400  C -1.78862400 -2.05925500 1.23285400  H -2.25240700 -3.05634000 -1.20498500  H -2.25240700 -3.05634000 1.20498500  H -2.59230400 -1.32151800 -1.29113100  H -2.59230400 -1.32151800 1.29113100  N -1.03515900 -1.79777000 0.00000000  H -0.20177600 -2.38048100 0.00000000  C 1.75755900 -0.87346900 3.06625600  C 1.75755900 -0.87346900 -3.06625600  H 1.96487900 -1.76195300 2.45846500  H 1.96487900 -1.76195300 -2.45846500  C -0.70719200 0.73804600 3.64555900  C -0.70719200 0.73804600 -3.64555900  C -2.21548400 0.83579000 3.42612600  C -2.21548400 0.83579000 -3.42612600  N 0.98141600 1.65021300 0.00000000  O 1.64308400 2.62496600 0.00000000  H -0.52606500 0.25589300 -4.61251200  H -0.52606500 0.25589300 4.61251200  C -0.07892700 2.13057700 -3.65269200  C -0.07892700 2.13057700 3.65269200  H 0.98049700 2.11035600 -3.91116500  H 0.98049700 2.11035600 3.91116500  H -0.17526900 2.60474100 -2.67368200  H -0.17526900 2.60474100 2.67368200  H -0.58588700 2.76417300 -4.38670800  H -0.58588700 2.76417300 4.38670800  C 2.87272000 0.12717200 2.77725200  C 2.87272000 0.12717200 -2.77725200  H 2.76356200 1.04502900 3.35834600  H 2.76356200 1.04502900 -3.35834600  H 2.89183800 0.39043600 1.71950200  H 2.89183800 0.39043600 -1.71950200  H 3.84022400 -0.31132400 3.04056800  H 3.84022400 -0.31132400 -3.04056800  C 1.71586400 -1.27851000 4.53655200  C 1.71586400 -1.27851000 -4.53655200  H 0.92752900 -2.00479300 4.75100400  H 0.92752900 -2.00479300 -4.75100400  H 1.56389000 -0.41423500 5.18789000  H 1.56389000 -0.41423500 -5.18789000  H 2.66837400 -1.73363400 4.82506000  H 2.66837400 -1.73363400 -4.82506000  H -2.65651100 1.46298000 4.20691800  H -2.65651100 1.46298000 -4.20691800  H -2.45000600 1.29227800 2.46325900  H -2.45000600 1.29227800 -2.46325900  H -2.71161700 -0.13607300 3.47777900  H -2.71161700 -0.13607300 -3.47777900 | **2V-C1**  O 0.03835600 -2.98731600 -0.89080300  N 0.01762900 -1.83561200 -0.59175200  V 0.00330700 -0.11523100 -0.32564200  H 0.01764000 1.58483500 -0.03351200  P 2.35538700 0.22404500 0.14115400  P -2.35837100 0.15681000 0.14859900  C 2.45878800 0.02479200 2.00123000  C -2.44454000 -0.00189000 2.01176600  H 2.47988200 1.01979400 2.45261900  H -2.46344400 1.00573800 2.43647200  H 3.37833300 -0.48076000 2.30413300  H -3.35772100 -0.50474500 2.33787400  C 1.24146900 -0.74229300 2.50084100  C -1.21519300 -0.74779500 2.51527000  H 1.21541100 -0.73541500 3.60054900  H -1.18311400 -0.72558100 3.61456600  H 1.28532000 -1.78485000 2.17760300  H -1.24833800 -1.79529600 2.20700800  N 0.00839000 -0.16379100 1.94650800  H 0.00688700 0.83598000 2.13257400  C -3.25152700 1.77674100 -0.22622500  C 3.17924200 1.88044200 -0.19332600  H -3.11467700 1.87604200 -1.30852400  H 4.20646300 1.79572600 0.17454000  C -3.57858300 -1.13121100 -0.46535400  C 3.63051500 -1.00361600 -0.51490300  C -3.26909600 -2.52726200 0.06729600  C 5.08961400 -0.63429600 -0.25664900  N -0.01358800 0.21525700 -2.02316000  O -0.03117500 0.44927700 -3.17685900  H 3.44939600 -0.99468500 -1.59486300  H -4.56189900 -0.83485500 -0.08656000  C 3.33790800 -2.41532900 -0.01001700  C -3.60577700 -1.11961800 -1.99264200  H 2.31569300 -2.72729800 -0.21690600  H -3.89842700 -0.14814500 -2.39785900  H 3.52088800 -2.50117500 1.06550400  H -2.62347100 -1.36869600 -2.39950200  H 4.00769400 -3.12601900 -0.50304800  H -4.32218900 -1.85986400 -2.36107500  C -4.74733200 1.78243300 0.08415800  C 2.50942300 3.04838700 0.52220700  H -4.94132900 1.57632700 1.14111900  H 1.45736100 3.11932100 0.24046700  H -5.30841300 1.06055000 -0.51042200  H 2.56751900 2.96624300 1.61028900  H -5.16276200 2.77134900 -0.13239200  H 3.00994900 3.98076100 0.24346400  C -2.56167600 2.96913800 0.43141400  C 3.20179400 2.11948400 -1.70302900  H -1.48314900 2.93634300 0.27011500  H 3.72231700 1.32799900 -2.24665300  H -2.75376400 2.99975600 1.50856300  H 2.18520800 2.18076900 -2.09682400  H -2.95196100 3.90039500 0.01097500  H 3.71011200 3.06213800 -1.92620600  H -4.02573000 -3.22921900 -0.29695100  H 5.74053000 -1.42756700 -0.63677100  H -2.29626400 -2.88368800 -0.27114400  H 5.30020400 -0.53186000 0.81250800  H -3.29389900 -2.57008200 1.15894400  H 5.38781000 0.29191400 -0.74930300 |
| **1Nb-cs**  O -0.49109600 3.09991400 0.00000000  N -0.47029600 1.91423300 0.00000000  P 0.16758700 -0.29744900 2.53672900  P 0.16758700 -0.29744900 -2.53672900  C 1.29754900 -1.76738200 2.46710800  C 1.29754900 -1.76738200 -2.46710800  H 0.63419000 -2.63721600 2.48566600  H 0.63419000 -2.63721600 -2.48566600  H 1.94889500 -1.82992600 3.34389100  H 1.94889500 -1.82992600 -3.34389100  C 2.11265100 -1.79398700 1.17744700  C 2.11265100 -1.79398700 -1.17744700  H 2.46383400 -2.82962200 1.03511100  H 2.46383400 -2.82962200 -1.03511100  H 3.03118600 -1.19766000 1.30623700  H 3.03118600 -1.19766000 -1.30623700  N 1.37193900 -1.35712000 0.00000000  C -1.21300800 -0.91995400 -3.64853400  C -1.21300800 -0.91995400 3.64853400  H -1.46326300 -1.86579600 -3.15301900  H -1.46326300 -1.86579600 3.15301900  C 1.11366000 1.00071100 -3.50422600  C 1.11366000 1.00071100 3.50422600  C 2.41908700 1.34515000 -2.78946000  C 2.41908700 1.34515000 2.78946000  N -2.14959200 -0.20006400 0.00000000  O -3.30484900 -0.46728300 0.00000000  H 1.35449600 0.55032600 4.47356400  H 1.35449600 0.55032600 -4.47356400  C 0.27582500 2.25820700 3.72668500  C 0.27582500 2.25820700 -3.72668500  H -0.59902800 2.07079200 4.34961500  H -0.59902800 2.07079200 -4.34961500  H -0.06675100 2.67961900 2.77907800  H -0.06675100 2.67961900 -2.77907800  H 0.88033000 3.01774000 4.23148900  H 0.88033000 3.01774000 -4.23148900  C -2.46544700 -0.04709100 -3.60839700  C -2.46544700 -0.04709100 3.60839700  H -2.32713900 0.89194100 -4.14700000  H -2.32713900 0.89194100 4.14700000  H -2.76093600 0.18730900 -2.58595200  H -2.76093600 0.18730900 2.58595200  H -3.29501800 -0.57595000 -4.08685900  H -3.29501800 -0.57595000 4.08685900  C -0.77179600 -1.22575700 -5.07736900  C -0.77179600 -1.22575700 5.07736900  H 0.09732200 -1.88663800 -5.11415100  H 0.09732200 -1.88663800 5.11415100  H -0.52676700 -0.31240500 -5.62517300  H -0.52676700 -0.31240500 5.62517300  H -1.58332100 -1.71939400 -5.62044100  H -1.58332100 -1.71939400 5.62044100  H 2.95142700 2.12015100 -3.34869600  H 2.95142700 2.12015100 3.34869600  H 2.22744100 1.73333300 -1.78576400  H 2.22744100 1.73333300 1.78576400  H 3.08535600 0.48591900 -2.70090800  H 3.08535600 0.48591900 2.70090800  Nb -0.27441900 0.03412800 0.00000000 | **1Nb-C1**  C -2.49146000 -0.60313800 1.99366800  H -2.54767100 0.32769700 2.56419100  H -3.35629600 -1.21323000 2.26970700  C -1.18445800 -1.31432300 2.33714400  H -1.06377800 -1.26562500 3.43216900  H -1.27968600 -2.38913800 2.10820400  C 1.17035600 -1.23922000 2.38453900  H 1.33677700 -2.30796900 2.16925700  H 1.00731100 -1.18811900 3.47394000  C 2.44467500 -0.45471000 2.07921400  H 3.33320300 -1.00271800 2.40510900  H 2.42164300 0.48813100 2.63039800  C -3.70666300 1.36882000 0.15914200  H -3.75945400 1.61244800 -0.90694800  C -5.11226400 1.06433000 0.67072100  H -5.09943100 0.77072300 1.72383800  H -5.60312400 0.27099100 0.10431100  H -5.73918300 1.95748800 0.59030700  C -3.09997900 2.57379900 0.87501400  H -3.73506200 3.45118300 0.72324900  H -2.10559600 2.81094100 0.49592800  H -3.02668900 2.41086700 1.95365900  C -3.46311000 -1.45482200 -0.68644400  H -4.42622100 -1.56959900 -0.17725600  C -3.70408600 -1.06090300 -2.14241300  H -2.75980200 -0.87638000 -2.65967100  H -4.32342700 -0.16651000 -2.23619600  H -4.21895300 -1.87191800 -2.66566700  C -2.70520400 -2.77713200 -0.59499900  H -3.25154300 -3.55513900 -1.13628300  H -2.58472200 -3.11491100 0.43584700  H -1.71346100 -2.69269300 -1.04516600  C 3.63292000 1.51284000 0.20874300  H 4.57297500 1.24362900 0.70286000  C 3.91151200 1.87573300 -1.24949300  H 2.98014700 2.08330400 -1.78191600  H 4.43947000 1.08490500 -1.78581000  H 4.53156400 2.77541100 -1.29683600  C 3.01196900 2.69745600 0.94596000  H 3.68734100 3.55630000 0.89171500  H 2.83297600 2.49157100 2.00287700  H 2.06456300 2.99029700 0.48957200  C 3.50391500 -1.34108400 -0.57001400  H 3.48215000 -1.03514200 -1.62117300  C 2.78078400 -2.68266900 -0.46421600  H 3.26067000 -3.41688200 -1.11732500  H 1.73391600 -2.60293500 -0.76249300  H 2.81776400 -3.07663600 0.55436200  C 4.95610500 -1.45687700 -0.11615600  H 5.02764300 -1.71581100 0.94378800  H 5.52214300 -0.53810900 -0.27804900  H 5.45723700 -2.25183600 -0.67676300  N -0.02824300 1.94284100 -1.00115400  N -0.01077500 -0.74598300 1.68400100  O -0.04687800 3.06922200 -1.37052700  P -2.53656100 -0.09786700 0.21193000  P 2.52068900 0.00757400 0.28768700  N 0.06393700 -0.53803900 -1.99096000  O 0.11752500 -1.08949700 -3.03931000  Nb -0.00212200 0.19955300 -0.25753600 |
| **2Nb-cs**  O 2.50122800 1.99518800 0.00000000  N 1.49340400 1.36264900 0.00000000  H -1.51324200 -1.00448000 0.00000000  P -0.09437800 -0.38509400 2.48507500  P -0.09437800 -0.38509400 -2.48507500  C 0.91636500 -1.96797400 2.45107600  C 0.91636500 -1.96797400 -2.45107600  H 0.20549500 -2.79974400 2.41951500  H 0.20549500 -2.79974400 -2.41951500  H 1.50161600 -2.08421000 3.36619600  H 1.50161600 -2.08421000 -3.36619600  C 1.83203900 -2.03525400 1.23394100  C 1.83203900 -2.03525400 -1.23394100  H 2.32903500 -3.01625400 1.20032700  H 2.32903500 -3.01625400 -1.20032700  H 2.61319200 -1.27364800 1.29486100  H 2.61319200 -1.27364800 -1.29486100  N 1.07167000 -1.79558300 0.00000000  H 0.24570600 -2.39068700 0.00000000  C -1.70358400 -0.99463300 -3.24037600  C -1.70358400 -0.99463300 3.24037600  H -1.91056500 -1.85954700 -2.59984400  H -1.91056500 -1.85954700 2.59984400  C 0.75929900 0.64872300 -3.79884300  C 0.75929900 0.64872300 3.79884300  C 2.24209200 0.82261500 -3.47783700  C 2.24209200 0.82261500 3.47783700  N -1.19378800 1.86045600 0.00000000  O -1.88319500 2.82015000 0.00000000  H 0.66489900 0.10107500 4.74309900  H 0.66489900 0.10107500 -4.74309900  C 0.07735000 2.00891300 3.93299100  C 0.07735000 2.00891300 -3.93299100  H -0.95544600 1.92673000 4.27402200  H -0.95544600 1.92673000 -4.27402200  H 0.07457100 2.53745400 2.97672200  H 0.07457100 2.53745400 -2.97672200  H 0.61645600 2.62486500 4.65884300  H 0.61645600 2.62486500 -4.65884300  C -2.84969100 -0.00877000 -3.03112500  C -2.84969100 -0.00877000 3.03112500  H -2.73955400 0.88856900 -3.64321300  H -2.73955400 0.88856900 3.64321300  H -2.91410500 0.29441900 -1.98527400  H -2.91410500 0.29441900 1.98527400  H -3.79672000 -0.48028700 -3.31065100  H -3.79672000 -0.48028700 3.31065100  C -1.59498600 -1.45881200 -4.68934400  C -1.59498600 -1.45881200 4.68934400  H -0.78680200 -2.17909300 -4.84079200  H -0.78680200 -2.17909300 4.84079200  H -1.43047500 -0.61950100 -5.36962200  H -1.43047500 -0.61950100 5.36962200  H -2.52711100 -1.94291500 -4.99619700  H -2.52711100 -1.94291500 4.99619700  H 2.71201700 1.43953800 -4.24962000  H 2.71201700 1.43953800 4.24962000  H 2.38565100 1.32317400 -2.51855000  H 2.38565100 1.32317400 2.51855000  H 2.78042500 -0.12762500 -3.45492100  H 2.78042500 -0.12762500 3.45492100  Nb -0.10332100 0.31095000 0.00000000 | **2Nb-C1**  O 0.03891800 -3.08967000 -0.92251500  N 0.01282200 -1.91626100 -0.72079600  H 0.02694000 1.81865000 0.05187900  P 2.50255300 0.23818100 0.19612700  P -2.51443600 0.17986700 0.19040300  C 2.45792300 0.10698700 2.06574000  C -2.47266500 0.04632100 2.05932700  H 2.43519700 1.12324400 2.46678700  H -2.47625600 1.06477500 2.45820600  H 3.36532400 -0.36504500 2.45004200  H -3.36906500 -0.44889500 2.44030000  C 1.23106700 -0.65956700 2.54907200  C -1.22752100 -0.68726800 2.54765700  H 1.19344500 -0.63616400 3.64840900  H -1.19330300 -0.66008400 3.64697400  H 1.28795700 -1.70762300 2.24601100  H -1.25731500 -1.73731200 2.24733800  N -0.00450700 -0.10248600 1.97801700  H -0.01493200 0.90406200 2.13043100  C -3.49578400 1.75700800 -0.13558500  C 3.42119200 1.84227600 -0.14118200  H -3.48356600 1.81833700 -1.22915900  H 4.41813400 1.72835100 0.29573400  C -3.70458600 -1.17149500 -0.33819800  C 3.74975600 -1.07885000 -0.32311400  C -3.29053200 -2.54327200 0.18563200  C 5.20209500 -0.77911900 0.03939000  N -0.00045000 0.29477100 -2.30063600  O -0.00126800 0.51340100 -3.46093600  H 3.65216300 -1.09363500 -1.41357700  H -4.67694900 -0.91877900 0.09642600  C 3.33550400 -2.45398500 0.19631500  C -3.81930600 -1.17677800 -1.86138900  H 2.30820900 -2.70312000 -0.06605800  H -4.18789600 -0.22721000 -2.25614900  H 3.44795200 -2.52072000 1.28276300  H -2.84840200 -1.37688700 -2.32064200  H 3.98388600 -3.22043900 -0.23778800  H -4.51393700 -1.95874200 -2.18175900  C -4.94678900 1.72339300 0.34034000  C 2.75523300 3.06381300 0.48337800  H -5.01384200 1.56312600 1.42044300  H 1.71672200 3.14825700 0.15735100  H -5.54058600 0.95395800 -0.15476100  H 2.76710500 3.03540300 1.57570800  H -5.42316300 2.68524800 0.12799500  H 3.29695000 3.96481500 0.17983500  C -2.77458000 2.99127800 0.40000500  C 3.54974100 2.01238700 -1.65524800  H -1.71773600 2.98414200 0.12751700  H 4.07538300 1.18041300 -2.12922200  H -2.84734100 3.05508400 1.49038200  H 2.56353800 2.09137900 -2.11825300  H -3.24161000 3.89393200 -0.00434000  H 4.10624100 2.92617500 -1.88249800  H -4.01633000 -3.29184600 -0.14651300  H 5.83583000 -1.61592000 -0.26942600  H -2.31161600 -2.84042000 -0.19145900  H 5.33564000 -0.65744500 1.11872100  H -3.26956800 -2.58155500 1.27746200  H 5.58622300 0.11589100 -0.45148500  Nb -0.00004700 -0.02548600 -0.43372900 |
| **1Ta-cs**  O -0.31095700 3.08604700 0.00000000  N -0.35337300 1.89384400 0.00000000  P 0.18681500 -0.30488800 2.51803800  P 0.18681500 -0.30488800 -2.51803800  C 1.27121300 -1.80852800 2.47064600  C 1.27121300 -1.80852800 -2.47064600  H 0.58324500 -2.65856800 2.50058100  H 0.58324500 -2.65856800 -2.50058100  H 1.92392200 -1.87973500 3.34538400  H 1.92392200 -1.87973500 -3.34538400  C 2.07992800 -1.86813100 1.17805500  C 2.07992800 -1.86813100 -1.17805500  H 2.38897400 -2.91540800 1.03157600  H 2.38897400 -2.91540800 -1.03157600  H 3.01987800 -1.30647400 1.30069800  H 3.01987800 -1.30647400 -1.30069800  N 1.35352400 -1.40050000 0.00000000  C -1.22508500 -0.86610800 -3.62085700  C -1.22508500 -0.86610800 3.62085700  H -1.50057400 -1.81008300 -3.13541100  H -1.50057400 -1.81008300 3.13541100  C 1.16478200 0.98047800 -3.46928100  C 1.16478200 0.98047800 3.46928100  C 2.48270000 1.27616900 -2.75559700  C 2.48270000 1.27616900 2.75559700  N -2.09362700 -0.17750100 0.00000000  O -3.25759500 -0.43721400 0.00000000  H 1.38761100 0.53643700 4.44589500  H 1.38761100 0.53643700 -4.44589500  C 0.36321800 2.26525700 3.66905300  C 0.36321800 2.26525700 -3.66905300  H -0.52035200 2.11240700 4.28907400  H -0.52035200 2.11240700 -4.28907400  H 0.04041300 2.68453200 2.71374400  H 0.04041300 2.68453200 -2.71374400  H 0.98790300 3.01196600 4.16838100  H 0.98790300 3.01196600 -4.16838100  C -2.44822400 0.04579900 -3.55661200  C -2.44822400 0.04579900 3.55661200  H -2.28268600 0.98960200 -4.07873500  H -2.28268600 0.98960200 4.07873500  H -2.73129700 0.26893700 -2.52841200  H -2.73129700 0.26893700 2.52841200  H -3.29580000 -0.44846600 -4.04041200  H -3.29580000 -0.44846600 4.04041200  C -0.80527200 -1.16516700 -5.05766100  C -0.80527200 -1.16516700 5.05766100  H 0.04401900 -1.85026500 -5.11202200  H 0.04401900 -1.85026500 5.11202200  H -0.53954100 -0.25186500 -5.59576100  H -0.53954100 -0.25186500 5.59576100  H -1.63594100 -1.62796900 -5.59873000  H -1.63594100 -1.62796900 5.59873000  H 3.03789000 2.03802400 -3.31054900  H 3.03789000 2.03802400 3.31054900  H 2.30550200 1.66340100 -1.74899400  H 2.30550200 1.66340100 1.74899400  H 3.12175400 0.39556300 -2.67588300  H 3.12175400 0.39556300 2.67588300  Ta -0.22836500 0.02087400 0.00000000 | **1Ta-C1**  C -2.49311100 -0.59567100 2.02823500  H -2.56208200 0.34386800 2.58258000  H -3.35480200 -1.20880400 2.30612900  C -1.18272700 -1.29111700 2.39108300  H -1.05720700 -1.20901200 3.48248900  H -1.27180500 -2.37157300 2.19249600  C 1.17328000 -1.21779100 2.43407600  H 1.33255600 -2.29165300 2.24513800  H 1.00602900 -1.13705600 3.51994400  C 2.45215700 -0.44791100 2.10964000  H 3.33832400 -1.00169400 2.43137500  H 2.44462700 0.50121400 2.65008000  C -3.67783900 1.34699400 0.13427300  H -3.69735600 1.57679400 -0.93593300  C -5.09834500 1.04895700 0.60745100  H -5.11778900 0.76934400 1.66438800  H -5.57322200 0.24904300 0.03675500  H -5.72095500 1.94176100 0.49677100  C -3.09126300 2.56007700 0.85302800  H -3.72621900 3.43293100 0.67674600  H -2.08984700 2.79819700 0.49450900  H -3.04473100 2.40845300 1.93483600  C -3.42309700 -1.49494800 -0.65486300  H -4.39333700 -1.60400300 -0.15806100  C -3.64188400 -1.12360600 -2.12036600  H -2.68981200 -0.94903600 -2.62636300  H -4.25932700 -0.23069600 -2.23764400  H -4.15000600 -1.94302600 -2.63706600  C -2.66311300 -2.81349500 -0.53227800  H -3.20605500 -3.60297600 -1.06013200  H -2.54685700 -3.13073900 0.50563400  H -1.67039500 -2.73610200 -0.98121800  C 3.60172600 1.50041300 0.18359300  H 4.55774700 1.23909800 0.65055900  C 3.83145400 1.84740900 -1.28712600  H 2.88219800 2.04640500 -1.78999500  H 4.34442500 1.05225300 -1.83160900  H 4.44679300 2.74825600 -1.36351400  C 2.99930300 2.69044300 0.92737100  H 3.67499100 3.54722100 0.84975300  H 2.84733700 2.49295600 1.99018500  H 2.04218100 2.98188400 0.49148600  C 3.46893100 -1.36907500 -0.54728000  H 3.41466600 -1.08277000 -1.60266000  C 2.75665300 -2.71194200 -0.39576900  H 3.22514000 -3.45639800 -1.04541300  H 1.70280900 -2.64411800 -0.67156400  H 2.82102200 -3.08502800 0.62939800  C 4.93370200 -1.46726700 -0.13141200  H 5.03645100 -1.70137400 0.93184400  H 5.49006300 -0.54998800 -0.33059400  H 5.42281800 -2.27260700 -0.68765000  N -0.02870600 1.90542900 -0.92044900  N -0.00850400 -0.74057000 1.71734500  O -0.04740800 3.04958500 -1.25687100  P -2.51642300 -0.12210600 0.23854500  P 2.50344300 -0.01022600 0.31223600  N 0.06331000 -0.57811000 -1.92827600  O 0.11487700 -1.15950100 -2.96829500  Ta -0.00138500 0.16530400 -0.21016900 |
| **2Ta-cs**  O -0.00002900 2.47678300 1.92685600  N 0.00002400 1.45733900 1.29775400  H -0.00002500 -1.46961000 -1.10512300  P 2.47283200 -0.06532700 -0.41567300  P -2.47279300 -0.06521800 -0.41571100  C 2.45618100 1.00736100 -1.95657200  C -2.45607000 1.00742700 -1.95664000  H 2.43812200 0.33197600 -2.81780600  H -2.43800800 0.33202000 -2.81785600  H 3.36769000 1.60361300 -2.03814300  H -3.36756100 1.60370300 -2.03825100  C 1.23242800 1.91512500 -1.99185300  C -1.23229300 1.91515600 -1.99190800  H 1.19657000 2.45320600 -2.95002200  H -1.19639100 2.45321500 -2.95008800  H 1.28033600 2.66088800 -1.19509700  H -1.28020000 2.66093900 -1.19517000  N 0.00005300 1.13440000 -1.79227500  H 0.00005500 0.35302200 -2.44484100  C -3.23781300 -1.64982700 -1.07387600  C 3.23775800 -1.64994900 -1.07391700  H -2.60611300 -1.82807100 -1.95167800  H 2.60630000 -1.82787000 -1.95195800  C -3.75674300 0.74512400 0.68604400  C 3.75681000 0.74496400 0.68609800  C -3.44696600 2.22622700 0.89323500  C 3.44738300 2.22620400 0.89282500  N -0.00000700 -1.22999200 1.75654100  O -0.00002700 -1.94700800 2.70398400  H 4.71739900 0.65429700 0.16692700  H -4.71726700 0.65483500 0.16668600  C 3.83683700 0.02141300 2.02919200  C -3.83717400 0.02120400 2.02891300  H 4.16540200 -1.01364100 1.92794700  H -4.16594800 -1.01375000 1.92730000  H 2.86405200 0.01777000 2.52618700  H -2.86448000 0.01719700 2.52608200  H 4.55034300 0.53212900 2.68253500  H -4.55068600 0.53188700 2.68227600  C -3.02534900 -2.83067200 -0.13050600  C 3.02473900 -2.83098200 -0.13090700  H -3.63536300 -2.75228200 0.77144700  H 3.63452700 -2.75298500 0.77123000  H -1.97916400 -2.90722700 0.16857200  H 1.97845300 -2.90736100 0.16786600  H -3.30704400 -3.75971900 -0.63523600  H 3.30634100 -3.75996800 -0.63580100  C -4.69050600 -1.51946000 -1.52077400  C 4.69062100 -1.51977200 -1.52032100  H -4.84624400 -0.68441000 -2.20876500  H 4.84674900 -0.68460100 -2.20807500  H -5.36261900 -1.38506100 -0.66963200  H 5.36248400 -1.38569500 -0.66893100  H -5.00431100 -2.43190600 -2.03675400  H 5.00441400 -2.43216500 -2.03640200  H -4.20802700 2.66766900 1.54360600  H 4.20844100 2.66763100 1.54320800  H -2.47663700 2.36868100 1.37216200  H 2.47700400 2.36904200 1.37153500  H -3.45779200 2.79177600 -0.04136600  H 3.45852000 2.79148600 -0.04193400  Ta 0.00001400 -0.11383800 0.24245300 | **2Ta-C1**  O 0.03550200 -3.07391300 -0.72676400  N 0.01238100 -1.88235400 -0.59475300  H 0.02087700 1.82187600 0.13053500  P 2.48742300 0.23649200 0.24301200  P -2.49780200 0.17690900 0.23339300  C 2.46449600 0.05773500 2.10851500  C -2.47548300 0.00747900 2.09896300  H 2.46141600 1.06171100 2.53979700  H -2.49086900 1.01628700 2.52107700  H 3.36738100 -0.44041300 2.46938400  H -3.36935600 -0.50520200 2.46184800  C 1.22993400 -0.70608800 2.57501100  C -1.22655700 -0.72799400 2.57318500  H 1.19048500 -0.70946100 3.67379500  H -1.19112200 -0.72602800 3.67206900  H 1.27242900 -1.74570300 2.24313500  H -1.24610800 -1.76965600 2.24536900  N -0.00341900 -0.12036500 2.01916700  H -0.01176800 0.87702900 2.22311900  C -3.46978000 1.76214100 -0.08159400  C 3.39361400 1.85190300 -0.07259400  H -3.42115600 1.85292900 -1.17204100  H 4.40124100 1.72631700 0.33547500  C -3.67392200 -1.16476500 -0.34469500  C 3.72064000 -1.06639100 -0.33628600  C -3.28009100 -2.54527600 0.17205700  C 5.18074300 -0.76683100 -0.00543300  N 0.00275700 0.28763000 -2.22394300  O 0.00482500 0.48936400 -3.39379600  H 3.59320000 -1.05801500 -1.42367400  H -4.65575900 -0.91240800 0.06826600  C 3.32527500 -2.45369300 0.16555600  C -3.74964900 -1.14792100 -1.87033200  H 2.29708100 -2.71064200 -0.08555000  H -4.10163600 -0.19044700 -2.26124900  H 3.45650600 -2.53882700 1.24871500  H -2.76907100 -1.34850300 -2.30769800  H 3.97562800 -3.20480100 -0.29194200  H -4.44174000 -1.92049600 -2.21772800  C -4.93567500 1.71313700 0.34515500  C 2.74454300 3.05517800 0.60332700  H -5.03880500 1.51588400 1.41632600  H 1.70086400 3.15420900 0.29963100  H -5.51255900 0.96207800 -0.19580000  H 2.77875400 2.99348300 1.69382500  H -5.40453600 2.68230700 0.15028000  H 3.28354900 3.96323000 0.31665700  C -2.77074700 2.98298000 0.51141000  C 3.48311400 2.06436400 -1.58424700  H -1.70652500 2.98823200 0.27062800  H 3.99388600 1.24502700 -2.09493000  H -2.87919300 3.01654800 1.60014300  H 2.48554700 2.15747500 -2.01926500  H -3.22863400 3.89470700 0.11725900  H 4.03604900 2.98317400 -1.79959900  H -4.00751300 -3.28248600 -0.18139400  H 5.80829400 -1.59568800 -0.34625300  H -2.29722200 -2.84913800 -0.18887100  H 5.34180800 -0.66538500 1.07230500  H -3.28129500 -2.59547500 1.26374900  H 5.54967000 0.13836300 -0.48923700  Ta 0.00039000 -0.00406600 -0.36563100 |
| **1V + H2-TS**  N 1.13192300 1.39023800 0.00000000  O 1.93879500 2.25064900 0.00000000  V -0.08602300 0.16212200 0.00000000  P -0.05175600 -0.35572700 2.38619900  P -0.05175600 -0.35572700 -2.38619900  C 0.96209600 -1.91427500 2.43214700  C 0.96209600 -1.91427500 -2.43214700  H 0.25281100 -2.74657600 2.39982200  H 0.25281100 -2.74657600 -2.39982200  H 1.54076800 -2.00766400 3.35390600  H 1.54076800 -2.00766400 -3.35390600  C 1.85486300 -1.96298200 1.19744900  C 1.85486300 -1.96298200 -1.19744900  H 2.30191100 -2.97001300 1.13233400  H 2.30191100 -2.97001300 -1.13233400  H 2.70161400 -1.26528200 1.33148900  H 2.70161400 -1.26528200 -1.33148900  N 1.10414200 -1.66572000 0.00000000  C -1.65269200 -0.93032400 -3.18823200  C -1.65269200 -0.93032400 3.18823200  H -1.91105900 -1.77496900 -2.53822500  H -1.91105900 -1.77496900 2.53822500  C 0.75830300 0.82459100 -3.59721900  C 0.75830300 0.82459100 3.59721900  C 2.26972700 0.89774800 -3.38770400  C 2.26972700 0.89774800 3.38770400  N -1.31116700 1.39385400 0.00000000  O -2.11021900 2.25967100 0.00000000  H 0.56723000 0.41670900 4.59580700  H 0.56723000 0.41670900 -4.59580700  C 0.13709900 2.21707000 3.49594600  C 0.13709900 2.21707000 -3.49594600  H -0.93451100 2.21685000 3.69647900  H -0.93451100 2.21685000 -3.69647900  H 0.28922100 2.63807100 2.50055800  H 0.28922100 2.63807100 -2.50055800  H 0.61033500 2.88644500 4.22059000  H 0.61033500 2.88644500 -4.22059000  C -2.78791700 0.08547200 -3.08872300  C -2.78791700 0.08547200 3.08872300  H -2.64449100 0.92065200 -3.77751800  H -2.64449100 0.92065200 3.77751800  H -2.88659100 0.49189600 -2.08211300  H -2.88659100 0.49189600 2.08211300  H -3.73514900 -0.39222000 -3.35658300  H -3.73514900 -0.39222000 3.35658300  C -1.49101400 -1.45076800 -4.61426100  C -1.49101400 -1.45076800 4.61426100  H -0.69983000 -2.19859900 -4.70061500  H -0.69983000 -2.19859900 4.70061500  H -1.27044200 -0.64122900 -5.31454900  H -1.27044200 -0.64122900 5.31454900  H -2.42286300 -1.91759000 -4.94786900  H -2.42286300 -1.91759000 4.94786900  H -1.24934100 -1.35757400 0.00000000  H -0.40353400 -1.70876000 0.00000000  H 2.70360100 1.58290200 -4.12220400  H 2.70360100 1.58290200 4.12220400  H 2.51685500 1.28019100 -2.39610300  H 2.51685500 1.28019100 2.39610300  H 2.75840300 -0.06968100 -3.51482000  H 2.75840300 -0.06968100 3.51482000 | **2V+PhCN-TS-HM transfer**  N -0.01348400 -2.53636900 -0.66776900  O -0.01953700 -3.67010500 -1.01784500  V -0.00473500 -0.84934000 -0.27328500  P 2.38650500 -0.70348100 0.18874100  P -2.39416100 -0.67881100 0.18914800  C 2.43913100 -0.93427800 2.03816600  C -2.44908500 -0.90903400 2.03858300  H 2.41117700 0.06618600 2.47910400  H -2.41089600 0.09104400 2.47961900  H 3.35661700 -1.41837000 2.37829600  H -3.37143700 -1.38379300 2.37872200  C 1.21123500 -1.70922700 2.49094600  C -1.22914000 -1.69662600 2.49111400  H 1.17090000 -1.73164100 3.58916600  H -1.18883800 -1.71956200 3.58932300  H 1.24849400 -2.74418800 2.14254100  H -1.27715800 -2.73111200 2.14261200  N -0.00578300 -1.08216900 1.94886700  C -3.29582300 0.95452700 -0.01857300  C 3.30585200 0.92016900 -0.01842300  H -2.61221200 1.64132600 0.49136300  H 2.62934900 1.61439300 0.49100400  C -3.55608700 -1.97415100 -0.52475900  C 3.53501600 -2.01077300 -0.52516100  C -3.42378100 -3.32728300 0.17140400  C 3.38927400 -3.36235400 0.17130200  N -0.00254900 -0.39311600 -1.94169100  O -0.00106100 -0.07918100 -3.07905200  C 3.29465700 -2.16666000 -2.02737600  C -3.31732500 -2.13202500 -2.02701700  H 3.39563500 -1.22841400 -2.57286100  H -3.40929300 -1.19272400 -2.57227500  H 2.29312000 -2.55448300 -2.21809100  H -2.31951200 -2.52931900 -2.21777400  H 4.01667400 -2.87516800 -2.44495600  H -4.04609500 -2.83348100 -2.44476300  C -3.38710900 1.38621500 -1.48051000  C 3.40312500 1.35083200 -1.48027200  H -4.14657800 0.81337300 -2.01813700  H 4.15666800 0.76960800 -2.01724100  H -2.43733500 1.26729800 -2.00375000  H 2.45260000 1.24249000 -2.00440900  H -3.67513500 2.43962200 -1.53911000  H 3.70287400 2.40098100 -1.53860200  C -4.65815800 1.02897200 0.66618100  C 4.66838600 0.97971400 0.66737900  H -4.60932000 0.77832600 1.72752400  H 4.61587600 0.72998300 1.72874600  H -5.38690400 0.36517900 0.19373800  H 5.39012200 0.30770300 0.19576600  H -5.05444000 2.04610200 0.58900800  H 5.07598500 1.99236000 0.59017700  H 0.00331100 0.90029600 0.23392100  H -0.00067700 -0.09604100 2.26754400  N 0.00874900 1.75113600 2.54268000  C 0.01092500 2.14401200 1.43116100  C 0.01747100 3.31578700 0.56170100  C 0.01678200 3.24163700 -0.82719300  C 0.02318000 4.40410300 -1.58626200  C 0.03029400 5.64579100 -0.96449200  C 0.02467900 4.56922200 1.18837900  C 0.03104100 5.72482200 0.42506300  H 0.01122300 2.26317500 -1.29113600  H 0.02257300 4.33635000 -2.66825500  H 0.03526800 6.55231800 -1.55964800  H 0.02513500 4.61644000 2.27076100  H 0.03658400 6.69192700 0.91539900  H -4.12064500 -4.03785300 -0.28325700  H 4.07877100 -4.08001000 -0.28346000  H -2.41941600 -3.73784000 0.05210100  H 2.38077700 -3.76276900 0.05236400  H -3.65976100 -3.28050000 1.23624600  H 3.62604300 -3.31777800 1.23605800  H -4.57237600 -1.59896600 -0.36151600  H 4.55500800 -1.64570200 -0.36212000 |
| **2V + PhCN-interm**  N 0.00157300 2.52436700 -0.66208100  O 0.00229700 3.66383300 -0.98239400  V 0.00055400 0.85399700 -0.26100900  P -2.40669100 0.68359800 0.18971700  P 2.40760700 0.68062100 0.18974000  C -2.44791600 0.84210100 2.04252900  C 2.44902700 0.83920700 2.04254600  H -2.41717400 -0.17583500 2.44029800  H 2.41707300 -0.17865600 2.44040300  H -3.36165400 1.31526700 2.40714400  H 3.36332400 1.31130500 2.40713800  C -1.21143800 1.59094400 2.51576700  C 1.21345300 1.58957600 2.51571800  H -1.15101700 1.53656600 3.61175400  H 1.15295900 1.53540900 3.61171200  H -1.26276700 2.64934200 2.24582000  H 1.26605700 2.64787600 2.24563300  N 0.00066600 1.00127900 1.91834500  C 3.31239700 -0.94101300 -0.08484600  C -3.31340500 -0.93692100 -0.08502100  H 2.63747900 -1.65218200 0.40335700  H -2.63934100 -1.64889100 0.40319400  C 3.54742300 2.01375400 -0.48374800  C -3.54493500 2.01808900 -0.48370100  C 3.39505300 3.34049600 0.25762700  C -3.39117100 3.34460300 0.25779800  N 0.00029500 0.39634000 -1.93293700  O 0.00004600 0.10586800 -3.07467600  H -4.56504500 1.65082000 -0.32698900  H 4.56710500 1.64534200 -0.32693000  C -3.31231300 2.21929900 -1.98153300  C 3.31516400 2.21515400 -1.98160300  H -3.42192600 1.29898500 -2.55494600  H 3.42386700 1.29469100 -2.55494500  H -2.31100100 2.60950100 -2.16803500  H 2.31430900 2.60645500 -2.16825400  H -4.03393800 2.94339400 -2.37175800  H 4.03763200 2.93844700 -2.37175400  C 3.40614900 -1.32096900 -1.56091200  C -3.40749600 -1.31665900 -1.56111200  H 4.16179200 -0.72545100 -2.07879200  H -4.16235100 -0.72017600 -2.07903400  H 2.45619800 -1.19373500 -2.08176800  H -2.45733100 -1.19054700 -2.08185500  H 3.70111500 -2.36973900 -1.65349000  H -3.70374000 -2.36506000 -1.65378600  C 4.67579800 -1.02850200 0.59689800  C -4.67694000 -1.02286500 0.59664000  H 4.62497900 -0.81701400 1.66650000  H -4.62597600 -0.81140900 1.66624200  H 5.39942700 -0.34325700 0.14772400  H -5.39976800 -0.33683500 0.14738000  H 5.07811700 -2.03958600 0.48336000  H -5.08036800 -2.03350800 0.48309300  H -0.00057200 -1.05934800 0.33634800  H 0.00004900 -0.04602900 2.22644100  N -0.00122400 -1.65431400 2.39560200  C -0.00128900 -1.93701700 1.20782300  C -0.00209800 -3.23914300 0.49295700  C -0.00197300 -3.30144100 -0.89696200  C -0.00274700 -4.52906900 -1.54813800  C -0.00367200 -5.70544600 -0.81004200  C -0.00304100 -4.42567400 1.23147700  C -0.00381900 -5.64926800 0.58187400  H -0.00128300 -2.37749900 -1.46625500  H -0.00264100 -4.56605200 -2.63205500  H -0.00428200 -6.66501700 -1.31555100  H -0.00314400 -4.35787400 2.31348800  H -0.00455600 -6.56684000 1.16051400  H 4.08642600 4.07372700 -0.16822900  H -4.08162900 4.07865400 -0.16813300  H 2.38694900 3.74408500 0.14742600  H -2.38259100 3.74703900 0.14779500  H 3.62493300 3.25869500 1.32143600  H -3.62133900 3.26299600 1.32156400 | **2V + PhCN-TS-HN transfer**  N -2.56195100 -0.62447600 0.00000000  O -3.71102700 -0.90462300 0.00000000  V -0.88859900 -0.25111400 0.00000000  P -0.69856800 0.18358800 2.41115100  P -0.69856800 0.18358800 -2.41115100  C -0.74254700 2.04011000 2.45295900  C -0.74254700 2.04011000 -2.45295900  H 0.29798200 2.37458400 2.44138300  H 0.29798200 2.37458400 -2.44138300  H -1.20791600 2.43221900 3.35943700  H -1.20791600 2.43221900 -3.35943700  C -1.44116600 2.55373100 1.20242500  C -1.44116600 2.55373100 -1.20242500  H -1.28784700 3.64046600 1.12914800  H -1.28784700 3.64046600 -1.12914800  H -2.52240700 2.38937700 1.26436200  H -2.52240700 2.38937700 -1.26436200  N -0.90561300 1.89401600 0.00000000  C 0.90357000 -0.19144500 -3.31646100  C 0.90357000 -0.19144500 3.31646100  H 1.63984900 0.27816400 -2.65500200  H 1.63984900 0.27816400 2.65500200  C -2.07523200 -0.40698700 -3.54383300  C -2.07523200 -0.40698700 3.54383300  C -3.36099200 0.39683700 -3.35896800  C -3.36099200 0.39683700 3.35896800  N -0.45945500 -1.93292300 0.00000000  O -0.18861700 -3.07992000 0.00000000  C -2.34602700 -1.89738400 3.33635500  C -2.34602700 -1.89738400 -3.33635500  H -1.45799500 -2.51276900 3.47935500  H -1.45799500 -2.51276900 -3.47935500  H -2.72288600 -2.08639900 2.33037800  H -2.72288600 -2.08639900 -2.33037800  H -3.10433400 -2.23604400 4.04879900  H -3.10433400 -2.23604400 -4.04879900  C 1.21815900 -1.68438200 -3.38042600  C 1.21815900 -1.68438200 3.38042600  H 0.59914700 -2.19122800 -4.12438200  H 0.59914700 -2.19122800 4.12438200  H 1.06977600 -2.18039400 -2.42039300  H 1.06977600 -2.18039400 2.42039300  H 2.26107500 -1.82886100 -3.67576800  H 2.26107500 -1.82886100 3.67576800  C 1.01703300 0.45830900 -4.69363200  C 1.01703300 0.45830900 4.69363200  H 0.84764200 1.53628100 -4.66469900  H 0.84764200 1.53628100 4.66469900  H 0.31335200 0.02156700 -5.40699400  H 0.31335200 0.02156700 5.40699400  H 2.02220100 0.29645000 -5.09429200  H 2.02220100 0.29645000 5.09429200  H 1.13571200 0.25135900 0.00000000  H 0.27420700 2.18006700 0.00000000  N 1.65130000 2.29696600 0.00000000  C 1.96533100 1.10435400 0.00000000  C 3.30134800 0.46250600 0.00000000  C 3.42669900 -0.92454000 0.00000000  C 4.68259800 -1.51909300 0.00000000  C 5.82380700 -0.72761000 0.00000000  C 4.45314400 1.25376000 0.00000000  C 5.70484300 0.66041300 0.00000000  H 2.53115900 -1.53821700 0.00000000  H 4.76951800 -2.60010300 0.00000000  H 6.80536900 -1.18891000 0.00000000  H 4.33623300 2.33158100 0.00000000  H 6.59550900 1.27958100 0.00000000  H -4.12344200 0.02209500 -4.04835000  H -4.12344200 0.02209500 4.04835000  H -3.75654500 0.28842900 -2.34764500  H -3.75654500 0.28842900 2.34764500  H -3.22751800 1.45936200 -3.56930000  H -3.22751800 1.45936200 3.56930000  H -1.71309200 -0.24846400 -4.56549100  H -1.71309200 -0.24846400 4.56549100 |
| **2V + Ph-CHNH-TS**  O 2.13105000 2.88896700 -1.01501000  P -1.45728300 1.81135600 0.16412500  P 2.54132000 -0.88755300 0.17225700  C -1.42313200 1.95332300 2.02185500  C 2.63002300 -0.82946300 2.03173400  H -2.00548900 1.11184700 2.40732000  H 2.04261900 -1.67487000 2.40228300  H -1.89412300 2.86853200 2.38611900  H 3.64782600 -0.94229700 2.41137200  C 0.00899900 1.84163900 2.52112600  C 2.00470500 0.46379300 2.53352600  H 0.01355000 1.78492300 3.61926600  H 1.93676600 0.43518500 3.63023000  H 0.58740100 2.72530800 2.23930800  H 2.62308800 1.32463300 2.26722800  N 0.66578800 0.65394200 1.94950400  C 2.55820300 -2.74077200 -0.15540800  C -3.14061800 1.04199800 -0.13334600  H 1.65052900 -3.06821100 0.36144500  H -3.01709600 0.06089200 0.33662300  C 4.22009400 -0.29614800 -0.43813400  C -1.60778800 3.57341700 -0.47721700  C 4.74545900 0.90622100 0.34351700  C -0.72578100 4.55826200 0.28794600  O 0.14556900 -0.10748900 -3.07110800  H -2.65439400 3.85979000 -0.32609000  H 4.90824100 -1.13261600 -0.27741700  C -1.28862200 3.63117000 -1.97207400  C 4.16880800 0.02290800 -1.93275400  H -1.89532600 2.94388800 -2.56143200  H 3.81472400 -0.81571100 -2.53238100  H -0.24075600 3.39009600 -2.15403400  H 3.51136100 0.87089500 -2.12605700  H -1.47058000 4.64283900 -2.34784100  H 5.17033800 0.28562700 -2.28703200  C 2.39073600 -3.07698000 -1.63588000  C -3.41892900 0.80445400 -1.61585200  H 3.31348400 -2.89888600 -2.19252100  H -3.66214900 1.73665100 -2.13161000  H 1.59639000 -2.49258600 -2.10282600  H -2.57051200 0.34189800 -2.12159700  H 2.14593700 -4.13688700 -1.75107400  H -4.27818500 0.13767300 -1.72606600  C 3.73483900 -3.49452100 0.45992000  C -4.30550700 1.76233500 0.54090500  H 3.84539800 -3.29823100 1.52820700  H -4.15218200 1.90174500 1.61302600  H 4.67868500 -3.24601600 -0.03138400  H -4.48951600 2.74350100 0.09547400  H 3.58576100 -4.57188000 0.33916000  H -5.22116200 1.17669900 0.41524500  H -0.55245100 -0.87083300 0.18517600  H 0.09260900 -0.18259100 2.24342200  C -0.97776300 -2.01341900 1.19905900  C -2.20571500 -2.49064200 0.48044800  C -2.15885600 -2.77792400 -0.88504800  C -3.26559600 -3.29118100 -1.54248000  C -4.44614400 -3.52710800 -0.84401200  C -3.38791100 -2.74533400 1.17352300  C -4.50296100 -3.25270200 0.51530800  H -1.24755000 -2.56948300 -1.43523500  H -3.21080400 -3.50332600 -2.60464200  H -5.31314900 -3.92827600 -1.35716500  H -3.43029600 -2.57620600 2.24408200  H -5.41280900 -3.44895400 1.07227100  H 5.72627200 1.19015300 -0.04978900  H 4.09033800 1.77170800 0.23384200  H 4.87364600 0.69354700 1.40659400  H -0.86451400 5.56268200 -0.12342800  H -0.97111100 4.60852800 1.35053000  H 0.33166200 4.30961400 0.18312300  H -0.09253700 -2.56487400 0.88686400  N 0.32314100 0.15732200 -1.93742300  V 0.58035300 0.53959500 -0.26862200  N 1.52289300 1.93328100 -0.65926300  N -0.95711500 -1.59321200 2.44870800  H -1.88374800 -1.27495700 2.73226700 | **2V + Ph-CHNCH2Ph-TS**  O -3.12840300 0.80612300 2.12888500  P -1.14049300 2.02475600 -1.25155400  P -1.15181200 -2.45939600 0.59674900  C 0.33517900 1.61295600 -2.31126200  C 0.14580400 -3.02607800 -0.61204500  H 1.21983800 1.85958200 -1.71934100  H 1.10821500 -2.89936100 -0.10921700  H 0.37923700 2.21307600 -3.22316400  H 0.04027000 -4.07774100 -0.88567500  C 0.33914800 0.13038500 -2.65177300  C 0.12240600 -2.13973600 -1.84664300  H 1.28236600 -0.13355500 -3.14944400  H 0.99167800 -2.37056300 -2.47756300  H -0.46877300 -0.09619300 -3.35213200  H -0.77536000 -2.31796500 -2.44405100  N 0.14332100 -0.71493900 -1.45976400  C -0.36894000 -2.98134800 2.22966700  C -0.52377400 3.51137000 -0.28967900  H 0.60899700 -2.49263500 2.16872900  H 0.32341800 3.07088000 0.24397100  C -2.59715000 -3.64291900 0.37527600  C -2.41626600 2.71141500 -2.45132600  C -2.90899400 -3.93419000 -1.09133400  C -2.55123500 1.86425200 -3.71525600  O -3.91111300 -0.65744800 -1.63380100  C -3.77626300 2.86755800 -1.76945200  C -3.83956900 -3.12218200 1.09761200  H -3.73012100 3.48432900 -0.87220700  H -3.66401100 -2.93899700 2.15825300  H -4.18471000 1.89617500 -1.48867400  H -4.18741400 -2.18960400 0.65220000  H -4.48120400 3.33998000 -2.46055500  H -4.64767100 -3.85564100 1.01721300  C -1.10736800 -2.41572200 3.44087100  C -1.51207500 3.99348800 0.76987500  H -2.04761400 -2.94204100 3.61900500  H -2.33743300 4.55509900 0.32657700  H -1.33835700 -1.35566100 3.32168100  H -1.92843500 3.16773500 1.34724600  H -0.49740200 -2.53578100 4.34133400  H -1.00176900 4.66501000 1.46612600  C -0.11719100 -4.48024400 2.37653200  C -0.01468100 4.66792200 -1.14560400  H 0.40981200 -4.90209800 1.51801200  H 0.72331600 4.35290400 -1.88683400  H -1.04671400 -5.03772200 2.51378200  H -0.82879800 5.17200600 -1.67254300  H 0.49953000 -4.66457100 3.26156200  H 0.46239200 5.41677700 -0.50588200  H 0.01987000 0.59307000 0.79563100  H 0.97019300 -0.60622400 -0.82065400  N 2.18265900 -0.37525100 0.53723700  H -2.04871700 3.70148400 -2.74253900  H -2.28295700 -4.58062500 0.84438900  H -3.73302000 -4.65217300 -1.14638100  H -3.30478900 2.31098100 -4.37092400  H -3.22545700 -3.03646600 -1.62286100  H -2.88417900 0.85120600 -3.48341000  H -2.06204400 -4.37583400 -1.61992400  H -1.62157400 1.80788400 -4.28498500  C 3.27729100 0.37264300 -0.02688400  H 2.95254300 1.21207000 -0.66647900  H 3.89535700 0.83619000 0.75901100  C 4.18254900 -0.50178200 -0.86714900  C 4.36289500 -1.85017000 -0.56698100  C 4.89253100 0.04163700 -1.93687400  C 5.23281100 -2.63360400 -1.31515100  H 3.80406000 -2.27161900 0.26012700  C 5.76337200 -0.73822700 -2.68797600  H 4.76101400 1.09078500 -2.18739000  C 5.93688200 -2.08166300 -2.37893000  H 5.36347200 -3.68158600 -1.06590800  H 6.30439200 -0.29678100 -3.51820700  H 6.61448500 -2.69394000 -2.96381900  C 1.36465700 0.15953500 1.43615000  H 0.81608100 -0.58169600 2.00910400  C 1.61997000 1.35712300 2.30576000  C 1.21990300 1.26812800 3.64213500  C 2.24242400 2.53846200 1.89148500  C 1.44118200 2.30496300 4.53619400  H 0.72662400 0.36451300 3.98481100  C 2.46566300 3.57986700 2.78378400  H 2.55256400 2.66121000 0.86322300  C 2.06957700 3.46814200 4.10985600  H 1.12128500 2.20477000 5.56755500  H 2.95370600 4.48467500 2.43779900  H 2.24687500 4.28157600 4.80449600  N -2.47155400 0.44644500 1.22168200  N -2.89513900 -0.48716800 -1.04265000  V -1.50094800 -0.09444200 -0.10697600 |
| **2V + Ph-CHNPh-TS**  O -1.80382800 0.29190900 3.12889600  P 0.22496300 2.39100200 0.26951800  P -2.45381800 -1.56966700 -0.50798200  C 0.93191300 2.28724100 -1.44965400  C -1.90412700 -1.65992200 -2.28765500  H 1.82445200 1.65895900 -1.38971700  H -1.01889600 -2.30208600 -2.31527200  H 1.24692500 3.25971400 -1.83402400  H -2.65914900 -2.10581800 -2.93918400  C -0.07878200 1.64469200 -2.38682800  C -1.52196300 -0.27046000 -2.77707200  H 0.38133300 1.48465800 -3.37165800  H -1.07601800 -0.34324000 -3.77894400  H -0.94136400 2.29984100 -2.53217200  H -2.40190900 0.37217600 -2.85674000  N -0.57473800 0.36666300 -1.84433500  C -2.05035900 -3.30994000 0.10407900  C 1.76151300 2.36216700 1.34534200  H -1.03774800 -3.45884200 -0.28515500  H 2.12154400 1.34502500 1.16604900  C -4.33265900 -1.53776700 -0.58865400  C -0.43319600 4.14711600 0.43380500  C -4.87287200 -0.56111900 -1.63098000  C -1.16768500 4.62542300 -0.81728800  O -3.63988500 2.19927800 0.01614600  C -1.34070500 4.27965200 1.65828700  C -4.92346200 -1.24470600 0.78965900  H -0.86314700 3.94569500 2.57885000  H -4.61709300 -1.97529000 1.53979300  H -2.25587400 3.70178600 1.52748100  H -4.62257300 -0.25725100 1.14252800  H -1.62365200 5.32842600 1.79241900  H -6.01612200 -1.26516700 0.73615600  C -1.97612400 -3.38596500 1.62743000  C 1.43937400 2.47690800 2.83387600  H -2.96331900 -3.29942300 2.08600800  H 1.18839600 3.50344300 3.11077900  H -1.34750700 -2.59701000 2.04194700  H 0.61079900 1.83104000 3.12841300  H -1.55841500 -4.34962500 1.93316600  H 2.31554800 2.18962500 3.42205800  C -2.92002500 -4.42248400 -0.47633400  C 2.85083200 3.34951500 0.93641900  H -2.99440400 -4.37231000 -1.56531900  H 3.15285700 3.23266400 -0.10576400  H -3.93149500 -4.40397800 -0.06396100  H 2.53746300 4.38597400 1.08689200  H -2.48843200 -5.39526200 -0.22212300  H 3.74036900 3.19251800 1.55436900  H 0.33746400 -0.35856000 0.52966000  H 0.23051600 -0.27991700 -1.75648500  N 1.64592200 -1.52302800 -1.27825400  H 0.44883800 4.78158100 0.57566800  H -4.62953500 -2.54597000 -0.89298800  H -5.96521100 -0.62559400 -1.64678000  H -1.51641700 5.65085600 -0.66176100  H -4.61207400 0.47052300 -1.39580700  H -2.04817400 4.01301700 -1.01971200  H -4.52429400 -0.79219200 -2.63958400  H -0.53175900 4.63221800 -1.70453800  C 1.29972400 -1.69314700 -0.02295900  H 0.37272800 -2.24114300 0.09782400  C 2.20712900 -1.89652400 1.15478200  C 3.34242800 -2.69691100 0.99603000  C 1.87740700 -1.45279300 2.43487600  C 4.13485100 -3.02554000 2.08663500  H 3.60034500 -3.06500800 0.01007900  C 2.67169900 -1.78137400 3.52600900  H 0.99586900 -0.83648000 2.56437900  C 3.80544900 -2.56575900 3.35615900  H 5.01187800 -3.64736100 1.94334300  H 2.40046500 -1.42242000 4.51288800  H 4.42662400 -2.82078300 4.20769800  C 2.85708400 -0.97418600 -1.69680000  C 3.21589700 -1.22103600 -3.03331400  C 3.71536900 -0.16066700 -0.93744400  C 4.37966000 -0.70454800 -3.57735400  H 2.55330700 -1.84146900 -3.62663900  C 4.87672100 0.36210000 -1.49084000  H 3.47906600 0.05163400 0.09630900  C 5.22190300 0.09432400 -2.80972000  H 4.63125600 -0.92349900 -4.60982500  H 5.52170400 0.98399300 -0.87863800  H 6.13192400 0.50289000 -3.23396300  N -1.60025000 0.36898500 1.97197500  V -1.29768200 0.48886000 0.27222700  N -2.69805100 1.47715300 0.04982300 | **2V + Ph-CCH-TS-HM transfer to C-H**  N -1.30591000 -2.38663100 0.00000000  O -2.16915400 -3.18969300 0.00000000  P 0.01131400 -0.70238800 -2.37519200  P 0.01131400 -0.70238800 2.37519200  C 1.14341900 0.78237000 -2.45085900  C 1.14341900 0.78237000 2.45085900  H 0.50463600 1.66988300 -2.45294300  H 0.50463600 1.66988300 2.45294300  H 1.73908500 0.81022100 -3.36558100  H 1.73908500 0.81022100 3.36558100  C 2.04038700 0.81053700 -1.22297400  C 2.04038700 0.81053700 1.22297400  H 2.59727100 1.75708300 -1.18701000  H 2.59727100 1.75708300 1.18701000  H 2.76939300 -0.00235200 -1.25518200  H 2.76939300 -0.00235200 1.25518200  N 1.23668300 0.64002100 0.00000000  C -1.52369100 -0.02939700 3.22422700  C -1.52369100 -0.02939700 -3.22422700  H -1.71368300 0.86220000 2.61633200  H -1.71368300 0.86220000 -2.61633200  C 0.76474900 -1.93680200 3.57446600  C 0.76474900 -1.93680200 -3.57446600  C 2.26683300 -2.10483500 3.35384200  C 2.26683300 -2.10483500 -3.35384200  O 1.97079500 -3.31521000 0.00000000  H 0.60604400 -1.53118200 -4.57945500  H 0.60604400 -1.53118200 4.57945500  C 0.05766600 -3.28692600 -3.45980900  C 0.05766600 -3.28692600 3.45980900  H -1.00960300 -3.22301100 -3.67413600  H -1.00960300 -3.22301100 3.67413600  H 0.17150700 -3.69834800 -2.45520300  H 0.17150700 -3.69834800 2.45520300  H 0.49609700 -3.99661200 -4.16789500  H 0.49609700 -3.99661200 4.16789500  C -2.73548500 -0.94527800 3.07293500  C -2.73548500 -0.94527800 -3.07293500  H -2.65844800 -1.83122000 3.70688400  H -2.65844800 -1.83122000 -3.70688400  H -2.86215300 -1.27832000 2.04237400  H -2.86215300 -1.27832000 -2.04237400  H -3.64208400 -0.41172300 3.37427700  H -3.64208400 -0.41172300 -3.37427700  C -1.32037700 0.40270100 4.67371500  C -1.32037700 0.40270100 -4.67371500  H -0.46176300 1.06691300 4.79843500  H -0.46176300 1.06691300 -4.79843500  H -1.18203300 -0.45592300 5.33550900  H -1.18203300 -0.45592300 -5.33550900  H -2.20480400 0.94092900 5.02831000  H -2.20480400 0.94092900 -5.02831000  H -1.27790100 0.14048900 0.00000000  H 0.51203700 1.36400700 0.00000000  C -2.03415700 1.62875600 0.00000000  H 2.65999500 -2.82586100 4.07694700  H 2.48237900 -2.49192700 2.35676000  H 2.82017400 -1.17412300 3.49552900  H 2.65999500 -2.82586100 -4.07694700  H 2.82017400 -1.17412300 -3.49552900  H 2.48237900 -2.49192700 -2.35676000  C -1.41732700 2.69785800 0.00000000  C -0.61883800 3.85854300 0.00000000  C -0.21872800 4.46843400 1.20716900  C -0.21872800 4.46843400 -1.20716900  C 0.55718000 5.61482200 1.19962100  H -0.54017900 4.03605900 2.14758500  C 0.55718000 5.61482200 -1.19962100  H -0.54017900 4.03605900 -2.14758500  C 0.95650400 6.19590300 0.00000000  H 0.84871900 6.06515700 2.14252500  H 0.84871900 6.06515700 -2.14252500  H 1.56199200 7.09464200 0.00000000  H -2.99247000 1.15039600 0.00000000  N 1.19834100 -2.41241400 0.00000000  V -0.04354900 -1.20413400 0.00000000 |
| **2V + PhCCH-TS-HM transfer to Ph-C**  N -2.52475600 -0.70295500 0.00000000  O -3.65403300 -1.06955300 0.00000000  V -0.84811400 -0.27037000 0.00000000  P -0.68329100 0.18397700 2.38647200  P -0.68329100 0.18397700 -2.38647200  C -0.93652900 2.03080700 2.44290800  C -0.93652900 2.03080700 -2.44290800  H 0.06146300 2.47749700 2.40640300  H 0.06146300 2.47749700 -2.40640300  H -1.41530200 2.36773200 3.36435300  H -1.41530200 2.36773200 -3.36435300  C -1.72469400 2.47744700 1.22134500  C -1.72469400 2.47744700 -1.22134500  H -1.75016100 3.57615600 1.17541700  H -1.75016100 3.57615600 -1.17541700  H -2.75880100 2.12860800 1.27035800  H -2.75880100 2.12860800 -1.27035800  N -1.11109000 1.92993300 0.00000000  C 0.95103900 -0.00305900 -3.28960700  C 0.95103900 -0.00305900 3.28960700  H 1.63442400 0.50104200 -2.59815200  H 1.63442400 0.50104200 2.59815200  C -1.97180500 -0.54559800 -3.54664500  C -1.97180500 -0.54559800 3.54664500  C -3.33192600 0.13644100 -3.41306500  C -3.33192600 0.13644100 3.41306500  N -0.34101000 -1.92441400 0.00000000  O -0.00023700 -3.05481500 0.00000000  C -2.11375500 -2.04875600 3.30331500  C -2.11375500 -2.04875600 -3.30331500  H -1.16870500 -2.58403900 3.39437000  H -1.16870500 -2.58403900 -3.39437000  H -2.50807600 -2.24041900 2.30449900  H -2.50807600 -2.24041900 -2.30449900  H -2.81139100 -2.47605600 4.03027200  H -2.81139100 -2.47605600 -4.03027200  C 1.38932500 -1.46180500 -3.40062800  C 1.38932500 -1.46180500 3.40062800  H 0.81862400 -1.99194000 -4.16717000  H 0.81862400 -1.99194000 4.16717000  H 1.27575500 -1.99857700 -2.45795100  H 1.27575500 -1.99857700 2.45795100  H 2.44294500 -1.51045200 -3.68933000  H 2.44294500 -1.51045200 3.68933000  C 1.02103300 0.69747600 -4.64416300  C 1.02103300 0.69747600 4.64416300  H 0.76759100 1.75765400 -4.58372300  H 0.76759100 1.75765400 4.58372300  H 0.35740100 0.23162400 -5.37746800  H 0.35740100 0.23162400 5.37746800  H 2.03786100 0.62756100 -5.04257000  H 2.03786100 0.62756100 5.04257000  H 0.88466100 0.36062700 0.00000000  H -0.11530700 2.23409600 0.00000000  C 2.14728200 1.51161900 0.00000000  C 3.27136600 0.58411500 0.00000000  C 3.14659100 -0.80322300 0.00000000  C 4.27232300 -1.61656700 0.00000000  C 5.54279000 -1.05735800 0.00000000  C 4.56049500 1.14102100 0.00000000  C 5.68108400 0.32775200 0.00000000  H 2.15092900 -1.22772500 0.00000000  H 4.15113500 -2.69419300 0.00000000  H 6.42103900 -1.69354600 0.00000000  H 4.66294200 2.21999000 0.00000000  H 6.66875100 0.77614000 0.00000000  H -4.04049800 -0.32904600 -4.10482100  H -4.04049800 -0.32904600 4.10482100  H -3.73704000 0.01730400 -2.40633800  H -3.73704000 0.01730400 2.40633800  H -3.29764900 1.20071100 -3.65431300  H -3.29764900 1.20071100 3.65431300  H -1.59962500 -0.38126800 -4.56396600  H -1.59962500 -0.38126800 4.56396600  C 1.79046000 2.69530300 0.00000000  H 1.76911700 3.76123200 0.00000000 | **2V + PhCCH-interm to Ph-C**  O -3.59516900 -1.14594900 0.00000000  P -0.67416900 0.20163400 2.40642700  P -0.67416900 0.20163400 -2.40642700  C -1.00799100 2.03442600 2.44418000  C -1.00799100 2.03442600 -2.44418000  H -0.03051600 2.52422800 2.39960400  H -0.03051600 2.52422800 -2.39960400  H -1.49599500 2.35852400 3.36498600  H -1.49599500 2.35852400 -3.36498600  C -1.82290300 2.43330800 1.22444600  C -1.82290300 2.43330800 -1.22444600  H -1.90578300 3.52768200 1.17172400  H -1.90578300 3.52768200 -1.17172400  H -2.83594500 2.02893200 1.27470900  H -2.83594500 2.02893200 -1.27470900  N -1.18136200 1.91493100 0.00000000  C 0.96766700 0.08361600 -3.30563600  C 0.96766700 0.08361600 3.30563600  H 1.63730200 0.60264200 -2.61130600  H 1.63730200 0.60264200 2.61130600  C -1.93507400 -0.58996700 -3.55307500  C -1.93507400 -0.58996700 3.55307500  C -3.32003400 0.04298800 -3.43577400  C -3.32003400 0.04298800 3.43577400  O 0.00890100 -3.04797000 0.00000000  H -1.56189000 -0.42077300 4.56903500  H -1.56189000 -0.42077300 -4.56903500  C -2.01832000 -2.09538500 3.29789400  C -2.01832000 -2.09538500 -3.29789400  H -1.05027700 -2.59100000 3.36812400  H -1.05027700 -2.59100000 -3.36812400  H -2.42375700 -2.29735900 2.30565000  H -2.42375700 -2.29735900 -2.30565000  H -2.68389600 -2.55651200 4.03378500  H -2.68389600 -2.55651200 -4.03378500  C 1.45280000 -1.35779400 -3.44306800  C 1.45280000 -1.35779400 3.44306800  H 0.89210900 -1.89695900 -4.21080100  H 0.89210900 -1.89695900 4.21080100  H 1.37433300 -1.91156300 -2.50675100  H 1.37433300 -1.91156300 2.50675100  H 2.50392500 -1.36302500 -3.74265100  H 2.50392500 -1.36302500 3.74265100  C 1.00378300 0.80844700 -4.64890500  C 1.00378300 0.80844700 4.64890500  H 0.72574400 1.86078400 -4.56811700  H 0.72574400 1.86078400 4.56811700  H 0.34724500 0.33708300 -5.38522800  H 0.34724500 0.33708300 5.38522800  H 2.01923200 0.77202400 -5.05394100  H 2.01923200 0.77202400 5.05394100  H 1.04892100 0.66666800 0.00000000  H -0.21404500 2.28415500 0.00000000  C 1.99167400 1.38760500 0.00000000  C 3.20772100 0.54451900 0.00000000  C 3.13545600 -0.84772700 0.00000000  C 4.28476300 -1.63004400 0.00000000  C 5.53574300 -1.02961100 0.00000000  C 4.47739700 1.13859500 0.00000000  C 5.62274900 0.36148200 0.00000000  H 2.16006400 -1.32157300 0.00000000  H 4.19832800 -2.71150500 0.00000000  H 6.43532800 -1.63552800 0.00000000  H 4.52546800 2.22188500 0.00000000  H 6.59574900 0.84211400 0.00000000  H -4.00380400 -0.45349700 -4.13055100  H -3.73163700 -0.08336500 -2.43258500  H -3.32263500 1.10568500 -3.68534000  H -4.00380400 -0.45349700 4.13055100  H -3.32263500 1.10568500 3.68534000  H -3.73163700 -0.08336500 2.43258500  C 1.95402900 2.69751300 0.00000000  H 1.08151200 3.35411900 0.00000000  N -0.30331500 -1.91370400 0.00000000  V -0.83416100 -0.26334300 0.00000000  N -2.47735300 -0.75520300 0.00000000 |
| **2V + PhCCH-TS-HN transfer to C-H**  N -2.49388600 -0.71333000 0.00000000  O -3.61903700 -1.08916800 0.00000000  V -0.83733900 -0.26038600 0.00000000  P -0.67571400 0.18742200 2.40117000  P -0.67571400 0.18742200 -2.40117000  C -0.92185100 2.03339700 2.44853500  C -0.92185100 2.03339700 -2.44853500  H 0.07878500 2.47454800 2.41706700  H 0.07878500 2.47454800 -2.41706700  H -1.40611500 2.37674600 3.36462200  H -1.40611500 2.37674600 -3.36462200  C -1.69761600 2.47788600 1.21880000  C -1.69761600 2.47788600 -1.21880000  H -1.71004300 3.57613800 1.16513400  H -1.71004300 3.57613800 -1.16513400  H -2.73583100 2.14168000 1.26235500  H -2.73583100 2.14168000 -1.26235500  N -1.07923600 1.92080800 0.00000000  C 0.95350200 -0.00779700 -3.31268800  C 0.95350200 -0.00779700 3.31268800  H 1.64678900 0.49566000 -2.63031600  H 1.64678900 0.49566000 2.63031600  C -1.97630600 -0.54601400 -3.54313400  C -1.97630600 -0.54601400 3.54313400  C -3.33268300 0.14225700 -3.40419200  C -3.33268300 0.14225700 3.40419200  N -0.30504900 -1.90901800 0.00000000  O 0.02411800 -3.04206300 0.00000000  C -2.11936400 -2.04817100 3.29492700  C -2.11936400 -2.04817100 -3.29492700  H -1.17513800 -2.58464200 3.38666300  H -1.17513800 -2.58464200 -3.38666300  H -2.51347400 -2.23810000 2.29583100  H -2.51347400 -2.23810000 -2.29583100  H -2.81835000 -2.47577600 4.02021200  H -2.81835000 -2.47577600 -4.02021200  C 1.38584900 -1.46791600 -3.42820200  C 1.38584900 -1.46791600 3.42820200  H 0.80511500 -1.99703900 -4.18782900  H 0.80511500 -1.99703900 4.18782900  H 1.28449900 -2.00458600 -2.48409600  H 1.28449900 -2.00458600 2.48409600  H 2.43584400 -1.51791800 -3.72867500  H 2.43584400 -1.51791800 3.72867500  C 1.01187000 0.69379400 -4.66744700  C 1.01187000 0.69379400 4.66744700  H 0.76368800 1.75488400 -4.60345100  H 0.76368800 1.75488400 4.60345100  H 0.34013200 0.23058500 -5.39501600  H 0.34013200 0.23058500 5.39501600  H 2.02492700 0.62058600 -5.07414200  H 2.02492700 0.62058600 5.07414200  H 1.03869500 0.56453700 0.00000000  H -0.08163700 2.26163200 0.00000000  C 1.97538500 1.37130500 0.00000000  C 3.20905200 0.54698000 0.00000000  C 3.15493700 -0.84448300 0.00000000  C 4.31789600 -1.60556700 0.00000000  C 5.55806300 -0.98192400 0.00000000  C 4.46428500 1.16600500 0.00000000  C 5.62424200 0.40983800 0.00000000  H 2.18462300 -1.32882900 0.00000000  H 4.25191300 -2.68830600 0.00000000  H 6.46780200 -1.57246900 0.00000000  H 4.49782800 2.25022000 0.00000000  H 6.58927900 0.90587400 0.00000000  H -4.04602900 -0.32217500 -4.09153800  H -4.04602900 -0.32217500 4.09153800  H -3.73418300 0.02774700 -2.39557200  H -3.73418300 0.02774700 2.39557200  H -3.29473000 1.20557700 -3.64856500  H -3.29473000 1.20557700 3.64856500  H -1.60911400 -0.38579200 -4.56278500  H -1.60911400 -0.38579200 4.56278500  C 1.81591000 2.63899200 0.00000000  H 1.45528600 3.64179800 0.00000000 | **2V + PhCHCH2-TS-HM transfer**  O -2.44929000 2.53447900 -1.48332800  P 1.20148100 1.92945400 -0.03173100  P -2.42511200 -1.20373600 -0.07589600  C 2.16221800 0.93370700 -1.28297500  C -1.61357600 -2.24394800 -1.39833800  H 2.79194000 0.23241500 -0.72862600  H -1.03748500 -3.01927900 -0.88572700  H 2.82591800 1.55383600 -1.88969300  H -2.33927500 -2.75113900 -2.03761400  C 1.20141200 0.16053200 -2.17227600  C -0.67756600 -1.38265000 -2.23174100  H 1.76340100 -0.53615400 -2.80900400  H -0.07920400 -2.01871500 -2.89919900  H 0.65198200 0.83850500 -2.82947100  H -1.24531400 -0.69214400 -2.85949400  N 0.20390900 -0.57378000 -1.36912800  C -2.62110600 -2.47020500 1.30244500  C 2.40278100 1.96783300 1.41393300  H -1.59719900 -2.85057400 1.38284300  H 2.62021400 0.90057700 1.52078600  C -4.16573600 -0.89683300 -0.71445300  C 1.20042300 3.67717000 -0.72306600  C -4.17639900 -0.44110100 -2.17226800  C 0.79100000 3.71611800 -2.19403800  O -1.96828500 1.87151200 2.55642700  H 2.23249100 4.03533700 -0.64665200  H -4.68720200 -1.85771400 -0.65277600  C 0.29368200 4.58284500 0.10925200  C -4.88621500 0.12089500 0.16926200  H 0.60487200 4.64268500 1.15276300  H -4.95517100 -0.19963700 1.20940700  H -0.73768200 4.22683300 0.08674700  H -4.37290400 1.08360000 0.14970100  H 0.30880800 5.59810100 -0.29858600  H -5.90540900 0.27412300 -0.19806700  C -2.98007100 -1.83376600 2.64303300  C 1.75692700 2.43469800 2.71568700  H -4.01876200 -1.49778000 2.66592000  H 1.55804200 3.50827600 2.70969200  H -2.34647200 -0.97469600 2.86657700  H 0.81494200 1.91997300 2.90541100  H -2.86131800 -2.56674000 3.44674200  H 2.43094200 2.23743200 3.55501000  C -3.53440900 -3.64841300 0.97411400  C 3.71725900 2.69321800 1.14012700  H -3.28978600 -4.11664100 0.01766000  H 4.19505800 2.36071000 0.21566800  H -4.58461500 -3.34852900 0.94571700  H 3.57591000 3.77505100 1.08062200  H -3.44165400 -4.41642700 1.74804600  H 4.42054700 2.50750900 1.95774600  H 0.14112200 -0.41824500 1.21757200  H 0.71038800 -1.21951900 -0.74888300  C 0.96157300 -1.67316700 1.82278000  H -5.21158500 -0.29734600 -2.49636100  H -3.66039100 0.51134300 -2.29812800  H -3.72895000 -1.17506400 -2.84576300  H 0.82091100 4.75069900 -2.54921500  H 1.46340000 3.13853600 -2.83171400  H -0.22749000 3.35252800 -2.33581500  H 0.08077300 -1.94514800 2.38886000  C 1.48226400 -2.57990600 0.92453200  H 0.83687900 -3.38740600 0.58609500  V -0.88504700 0.68368100 0.13333800  N -1.52898000 1.39506400 1.57238500  N -1.79105100 1.74087700 -0.89133400  C 2.82213600 -2.59882900 0.37466400  C 3.13996700 -3.50037900 -0.66075500  C 3.86863200 -1.77832300 0.83902300  C 4.41086200 -3.56685700 -1.20675400  H 2.36366000 -4.16307300 -1.03217000  C 5.13879600 -1.84391200 0.28867100  H 3.69153900 -1.10186600 1.66751400  C 5.42367000 -2.73296200 -0.74306400  H 4.61500700 -4.27698600 -2.00147200  H 5.92155500 -1.20164400 0.67920200  H 6.41945600 -2.78442700 -1.16777600  H 1.62098800 -0.99924900 2.35853100 |
| **2V + Ph-CHCH2-interm**  O -2.44849800 2.50763100 -1.45878500  P 1.20536400 1.92673800 -0.03470500  P -2.46730400 -1.21386900 -0.06258000  C 2.16644900 0.88806900 -1.24201300  C -1.65192500 -2.26004700 -1.37186600  H 2.77789800 0.19379600 -0.65813400  H -1.09868400 -3.04478400 -0.84998800  H 2.84811500 1.47916400 -1.85717700  H -2.37340300 -2.75261300 -2.02685200  C 1.20582200 0.09981200 -2.11630000  C -0.68368100 -1.41252000 -2.18179100  H 1.76815800 -0.62882100 -2.71431000  H -0.06807600 -2.06250000 -2.81826000  H 0.67870200 0.75964400 -2.80933700  H -1.22468900 -0.72873700 -2.83979200  N 0.18656600 -0.60140500 -1.30207700  C -2.68757000 -2.47113100 1.31960100  C 2.38837300 2.02582500 1.42104200  H -1.65969900 -2.82822000 1.44440300  H 2.48094600 0.96794600 1.68569900  C -4.19708000 -0.86517700 -0.70522700  C 1.16419500 3.65681600 -0.76605600  C -4.19774900 -0.44311300 -2.17331200  C 0.85082600 3.64773200 -2.26104200  O -1.89393600 1.81668400 2.62056500  H 2.17314200 4.06076300 -0.62997600  H -4.74316700 -1.81051600 -0.62108800  C 0.16746100 4.54255100 -0.01790300  C -4.88999100 0.18954000 0.15732500  H 0.36740400 4.59340800 1.05219000  H -4.95020100 -0.09808800 1.20731700  H -0.85207000 4.17914700 -0.15059200  H -4.36457400 1.14397600 0.10233700  H 0.21457000 5.56179000 -0.41320500  H -5.91127100 0.34616300 -0.20239400  C -3.11881000 -1.83910100 2.64087500  C 1.79945800 2.75358800 2.62757900  H -4.16942000 -1.54201600 2.62144400  H 1.78573100 3.83498900 2.47560600  H -2.52532900 -0.95814200 2.88785400  H 0.78306400 2.42828900 2.85241900  H -3.00527400 -2.56407700 3.45219200  H 2.41813200 2.56283100 3.50936700  C -3.56033700 -3.67058900 0.95832800  C 3.77912100 2.55042300 1.07344500  H -3.25993600 -4.14255300 0.02014500  H 4.23905900 2.00345900 0.24840900  H -4.61401200 -3.39329200 0.87719200  H 3.75808700 3.61148300 0.81273300  H -3.48852800 -4.42904800 1.74358400  H 4.43824500 2.44765500 1.94076100  H 0.30882200 -0.64720100 1.30555300  H 0.71347600 -1.29213200 -0.69465000  C 0.90771500 -1.58266700 1.70364300  H -5.22933500 -0.27952000 -2.49894400  H -3.65794400 0.49268000 -2.32222200  H -3.77052200 -1.20338100 -2.83009400  H 0.84809200 4.67584400 -2.63504100  H 1.59068200 3.09472400 -2.84271100  H -0.13704900 3.22860900 -2.45892600  H 0.16439800 -2.05682500 2.34584800  C 1.45867100 -2.46013100 0.68282600  H 0.84102000 -3.29626100 0.36494300  V -0.89040500 0.66309600 0.14254200  N -1.48558800 1.34811700 1.61826200  N -1.79738600 1.72639700 -0.84647300  C 2.83019700 -2.53290700 0.29418300  C 3.24844700 -3.49566100 -0.66265300  C 3.85288800 -1.69556600 0.80619500  C 4.56070500 -3.59866000 -1.07724000  H 2.50478400 -4.17367200 -1.07234600  C 5.16860600 -1.80587000 0.38363900  H 3.61660600 -0.96840700 1.57529300  C 5.54376300 -2.74893500 -0.56709500  H 4.82844500 -4.35471000 -1.80907800  H 5.91787000 -1.14835200 0.81436700  H 6.57398100 -2.83181300 -0.89238300  H 1.65316500 -1.11487700 2.34934400 | **2V + Ph-CHCH2-TS-HN transfer**  O -2.46912000 2.41669300 -1.55491600  P 1.16770800 1.94564800 -0.03620200  P -2.46366700 -1.25491600 -0.04034400  C 2.16198800 0.89251000 -1.19626900  C -1.59094300 -2.33970100 -1.27250100  H 2.78519700 0.23667900 -0.58247800  H -1.04930900 -3.09391400 -0.69769300  H 2.83341300 1.47816800 -1.82759800  H -2.28246700 -2.86848600 -1.93166200  C 1.22436300 0.04483400 -2.04044900  C -0.60261900 -1.50817700 -2.07674700  H 1.81178900 -0.71764500 -2.56992500  H 0.07014000 -2.18203600 -2.62639700  H 0.72651000 0.65512000 -2.80036200  H -1.12720400 -0.90315400 -2.82251200  N 0.19296300 -0.61386300 -1.21033000  C -2.70314700 -2.44231000 1.39858700  C 2.31422600 2.09405700 1.44446700  H -1.67118200 -2.76251500 1.57839300  H 2.41766800 1.04308600 1.73321500  C -4.17823100 -0.96085100 -0.74713100  C 1.10979800 3.65675700 -0.80785700  C -4.13836200 -0.60075600 -2.23130200  C 0.82077700 3.60355900 -2.30701200  O -1.99573500 1.88093700 2.53292300  H 2.11081700 4.07851800 -0.66691500  H -4.71054800 -1.91193200 -0.64090200  C 0.09008100 4.54759000 -0.09810700  C -4.91765000 0.11487700 0.04790700  H 0.27372100 4.63002700 0.97295200  H -5.00771700 -0.13075900 1.10627300  H -0.92250700 4.16668000 -0.23494800  H -4.40823900 1.07634700 -0.02928700  H 0.12824900 5.55643000 -0.52007700  H -5.92896800 0.23747700 -0.35104800  C -3.19992900 -1.75972400 2.67083500  C 1.68984900 2.83698000 2.62361500  H -4.25625600 -1.49235700 2.59921000  H 1.66177200 3.91467100 2.44881600  H -2.63794000 -0.85328700 2.89779200  H 0.67443500 2.50031600 2.83567900  H -3.09883800 -2.44258200 3.51949800  H 2.29360600 2.67475700 3.52131400  C -3.53051200 -3.68162700 1.06608400  C 3.70355000 2.63377800 1.11430200  H -3.18084700 -4.19158000 0.16571500  H 4.18759500 2.07886800 0.30861200  H -4.58654000 -3.43664000 0.92963800  H 3.67075200 3.68923900 0.83279600  H -3.47198900 -4.39739700 1.89151800  H 4.34708200 2.55809200 1.99601900  H 0.33289600 -0.67262900 1.42799100  H 0.81820500 -1.36845100 -0.52527200  C 0.97703100 -1.58194700 1.69653400  H -5.16135200 -0.46969200 -2.59640800  H -3.60947000 0.33732100 -2.40345100  H -3.67605600 -1.37943400 -2.84069200  H 0.80977700 4.62124100 -2.70842600  H 1.57702100 3.04504100 -2.86126500  H -0.15707300 3.16418700 -2.51012200  H 0.31903500 -2.17484900 2.33524600  C 1.49073800 -2.31320500 0.51450500  H 0.94633000 -3.22936800 0.28618800  V -0.91290400 0.64731900 0.12500200  N -1.55085400 1.37352900 1.56704700  N -1.82777600 1.68175300 -0.88368800  C 2.90860900 -2.43733600 0.22952200  C 3.35181300 -3.39121200 -0.71558700  C 3.91390400 -1.63922000 0.81394900  C 4.68380700 -3.52376200 -1.05897500  H 2.61522400 -4.04145500 -1.17956000  C 5.25172600 -1.77390900 0.46599000  H 3.65192600 -0.91285600 1.57569800  C 5.65531900 -2.71017400 -0.47683800  H 4.97372100 -4.27479000 -1.78735100  H 5.99028500 -1.14172400 0.94953800  H 6.70036300 -2.81507900 -0.74400600  H 1.75454500 -1.16412700 2.33900500 |
| **2V + PhCHO-TS-HM transfer**  O 2.14918500 3.07142700 -0.43976000  P -1.47776400 1.67504200 0.15023500  P 2.61214500 -0.86027500 0.13880800  C -1.69016000 1.36108700 1.97538500  C 2.63454300 -0.98222300 2.00018500  H -2.21429000 0.40499400 2.06590900  H 2.13303200 -1.91881100 2.25677000  H -2.30471700 2.11894100 2.46672100  H 3.64689800 -1.01871000 2.40715400  C -0.32769400 1.26054200 2.64415000  C 1.85281300 0.17867100 2.59614200  H -0.44937400 0.96781800 3.69675000  H 1.73017200 0.02538000 3.67773900  H 0.17807300 2.22879500 2.63324800  H 2.38410300 1.12326700 2.45547000  N 0.53536400 0.29532800 1.94414200  C 2.64302900 -2.67845300 -0.34100200  C -3.06806200 0.97146200 -0.54991900  H 1.81019400 -3.06343100 0.25638100  H -2.98811100 -0.07404200 -0.23851800  C 4.30937100 -0.20156800 -0.32990500  C -1.63991800 3.53869800 -0.05304600  C 4.74791900 0.97268500 0.54306000  C -0.87400000 4.32136200 1.01160200  O 0.57998000 0.45087700 -3.17920100  H -2.70603400 3.76250500 0.06042700  H 5.00879000 -1.02731000 -0.16398600  C -1.18836300 3.96758600 -1.44996100  C 4.34133300 0.18783600 -1.80730500  H -1.72571300 3.45055300 -2.24488900  H 4.08801700 -0.64319400 -2.46679400  H -0.12332700 3.77799200 -1.58854600  H 3.63934200 0.99830100 -2.00968900  H -1.35788400 5.04119200 -1.57834000  H 5.34367800 0.53281300 -2.07867400  C 2.31055300 -2.90210800 -1.81428600  C -3.09931900 0.99093800 -2.07634100  H 3.14020500 -2.61505800 -2.46407300  H -3.27942500 1.99615600 -2.46448500  H 1.43336400 -2.33000400 -2.12092900  H -2.16939600 0.61871700 -2.50778000  H 2.11119400 -3.96259300 -1.99629300  H -3.91537100 0.35648200 -2.43343000  C 3.90061100 -3.43681600 0.07577200  C -4.34709500 1.55682600 0.04253300  H 4.15151400 -3.28442100 1.12804300  H -4.35945200 1.52128300 1.13398500  H 4.76604300 -3.14841700 -0.52574900  H -4.50193000 2.59415900 -0.26542800  H 3.75092900 -4.51067600 -0.07236700  H -5.20976600 0.98483800 -0.31154200  H -0.44908300 -0.87983500 -0.23626400  H 0.09124300 -0.63342300 2.00498500  C -0.84098200 -2.46985400 0.60784900  C -2.28458600 -2.55854100 0.24902100  C -2.66777600 -2.79965300 -1.06984500  C -4.00633000 -2.96566800 -1.39155300  C -4.97427400 -2.89800600 -0.39375600  C -3.25691400 -2.50405400 1.24651300  C -4.59704500 -2.66916600 0.92523400  H -1.90859800 -2.84227000 -1.84466700  H -4.29826300 -3.15069200 -2.41938600  H -6.02094600 -3.03257500 -0.64381900  H -2.93789500 -2.35399200 2.27178600  H -5.34994500 -2.63190600 1.70507800  H 5.75181500 1.28788800 0.24232700  H 4.08779000 1.83233000 0.42390700  H 4.79723300 0.71308700 1.60242200  H -1.01195800 5.39346500 0.84126300  H -1.22381500 4.10870900 2.02384300  H 0.19776300 4.12176400 0.95939200  O -0.45817600 -2.36641400 1.78176100  H -0.17702700 -2.87667900 -0.16864200  N 0.60858400 0.50285100 -2.00420900  V 0.65309800 0.57473800 -0.27541200  N 1.56606900 2.04461100 -0.31365200 | **2V + PhCHO-interm**  N 1.55839000 2.03554300 -0.37068900  O 2.16039700 3.04749500 -0.46979900  P -1.50803000 1.68374300 0.15955500  P 2.62800800 -0.87281000 0.14952500  C -1.74742900 1.27030600 1.95383600  C 2.61384800 -1.01055200 2.00226900  H -2.26240000 0.30531800 1.97587000  H 2.11321600 -1.95457500 2.22877000  H -2.37737200 1.99516600 2.47457200  H 3.61711500 -1.03567200 2.43127400  C -0.39527900 1.13229800 2.63560800  C 1.79234800 0.12982300 2.58366100  H -0.54121900 0.71797600 3.64335000  H 1.60625700 -0.07025400 3.64839600  H 0.07429600 2.11323500 2.76068300  H 2.33852500 1.07729500 2.52708600  N 0.50887500 0.26150500 1.86924000  C 2.64177500 -2.68175700 -0.35449400  C -3.08571300 1.02645300 -0.61136500  H 1.75751700 -3.04753600 0.17783900  H -3.02540700 -0.03656500 -0.35725100  C 4.31863900 -0.20076700 -0.31612400  C -1.62823700 3.55425400 0.03101800  C 4.76408200 0.94822600 0.58668200  C -0.85670800 4.27302400 1.13567700  O 0.55941400 0.41579000 -3.16659100  H -2.69193900 3.78436300 0.15376400  H 5.01449500 -1.03405600 -0.17419800  C -1.17267700 4.04228100 -1.34463600  C 4.34920600 0.22414200 -1.78392500  H -1.70920100 3.56192700 -2.16251200  H 4.07114400 -0.58312400 -2.46217300  H -0.10740200 3.86155800 -1.49093600  H 3.66822000 1.05745400 -1.96283700  H -1.34218300 5.12033700 -1.42490000  H 5.35810700 0.55098900 -2.05296900  C 2.42215400 -2.89314600 -1.85021400  C -3.10391100 1.13311600 -2.13456000  H 3.30966000 -2.63009800 -2.43025700  H -3.29865000 2.15582900 -2.46544200  H 1.58573100 -2.30444800 -2.22976100  H -2.16745300 0.80150700 -2.58496000  H 2.20941700 -3.94779300 -2.04769900  H -3.90716000 0.50697200 -2.53228100  C 3.85095700 -3.46527800 0.15082400  C -4.36741000 1.58579600 0.00146800  H 4.01603600 -3.33476000 1.22231300  H -4.39543700 1.47645700 1.08723700  H 4.76739400 -3.18317400 -0.37356100  H -4.50889100 2.64241000 -0.24057600  H 3.69538400 -4.53349700 -0.02727000  H -5.22824400 1.04470200 -0.40137800  H -0.64478500 -1.08845100 -0.15989000  H 0.06146500 -0.79081800 1.85869400  C -0.79872600 -2.11990200 0.38881200  C -2.26486400 -2.45375200 0.14744300  C -2.75406800 -2.66201700 -1.14212400  C -4.08583300 -2.99408000 -1.34886800  C -4.94718700 -3.12795200 -0.26352000  C -3.12751600 -2.60142600 1.22781500  C -4.46271800 -2.93451200 1.02399000  H -2.08406400 -2.56310100 -1.99224000  H -4.45359500 -3.15560900 -2.35675800  H -5.98677000 -3.39302800 -0.42283000  H -2.71603000 -2.47328100 2.22277000  H -5.12546400 -3.05343700 1.87500500  H 5.76605000 1.27148800 0.28874800  H 4.10443600 1.81192500 0.49580800  H 4.81717600 0.65978700 1.63790900  H -0.97210700 5.35391900 1.01160400  H -1.22063300 4.02068600 2.13320400  H 0.21137600 4.05386000 1.08689900  O -0.40607300 -2.08355500 1.66320900  H -0.20950000 -2.79493100 -0.26205800  N 0.59324200 0.47510900 -1.99401900  V 0.65875400 0.58298500 -0.26196500 |
| **2V +PhCHO -TS-HN transfer**  N 1.66041700 1.92919800 -0.47930600  O 2.33717700 2.88271800 -0.64030600  P -1.41757100 1.77834100 0.15624600  P 2.58227400 -0.97355400 0.15683900  C -1.60704500 1.53749300 1.98547700  C 2.44167500 -1.23921200 1.98463200  H -2.20396200 0.63001200 2.11250300  H 1.80411600 -2.11683600 2.12334700  H -2.13535800 2.36153100 2.46982700  H 3.40325600 -1.43618500 2.46311900  C -0.23661100 1.31165500 2.60598500  C 1.74387800 -0.03471500 2.60099400  H -0.37033000 0.97914500 3.64608900  H 1.48953200 -0.27133900 3.64456900  H 0.33024500 2.24951000 2.64659900  H 2.41474900 0.83214900 2.62875100  N 0.51907100 0.29761200 1.85636600  C 2.61441700 -2.71948600 -0.53146000  C -3.05031900 1.13663100 -0.50627800  H 1.61249000 -3.08340100 -0.28074800  H -3.02641400 0.09358500 -0.17360000  C 4.30610400 -0.31242100 -0.17558700  C -1.44136100 3.63331500 -0.13672400  C 4.76040700 0.70962800 0.86522900  C -0.58878400 4.39502000 0.87609400  O 0.47512200 0.20516000 -3.13835100  H -2.48538400 3.93551400 -0.00056300  H 4.96650600 -1.18078100 -0.09092700  C -1.00950900 3.97350600 -1.56326500  C 4.40925100 0.26305800 -1.60341000  H -1.60657300 3.46266700 -2.31821500  H 4.10022800 -0.44225400 -2.37529900  H 0.03552000 3.70967000 -1.72879900  H 3.76320300 1.13644700 -1.70773600  H -1.11266100 5.04996600 -1.73051800  H 5.43232800 0.57357100 -1.82739700  C 2.75617700 -2.74476000 -2.05184300  C -3.12432600 1.13083200 -2.03153900  H 3.74843000 -2.41525300 -2.36869200  H -3.28506300 2.13487700 -2.43103300  H 2.01614200 -2.11355500 -2.54629400  H -2.22203100 0.72248400 -2.48852700  H 2.62243200 -3.76730200 -2.41652900  H -3.96928400 0.51567400 -2.35205600  C 3.63405600 -3.63687900 0.13938700  C -4.28031600 1.79988800 0.10880300  H 3.51382100 -3.67354700 1.22346100  H -4.26859600 1.77334000 1.20004000  H 4.66099200 -3.33336700 -0.07994700  H -4.38249100 2.84143000 -0.20707300  H 3.51437800 -4.65678600 -0.23817200  H -5.18068100 1.27326300 -0.22023400  H -0.68233800 -1.21783300 -0.06489700  H -0.16327900 -0.74295600 1.92799500  C -1.00035500 -2.07562400 0.63170700  C -2.43025700 -2.40840300 0.24443000  C -2.76229100 -2.71724900 -1.07493400  C -4.06446200 -3.05390800 -1.41658000  C -5.05428200 -3.09231300 -0.43875900  C -3.42235100 -2.45524000 1.21783700  C -4.72813600 -2.79411100 0.87786100  H -1.99414200 -2.68930600 -1.84317700  H -4.30959100 -3.28941600 -2.44684700  H -6.07158200 -3.35916100 -0.70370500  H -3.14064600 -2.23194900 2.24024900  H -5.49259700 -2.83201800 1.64701200  H 5.77188500 1.04767700 0.62077900  H 4.11599400 1.59004200 0.86770800  H 4.79160100 0.29566900 1.87485200  H -0.65043100 5.46702400 0.66612200  H -0.92430700 4.24528300 1.90364700  H 0.46279800 4.11127800 0.80834700  O -0.81026200 -1.76626100 1.93450000  H -0.37095100 -2.91773600 0.28342100  N 0.54831700 0.33652700 -1.97160900  V 0.68274800 0.54394900 -0.25160600 | **2V + Ph-COCH3-TS**  O -2.07732800 2.94553500 0.80854900  P 1.47097700 1.72104100 -0.18385900  P -2.71169200 -0.76159700 -0.09040600  C 1.51326000 1.64444000 -2.04204000  C -2.70797600 -0.91353500 -1.94855800  H 2.04885900 0.72517300 -2.29635100  H -2.18821200 -1.84434500 -2.19138200  H 2.04648000 2.48524600 -2.49064200  H -3.71378900 -0.98526900 -2.36884300  C 0.09692200 1.54957400 -2.58706400  C -1.95720200 0.25943700 -2.56289400  H 0.13072600 1.40011600 -3.67545100  H -1.85412300 0.10371500 -3.64600000  H -0.45947900 2.47128300 -2.40067000  H -2.51774900 1.18647400 -2.42132000  N -0.63112600 0.43769400 -1.94771400  C -2.95715100 -2.54121500 0.46051100  C 3.16995900 1.08521200 0.28407100  H -2.05883300 -3.01280800 0.06039400  H 3.10988600 0.04074900 -0.02927800  C -4.35538000 0.06072900 0.32458900  C 1.55102400 3.55387800 0.24842600  C -4.71923000 1.20432100 -0.62037400  C 0.72276800 4.43817500 -0.68139100  O -0.28420600 0.05396600 3.13945200  H 2.60420200 3.82818400 0.12343300  H -5.10880500 -0.72492200 0.20475100  C 1.15325600 3.79987800 1.70518400  C -4.37792200 0.54349400 1.77597400  H 1.70776000 3.17754200 2.40684700  H -4.12567000 -0.24238900 2.48752900  H 0.09113800 3.61029800 1.85738100  H -3.67936400 1.36654900 1.92486000  H 1.34586900 4.84579200 1.96457900  H -5.38002300 0.90658300 2.02470500  C -2.90922700 -2.69702800 1.97966200  C 3.40129300 1.10134300 1.79373500  H -3.83423900 -2.35583400 2.44935900  H 3.57767400 2.11458200 2.16308000  H -2.07827300 -2.14501400 2.42182000  H 2.55915300 0.67636800 2.34247500  H -2.79030800 -3.75336500 2.23887200  H 4.28852000 0.50940200 2.03306300  C -4.17098700 -3.24837300 -0.13704800  C 4.32939000 1.74176000 -0.46085600  H -4.20436600 -3.17809000 -1.22639700  H 4.21887000 1.68100900 -1.54512800  H -5.11011000 -2.85225400 0.25686300  H 4.45006200 2.79404400 -0.18953300  H -4.14142000 -4.31162500 0.12075800  H 5.26294900 1.23435400 -0.19992400  H 0.32181400 -1.12610500 -0.02729700  H -0.07223200 -0.41460300 -2.13308300  C 1.16937500 -2.24342900 -1.10786000  C 2.45987600 -2.34539700 -0.32768500  C 2.50299100 -2.59243500 1.04414200  C 3.71617100 -2.79812800 1.68387700  C 4.90381800 -2.77068600 0.95879100  C 3.65352000 -2.31691600 -1.04767600  C 4.86926200 -2.52876100 -0.40838900  H 1.58279500 -2.58549400 1.61727500  H 3.73762300 -2.97518600 2.75365800  H 5.85113000 -2.93690100 1.46001300  H 3.60766500 -2.13291200 -2.11491700  H 5.79048900 -2.51001800 -0.98087600  H -5.69025700 1.61566900 -0.32818100  H -3.99495500 2.01797300 -0.56411300  H -4.80758500 0.88031300 -1.65920100  H 0.84474600 5.48493500 -0.38626300  H 1.03306600 4.35930800 -1.72505000  H -0.34113300 4.20652300 -0.61138600  O 1.16910500 -1.68714800 -2.22601500  N -0.42202100 0.22938400 1.98528300  C 0.25722400 -3.43675700 -0.88841400  H 0.77510300 -4.30943100 -1.30291000  H 0.05290800 -3.63565500 0.16232700  H -0.67010500 -3.30703400 -1.44288300  V -0.61728900 0.48280400 0.28286800  N -1.48411900 1.95072300 0.54570000 |
| **1Nb + H2-TS**  N 0.59572800 1.87150700 0.00000000  O 1.09489300 2.94506800 0.00000000  P 0.07746100 -0.38684300 2.52048700  P 0.07746100 -0.38684300 -2.52048700  C 1.35914200 -1.73900200 2.44922300  C 1.35914200 -1.73900200 -2.44922300  H 0.80187900 -2.67993600 2.41878900  H 0.80187900 -2.67993600 -2.41878900  H 1.97595200 -1.75248000 3.35144700  H 1.97595200 -1.75248000 -3.35144700  C 2.22653200 -1.62595500 1.19718200  C 2.22653200 -1.62595500 -1.19718200  H 2.82390300 -2.55101900 1.11891900  H 2.82390300 -2.55101900 -1.11891900  H 2.95772100 -0.80980400 1.33130500  H 2.95772100 -0.80980400 -1.33130500  N 1.43740700 -1.43052200 0.00000000  C -1.33229100 -1.25828700 -3.40878500  C -1.33229100 -1.25828700 3.40878500  H -1.44171100 -2.15321800 -2.78432500  H -1.44171100 -2.15321800 2.78432500  C 0.76984000 0.89295500 -3.70149400  C 0.76984000 0.89295500 3.70149400  C 2.17894600 1.31000400 -3.28555700  C 2.17894600 1.31000400 3.28555700  N -1.91197700 1.06293500 0.00000000  O -2.96891100 1.59051700 0.00000000  H 0.82387400 0.40977600 4.68326300  H 0.82387400 0.40977600 -4.68326300  C -0.14817400 2.11087200 3.78516300  C -0.14817400 2.11087200 -3.78516300  H -1.13734200 1.86517100 4.17265100  H -1.13734200 1.86517100 -4.17265100  H -0.27592300 2.56920000 2.80214500  H -0.27592300 2.56920000 -2.80214500  H 0.29115600 2.85917900 4.45135900  H 0.29115600 2.85917900 -4.45135900  C -2.65327100 -0.49554500 -3.34237800  C -2.65327100 -0.49554500 3.34237800  H -2.65613800 0.37178700 -4.00539000  H -2.65613800 0.37178700 4.00539000  H -2.87091600 -0.14640400 -2.33252400  H -2.87091600 -0.14640400 2.33252400  H -3.47161000 -1.14788600 -3.66130600  H -3.47161000 -1.14788600 3.66130600  C -1.00072200 -1.69709800 -4.83242800  C -1.00072200 -1.69709800 4.83242800  H -0.07222700 -2.26966900 -4.88874100  H -0.07222700 -2.26966900 4.88874100  H -0.91258900 -0.84032000 -5.50509500  H -0.91258900 -0.84032000 5.50509500  H -1.80234900 -2.33115800 -5.22313400  H -1.80234900 -2.33115800 5.22313400  H -0.91062500 -1.81492000 0.00000000  H 0.01922700 -1.89967500 0.00000000  H 2.55495700 2.06468100 -3.98256500  H 2.55495700 2.06468100 3.98256500  H 2.18250000 1.75134500 -2.28703400  H 2.18250000 1.75134500 2.28703400 | **2Nb+PhCN-TS-HM transfer**  N -2.67878600 -0.73418800 0.00000000  O -3.84185300 -0.97820200 0.00000000  P -0.65920000 0.23115700 2.52205600  P -0.65920000 0.23115700 -2.52205600  C -0.79266500 2.09396000 2.45876000  C -0.79266500 2.09396000 -2.45876000  H 0.23152500 2.47522500 2.41363800  H 0.23152500 2.47522500 -2.41363800  H -1.25275900 2.49891600 3.36279400  H -1.25275900 2.49891600 -3.36279400  C -1.54784300 2.56264600 1.22171400  C -1.54784300 2.56264600 -1.22171400  H -1.52762700 3.66111400 1.18064000  H -1.52762700 3.66111400 -1.18064000  H -2.59589200 2.25608600 1.26172700  H -2.59589200 2.25608600 -1.26172700  N -0.94864800 1.99842000 0.00000000  C 0.96284100 0.00688200 -3.44041600  C 0.96284100 0.00688200 3.44041600  H 1.65667500 0.50778800 -2.75637300  H 1.65667500 0.50778800 2.75637300  C -2.01355800 -0.33347600 -3.69496700  C -2.01355800 -0.33347600 3.69496700  C -3.33725000 0.37633900 -3.41854500  C -3.33725000 0.37633900 3.41854500  N -0.42005700 -2.23599400 0.00000000  O -0.14786500 -3.38671400 0.00000000  C -2.19827400 -1.84786400 3.59819900  C -2.19827400 -1.84786400 -3.59819900  H -1.28686400 -2.40071100 3.82618200  H -1.28686400 -2.40071100 -3.82618200  H -2.51571800 -2.13134500 2.59278000  H -2.51571800 -2.13134500 -2.59278000  H -2.97011300 -2.17206300 4.30270400  H -2.97011300 -2.17206300 -4.30270400  C 1.38230500 -1.45829200 -3.53336700  C 1.38230500 -1.45829200 3.53336700  H 0.80464100 -1.99363700 -4.29039100  H 0.80464100 -1.99363700 4.29039100  H 1.26010400 -1.97698300 -2.58114100  H 1.26010400 -1.97698300 2.58114100  H 2.43475900 -1.52446700 -3.82295100  H 2.43475900 -1.52446700 3.82295100  C 1.03111700 0.69793400 -4.79936100  C 1.03111700 0.69793400 4.79936100  H 0.77412000 1.75776800 -4.74515500  H 0.77412000 1.75776800 4.74515500  H 0.36824700 0.22389800 -5.52770400  H 0.36824700 0.22389800 5.52770400  H 2.04763700 0.62857900 -5.19829200  H 2.04763700 0.62857900 5.19829200  H 1.08987400 0.18001200 0.00000000  H 0.05094400 2.27302400 0.00000000  N 1.91748800 2.51439500 0.00000000  C 2.32361400 1.40813000 0.00000000  C 3.49928200 0.54375300 0.00000000  C 3.43336800 -0.84560200 0.00000000  C 4.60015000 -1.59794800 0.00000000  C 5.83854000 -0.96935900 0.00000000  C 4.74933200 1.17712300 0.00000000  C 5.90951400 0.42054700 0.00000000  H 2.45554400 -1.31271600 0.00000000  H 4.53875400 -2.68038900 0.00000000  H 6.74841400 -1.55944700 0.00000000  H 4.79044600 2.25981800 0.00000000  H 6.87378500 0.91650800 0.00000000  H -4.09765000 0.00809000 -4.11355200  H -4.09765000 0.00809000 4.11355200  H -3.69305300 0.16917400 -2.40729700  H -3.69305300 0.16917400 2.40729700  H -3.27279000 1.45775900 -3.55370400  H -3.27279000 1.45775900 3.55370400  H -1.68037400 -0.07197200 -4.70519100  H -1.68037400 -0.07197200 4.70519100  Nb -0.81162500 -0.38132800 0.00000000 |
| **2Nb + PhCN-interm**  N -2.62836500 -0.80296700 0.00000000  O -3.77720100 -1.09984300 0.00000000  P -0.65299800 0.23770100 2.53395700  P -0.65299800 0.23770100 -2.53395700  C -0.71641000 2.09939800 2.46117200  C -0.71641000 2.09939800 -2.46117200  H 0.32231400 2.43835300 2.41673300  H 0.32231400 2.43835300 -2.41673300  H -1.16602300 2.52627900 3.36042000  H -1.16602300 2.52627900 -3.36042000  C -1.44166100 2.58667100 1.21356900  C -1.44166100 2.58667100 -1.21356900  H -1.34835400 3.68053100 1.15491700  H -1.34835400 3.68053100 -1.15491700  H -2.50929400 2.35538700 1.26304600  H -2.50929400 2.35538700 -1.26304600  N -0.87333200 1.97262600 0.00000000  C 0.95161100 -0.05259700 -3.46416800  C 0.95161100 -0.05259700 3.46416800  H 1.67304500 0.42728800 -2.79335900  H 1.67304500 0.42728800 2.79335900  C -2.04303000 -0.28556900 -3.68130300  C -2.04303000 -0.28556900 3.68130300  C -3.33917900 0.46313900 -3.37815300  C -3.33917900 0.46313900 3.37815300  N -0.34387800 -2.21013800 0.00000000  O -0.03305400 -3.34887300 0.00000000  H -1.71792900 -0.02469000 4.69426100  H -1.71792900 -0.02469000 -4.69426100  C -2.27009300 -1.79472100 3.59641400  C -2.27009300 -1.79472100 -3.59641400  H -1.37649600 -2.37102600 3.83603500  H -1.37649600 -2.37102600 -3.83603500  H -2.59160400 -2.08025600 2.59309700  H -2.59160400 -2.08025600 -2.59309700  H -3.05491200 -2.08914300 4.29949700  H -3.05491200 -2.08914300 -4.29949700  C 1.31886600 -1.53161000 -3.56051200  C 1.31886600 -1.53161000 3.56051200  H 0.71827200 -2.04582500 -4.31422400  H 0.71827200 -2.04582500 4.31422400  H 1.18710000 -2.04904400 -2.60890900  H 1.18710000 -2.04904400 2.60890900  H 2.36640200 -1.63263500 -3.85682600  H 2.36640200 -1.63263500 3.85682600  C 1.02691200 0.63493800 -4.82483200  C 1.02691200 0.63493800 4.82483200  H 0.81064500 1.70352300 -4.76761600  H 0.81064500 1.70352300 4.76761600  H 0.33791900 0.18482500 -5.54406400  H 0.33791900 0.18482500 5.54406400  H 2.03524700 0.52776300 -5.23540200  H 2.03524700 0.52776300 5.23540200  H 1.23169500 0.31598900 0.00000000  H 0.18470300 2.24136700 0.00000000  N 1.80529500 2.38619600 0.00000000  C 2.09871600 1.20112900 0.00000000  C 3.40083300 0.48584700 0.00000000  C 3.45999000 -0.90398800 0.00000000  C 4.68566800 -1.55853800 0.00000000  C 5.86382700 -0.82300500 0.00000000  C 4.58863800 1.22167300 0.00000000  C 5.81080900 0.56906500 0.00000000  H 2.53309400 -1.47046300 0.00000000  H 4.72008500 -2.64256400 0.00000000  H 6.82223100 -1.33075500 0.00000000  H 4.52271500 2.30390200 0.00000000  H 6.72988600 1.14536800 0.00000000  H -4.12297100 0.12030900 -4.05986900  H -4.12297100 0.12030900 4.05986900  H -3.68297200 0.26421900 -2.36107700  H -3.68297200 0.26421900 2.36107700  H -3.24335900 1.54232200 -3.51085000  H -3.24335900 1.54232200 3.51085000  Nb -0.80389200 -0.36754600 0.00000000 | **2Nb + PhCN-TS-HN transfer**  N -0.00021800 -2.65200200 -0.79853200  O -0.00030800 -3.80225800 -1.08866100  P 2.53739500 -0.67188700 0.23381200  P -2.53758400 -0.67149200 0.23380000  C 2.46688200 -0.61650500 2.09378300  C -2.46716000 -0.61673200 2.09380600  H 2.44822100 0.44184500 2.36703800  H -2.44870400 0.44151700 2.36745900  H 3.35706100 -1.05886000 2.54701400  H -3.35729800 -1.05941100 2.54680200  C 1.20264300 -1.28309000 2.62258800  C -1.20286600 -1.28334400 2.62245600  H 1.13321500 -1.08497000 3.70285700  H -1.13346200 -1.08549300 3.70277600  H 1.25834900 -2.37072700 2.50393300  H -1.25849400 -2.37095700 2.50352600  N -0.00012900 -0.77015000 1.94694500  C -3.47847500 0.90502600 -0.16111100  C 3.47878900 0.90420100 -0.16160000  H -2.83091400 1.65622100 0.30536500  H 2.83127700 1.65580900 0.30428600  C -3.66906800 -2.10397400 -0.19804700  C 3.66845100 -2.10483400 -0.19765700  C -3.31712400 -3.35577900 0.60316300  C 3.31660700 -3.35614700 0.60436000  N 0.00004100 -0.37254300 -2.20032100  O 0.00015700 -0.04974200 -3.33617000  C 3.61994400 -2.40145500 -1.69607100  C -3.62118200 -2.39978300 -1.69663700  H 3.90976400 -1.54546600 -2.30549700  H -3.91137800 -1.54349700 -2.30546800  H 2.61518300 -2.70227100 -1.99876000  H -2.61651400 -2.70032000 -1.99992800  H 4.30317600 -3.22303300 -1.93083800  H -4.30441600 -3.22131600 -1.93155600  C -3.53556300 1.20790000 -1.65675500  C 3.53642400 1.20625900 -1.65738700  H -4.26754500 0.57794100 -2.16681000  H 4.26829400 0.57572000 -2.16689000  H -2.56863100 1.06439000 -2.14147200  H 2.56957100 1.06289900 -2.14230700  H -3.84016300 2.24670000 -1.81087700  H 3.84151000 2.24484800 -1.81197200  C -4.85877800 0.99381400 0.48462300  C 4.85891800 0.99299100 0.48450400  H -4.82982300 0.81928000 1.56207300  H 4.82957400 0.81916800 1.56205700  H -5.55781900 0.27995500 0.04165800  H 5.55789200 0.27864300 0.04222100  H -5.27598500 1.99270700 0.32652400  H 5.27646800 1.99165800 0.32588500  H 0.00005300 1.30883000 0.23151300  H -0.00024000 0.41619600 2.18921600  N -0.00022000 1.80474100 2.28828300  C 0.00000500 2.12766300 1.09866100  C 0.00027800 3.46393000 0.45661200  C 0.00061900 3.58822600 -0.93022500  C 0.00091400 4.84346500 -1.52597500  C 0.00086700 5.98520900 -0.73508000  C 0.00023300 4.61576300 1.24732100  C 0.00052700 5.86712500 0.65303900  H 0.00065700 2.69113800 -1.54280300  H 0.00117700 4.92957100 -2.60704900  H 0.00109800 6.96647900 -1.19702200  H -0.00002700 4.49891100 2.32521900  H 0.00049200 6.75830800 1.27150000  H -3.98792700 -4.17040700 0.31504500  H 3.98710400 -4.17107000 0.31636400  H -2.29683600 -3.68505000 0.39674000  H 2.29615500 -3.68530700 0.39854800  H -3.42587000 -3.21023400 1.67932300  H 3.42585400 -3.21006500 1.68039600  H -4.68110700 -1.78738600 0.07656700  H 4.68066100 -1.78828600 0.07637300  Nb -0.00007900 -0.83482500 -0.35535100 |
| **2Nb + Ph-CHNH-TS**  O -2.14612600 3.10981900 0.94752400  P 1.61923400 1.80536000 -0.21688000  P -2.65387200 -0.92603000 -0.21057600  C 1.57134100 1.73838600 -2.08261800  C -2.60653200 -0.89694800 -2.07681800  H 2.12119600 0.83673400 -2.36725100  H -2.02727600 -1.77132100 -2.38816300  H 2.08779100 2.58828700 -2.53473500  H -3.60492100 -0.99120500 -2.51040700  C 0.14631300 1.64207500 -2.61285800  C -1.91683700 0.35671500 -2.60131900  H 0.17699900 1.51699900 -3.70521200  H -1.82739800 0.28249700 -3.69463800  H -0.40455700 2.56394100 -2.40905000  H -2.50782800 1.24966000 -2.38269700  N -0.58281100 0.52032100 -1.99715500  C -2.70014300 -2.77408800 0.13594200  C 3.27905300 1.01449300 0.15016100  H -1.81126700 -3.11522200 -0.40596200  H 3.13324100 0.01373300 -0.27095000  C -4.35394400 -0.27860300 0.25863700  C 1.79625500 3.62426900 0.21899300  C -4.72575500 0.97884700 -0.52381600  C 0.86399000 4.50617400 -0.60899800  O -0.23437500 0.03126300 3.39389100  H 2.83149800 3.89709000 -0.01305400  H -5.06431800 -1.06990500 -0.00267800  C 1.53973600 3.84006100 1.71073300  C -4.42611900 -0.01228400 1.76171500  H 2.20617300 3.25355700 2.34314000  H -4.22422700 -0.90272000 2.35772400  H 0.51377100 3.57059500 1.96761700  H -3.70512000 0.75397700 2.05237900  H 1.68534100 4.89522400 1.96114200  H -5.42605200 0.34446300 2.02601300  C -2.49104400 -3.09860500 1.61346600  C 3.52207300 0.84445800 1.64796000  H -3.38820300 -2.89371500 2.20140500  H 3.78600900 1.79222000 2.12309300  H -1.66882500 -2.52353500 2.04284000  H 2.64672200 0.43651000 2.15574500  H -2.26376600 -4.16194000 1.73214000  H 4.35582300 0.15602100 1.80871500  C -3.90865400 -3.50630700 -0.44087900  C 4.46989900 1.67112700 -0.54236100  H -4.05510900 -3.30014400 -1.50333100  H 4.32955200 1.76760200 -1.62116200  H -4.82885100 -3.24505900 0.08723800  H 4.67648200 2.66511500 -0.13731600  H -3.77275400 -4.58659900 -0.33295000  H 5.36741400 1.06634100 -0.38248000  H 0.66085800 -1.00924500 -0.10273000  H -0.04722700 -0.36126500 -2.22461900  C 1.01474600 -2.20490800 -1.11203100  C 2.27852200 -2.65100700 -0.43592600  C 2.29740800 -2.88789800 0.93994200  C 3.43807300 -3.36627900 1.56423300  C 4.58912800 -3.61503000 0.82160000  C 3.43118500 -2.91751100 -1.17211200  C 4.58120900 -3.38917900 -0.54746900  H 1.40967300 -2.66483500 1.52262800  H 3.43380800 -3.54052600 2.63469700  H 5.48321100 -3.98809500 1.30886200  H 3.42387300 -2.78744900 -2.24897300  H 5.46751000 -3.59522300 -1.13790300  H -5.71707200 1.31843700 -0.20939800  H -4.02538000 1.79230300 -0.32715100  H -4.77071200 0.80501500 -1.60067900  H 0.99634000 5.55097100 -0.31271000  H 1.06666700 4.44620200 -1.68010700  H -0.18272400 4.24988000 -0.43381400  H 0.14342300 -2.73191800 -0.72524600  N -0.36838300 0.23856500 2.23930800  N -1.56412000 2.10293600 0.70069100  Nb -0.56146000 0.53068200 0.37470300  N 0.93208500 -1.83521900 -2.37438500  H 1.84681200 -1.54402100 -2.71861800 | **2Nb + Ph-CHNCH2Ph-TS**  O -2.76896700 0.31114500 3.02959200  P 0.43363900 2.36482200 0.77389100  P -2.50286800 -1.34237500 -1.10855100  C 1.46899900 2.25034800 -0.77556500  C -1.35764200 -1.41235600 -2.58454500  H 2.28026600 1.55053100 -0.56416000  H -0.58418100 -2.15006400 -2.35140500  H 1.93382900 3.20698200 -1.02356400  H -1.87529300 -1.75907800 -3.48267600  C 0.66525500 1.73701900 -1.96284800  C -0.69580200 -0.06499900 -2.85185600  H 1.34062800 1.60543200 -2.81940600  H 0.02485300 -0.17734000 -3.67405100  H -0.09752100 2.46329700 -2.25520400  H -1.43704200 0.67184400 -3.16963100  N -0.01502400 0.46379000 -1.65509900  C -2.52567400 -3.13903700 -0.54130200  C 1.71278800 2.09975800 2.12265300  H -1.45700700 -3.37382800 -0.50013000  H 2.03010900 1.07275800 1.91272000  C -4.21037600 -1.03770100 -1.83189500  C -0.07242000 4.17034000 0.91083500  C -4.21489300 0.08343400 -2.86821200  C -0.49865900 4.75696300 -0.43338400  O -3.45483200 2.68924400 -0.52207900  C -1.19325900 4.33736900 1.93751200  C -5.21510200 -0.74521600 -0.71839200  H -0.92945400 3.94704100 2.92026600  H -5.29486700 -1.56192600 -0.00003000  H -2.09792900 3.82482500 1.60745000  H -4.93579800 0.15668400 -0.17074400  H -1.43004700 5.39939800 2.05328900  H -6.20787300 -0.58589300 -1.14958300  C -3.07657300 -3.29307900 0.87477800  C 1.09286000 2.11054500 3.51829800  H -4.15924200 -3.15503400 0.90618200  H 0.86269000 3.12688400 3.84596200  H -2.62523100 -2.57670400 1.56253300  H 0.17428200 1.52242700 3.56212200  H -2.86687700 -4.30032200 1.24592600  H 1.79943100 1.69081300 4.23975700  C -3.17607100 -4.11578700 -1.51714500  C 2.93058900 3.01610500 2.04401500  H -2.78919600 -4.01432300 -2.53393700  H 3.41905200 2.98387500 1.06815800  H -4.26083800 -3.99052200 -1.55125100  H 2.66942500 4.05552300 2.25835600  H -2.98250000 -5.14298200 -1.19399300  H 3.67022300 2.71178300 2.79085900  H 0.09427600 -0.71324900 0.83349400  H 0.72082100 -0.23148500 -1.39419400  N 1.88826600 -1.54158700 -0.65416400  H 0.81625400 4.70894800 1.25771500  H -4.49286200 -1.96772100 -2.33546600  H -5.23251900 0.21652700 -3.24736100  H -0.78527000 5.80374200 -0.29551300  H -3.90332200 1.03394500 -2.43322000  H -1.36815900 4.23410000 -0.83570900  H -3.57858400 -0.13839600 -3.72719600  H 0.30047000 4.73640800 -1.17672200  C 3.19014600 -1.06153300 -0.24970900  H 3.11018400 -0.22308400 0.46237500  H 3.74984900 -1.83203200 0.30095300  C 4.03966300 -0.61887000 -1.41847800  C 3.76713500 -1.03929300 -2.71790600  C 5.15124900 0.19722800 -1.20282700  C 4.58463400 -0.65372200 -3.77480900  H 2.90432100 -1.67362000 -2.88161000  C 5.96893000 0.58449000 -2.25581700  H 5.38052500 0.53154600 -0.19468500  C 5.68769800 0.15954700 -3.54956800  H 4.35964200 -0.99383500 -4.78042600  H 6.82773800 1.21982800 -2.06699100  H 6.32455200 0.46048300 -4.37413600  C 1.06988900 -1.95039600 0.28460600  H 0.17371400 -2.43695700 -0.09294800  C 1.49879800 -2.50003300 1.62092900  C 2.30549700 -3.64383700 1.60615800  C 1.09350700 -1.99053600 2.85094500  C 2.70064800 -4.25161000 2.78922700  H 2.61740700 -4.06008600 0.65378100  C 1.48650700 -2.60095200 4.03705300  H 0.45928600 -1.11250900 2.86520700  C 2.29291900 -3.73031200 4.01186500  H 3.32494800 -5.13806600 2.75584700  H 1.15680700 -2.18940800 4.98495000  H 2.60054800 -4.20415800 4.93755700  N -2.24833600 0.41692400 1.97612400  N -2.64990800 1.85714600 -0.24961700  Nb -1.37946600 0.56414700 0.29663100 |
| **2Nb + Ph-CHNPh-TS**  O -1.85773400 0.22723400 3.39988700  P 0.32340500 2.51336500 0.29113800  P -2.43669100 -1.67668600 -0.59611900  C 0.99772700 2.34394200 -1.44117000  C -1.77106600 -1.67548200 -2.34267600  H 1.89723100 1.72665300 -1.36562100  H -0.87028200 -2.29674000 -2.33578600  H 1.30442200 3.30868000 -1.85223400  H -2.47554400 -2.12691200 -3.04554600  C 0.00050200 1.67519000 -2.37913200  C -1.39571400 -0.27204600 -2.80414500  H 0.47008200 1.53751200 -3.36308300  H -0.93513700 -0.33443600 -3.80029700  H -0.87700800 2.31005900 -2.52471200  H -2.28251700 0.35953200 -2.89481600  N -0.46862100 0.37660300 -1.85826000  C -2.03682700 -3.43245300 -0.03751200  C 1.88781700 2.52080000 1.32519100  H -0.98213300 -3.52263400 -0.31838700  H 2.29071400 1.53315500 1.08272700  C -4.30666500 -1.64235000 -0.78377800  C -0.36550100 4.25886300 0.39438000  C -4.77457100 -0.60269400 -1.79899800  C -1.17708100 4.63699100 -0.84283500  O -3.74802300 2.26110200 0.08845900  C -1.21445600 4.42692300 1.65498900  C -4.97248100 -1.41097500 0.57183800  H -0.66698200 4.19178700 2.56753700  H -4.71675900 -2.18022400 1.30159700  H -2.09405200 3.78258700 1.61762000  H -4.67991700 -0.44515200 0.98754300  H -1.55860900 5.46287100 1.73119400  H -6.06019800 -1.41449400 0.45461000  C -2.12307800 -3.59061800 1.47902400  C 1.59712600 2.54129700 2.82409100  H -3.15833700 -3.60020100 1.82600500  H 1.29770600 3.53561900 3.16298800  H -1.60300100 -2.78510200 1.99976200  H 0.81014300 1.83559100 3.09526400  H -1.67054700 -4.53957100 1.78044100  H 2.50049000 2.27066300 3.37804800  C -2.80015500 -4.53309200 -0.76938400  C 2.91296700 3.58036400 0.93332900  H -2.74839200 -4.42893800 -1.85570800  H 3.17354200 3.53937500 -0.12597200  H -3.85296700 -4.55691900 -0.47864700  H 2.56056300 4.58973500 1.16075000  H -2.37507900 -5.50816500 -0.51340100  H 3.83529000 3.42875000 1.50235300  H 0.53699800 -0.41958300 0.60400400  H 0.35280300 -0.25133800 -1.77275800  N 1.79899200 -1.48104900 -1.34228400  H 0.50253100 4.92439500 0.45412700  H -4.58752500 -2.63220200 -1.15714500  H -5.86621700 -0.63344700 -1.86537800  H -1.56102000 5.65479100 -0.72607400  H -4.49538200 0.40746100 -1.49765300  H -2.03915100 3.97911000 -0.96816500  H -4.38635300 -0.79286400 -2.80161800  H -0.58283800 4.61928400 -1.75847100  C 1.44141200 -1.77258200 -0.11591200  H 0.48832700 -2.28674000 -0.05177200  C 2.33442800 -2.12057200 1.03759900  C 3.45627600 -2.91910800 0.79712700  C 2.00573900 -1.80953900 2.35665100  C 4.23659500 -3.37825900 1.84894300  H 3.71300000 -3.18234500 -0.22224400  C 2.78692000 -2.26987000 3.40836000  H 1.13911000 -1.18648800 2.54446500  C 3.90739100 -3.05284900 3.15915200  H 5.10408800 -3.99570900 1.64257900  H 2.51852400 -2.01228700 4.42720200  H 4.51921000 -3.40904300 3.98065500  C 3.01522700 -0.88757800 -1.67597600  C 3.41929900 -1.00047900 -3.01703400  C 3.83090900 -0.13566300 -0.81386500  C 4.58911200 -0.41392600 -3.46988600  H 2.78869200 -1.57232400 -3.68897400  C 4.99790200 0.45835800 -1.27597900  H 3.55481900 -0.03086400 0.22685800  C 5.38963200 0.32330100 -2.60218900  H 4.87829900 -0.52892600 -4.50931800  H 5.61072400 1.03012800 -0.58672100  H 6.30402900 0.78609500 -2.95541000  N -1.64333100 0.32818800 2.24373100  Nb -1.26422400 0.46420200 0.39157400  N -2.81034700 1.53272700 0.15677900 | **2Nb + Ph-CCH-TS-HM transfer to C-H**  N 1.39997700 -2.62564700 0.00000000  O 2.22450100 -3.47181900 0.00000000  P -0.01850000 -0.60566000 2.50809400  P -0.01850000 -0.60566000 -2.50809400  C -1.08537800 0.93215900 2.46406000  C -1.08537800 0.93215900 -2.46406000  H -0.40298800 1.78624400 2.44770100  H -0.40298800 1.78624400 -2.44770100  H -1.69521300 1.02492800 3.36568100  H -1.69521300 1.02492800 -3.36568100  C -1.97114500 0.97713300 1.22556100  C -1.97114500 0.97713300 -1.22556100  H -2.49525500 1.94208400 1.18737900  H -2.49525500 1.94208400 -1.18737900  H -2.72853700 0.19051100 1.25956100  H -2.72853700 0.19051100 -1.25956100  N -1.17616900 0.77871500 0.00000000  C 1.52655300 0.04358600 -3.35609400  C 1.52655300 0.04358600 3.35609400  H 1.74857000 0.91457300 -2.72907500  H 1.74857000 0.91457300 2.72907500  C -0.87696300 -1.73552700 -3.73638100  C -0.87696300 -1.73552700 3.73638100  C -2.35710600 -1.90075600 -3.39845900  C -2.35710600 -1.90075600 3.39845900  O -2.17941400 -3.31038500 0.00000000  H -0.79326300 -1.25270900 4.71608100  H -0.79326300 -1.25270900 -4.71608100  C -0.18391900 -3.09625100 3.78119500  C -0.18391900 -3.09625100 -3.78119500  H 0.85415300 -3.02750500 4.10821000  H 0.85415300 -3.02750500 -4.10821000  H -0.19422300 -3.56786800 2.79593500  H -0.19422300 -3.56786800 -2.79593500  H -0.70758300 -3.75648800 4.47881500  H -0.70758300 -3.75648800 -4.47881500  C 2.70897800 -0.91382900 -3.23039400  C 2.70897800 -0.91382900 3.23039400  H 2.60038100 -1.78623700 -3.87800100  H 2.60038100 -1.78623700 3.87800100  H 2.82789100 -1.26726000 -2.20501700  H 2.82789100 -1.26726000 2.20501700  H 3.63026900 -0.40340500 -3.52638300  H 3.63026900 -0.40340500 3.52638300  C 1.31825200 0.51072500 -4.79345400  C 1.31825200 0.51072500 4.79345400  H 0.48332300 1.20888100 -4.89142000  H 0.48332300 1.20888100 4.89142000  H 1.13723200 -0.32980700 -5.46804600  H 1.13723200 -0.32980700 5.46804600  H 2.21651600 1.02255600 -5.15177400  H 2.21651600 1.02255600 5.15177400  H 1.42919700 0.27118300 0.00000000  H -0.42293600 1.47355400 0.00000000  C 2.14592600 1.76954400 0.00000000  H -2.82314500 -2.56941400 -4.12825800  H -2.49237300 -2.34596800 -2.41111700  H -2.90371200 -0.95597700 -3.43316900  H -2.82314500 -2.56941400 4.12825800  H -2.90371200 -0.95597700 3.43316900  H -2.49237300 -2.34596800 2.41111700  C 1.50771500 2.82845400 0.00000000  C 0.66815000 3.95758100 0.00000000  C 0.24403800 4.55454800 -1.20692100  C 0.24403800 4.55454800 1.20692100  C -0.57574300 5.66988300 -1.19905400  H 0.58456600 4.13793900 -2.14785200  C -0.57574300 5.66988300 1.19905400  H 0.58456600 4.13793900 2.14785200  C -0.99883300 6.23557000 0.00000000  H -0.88286700 6.10919500 -2.14236800  H -0.88286700 6.10919500 2.14236800  H -1.63815200 7.11050700 0.00000000  H 3.11935600 1.32268700 0.00000000  N -1.31317300 -2.49632200 0.00000000  Nb 0.10966700 -1.23763900 0.00000000 |
| **2Nb + PhCCH-TS-HM transfer to Ph-C**  N 2.66168000 -0.79806600 0.00000000  O 3.81972300 -1.06690200 0.00000000  P 0.65363200 0.22738200 -2.51844100  P 0.65363200 0.22738200 2.51844100  C 0.81234700 2.08844900 -2.45643300  C 0.81234700 2.08844900 2.45643300  H -0.20961400 2.47599300 -2.40533700  H -0.20961400 2.47599300 2.40533700  H 1.27080900 2.49008500 -3.36278100  H 1.27080900 2.49008500 3.36278100  C 1.57655700 2.55138900 -1.22290400  C 1.57655700 2.55138900 1.22290400  H 1.55744100 3.65044600 -1.17589800  H 1.55744100 3.65044600 1.17589800  H 2.62449300 2.24616600 -1.27098700  H 2.62449300 2.24616600 1.27098700  N 0.98689300 1.98095100 0.00000000  C -0.97718800 0.02744400 3.42540600  C -0.97718800 0.02744400 -3.42540600  H -1.65940000 0.52959700 2.73040100  H -1.65940000 0.52959700 -2.73040100  C 1.99474300 -0.35339600 3.69888500  C 1.99474300 -0.35339600 -3.69888500  C 3.32927200 0.33569500 3.42230500  C 3.32927200 0.33569500 -3.42230500  N 0.33384300 -2.21724100 0.00000000  O 0.01007200 -3.35510000 0.00000000  C 2.15772800 -1.87059000 -3.60681600  C 2.15772800 -1.87059000 3.60681600  H 1.23773500 -2.40925300 -3.83399200  H 1.23773500 -2.40925300 3.83399200  H 2.47357200 -2.16130100 -2.60289800  H 2.47357200 -2.16130100 2.60289800  H 2.92305800 -2.20400500 -4.31416200  H 2.92305800 -2.20400500 4.31416200  C -1.41211400 -1.43275200 3.52676800  C -1.41211400 -1.43275200 -3.52676800  H -0.84803100 -1.96712000 4.29481700  H -0.84803100 -1.96712000 -4.29481700  H -1.28688000 -1.96126100 2.58051500  H -1.28688000 -1.96126100 -2.58051500  H -2.46831000 -1.48499400 3.80488700  H -2.46831000 -1.48499400 -3.80488700  C -1.04847600 0.72833400 4.77914900  C -1.04847600 0.72833400 -4.77914900  H -0.78104400 1.78545800 4.72052700  H -0.78104400 1.78545800 -4.72052700  H -0.39547900 0.25305300 5.51568200  H -0.39547900 0.25305300 -5.51568200  H -2.06858500 0.67116600 5.17077500  H -2.06858500 0.67116600 -5.17077500  H -1.05712900 0.33602400 0.00000000  H -0.02179400 2.23809700 0.00000000  C -2.32711800 1.51303300 0.00000000  C -3.44288900 0.57625800 0.00000000  C -3.31349100 -0.81088800 0.00000000  C -4.43606400 -1.62838600 0.00000000  C -5.70901600 -1.07455600 0.00000000  C -4.73469700 1.12734200 0.00000000  C -5.85238300 0.30988300 0.00000000  H -2.31471700 -1.23070700 0.00000000  H -4.31063900 -2.70559700 0.00000000  H -6.58467900 -1.71432400 0.00000000  H -4.84169300 2.20592700 0.00000000  H -6.84165500 0.75477300 0.00000000  H 4.08436600 -0.04325400 4.11735200  H 4.08436600 -0.04325400 -4.11735200  H 3.68121400 0.12174500 2.41096500  H 3.68121400 0.12174500 -2.41096500  H 3.28144000 1.41824600 3.55623900  H 3.28144000 1.41824600 -3.55623900  H 1.66279900 -0.08395000 4.70750400  H 1.66279900 -0.08395000 -4.70750400  Nb 0.80782000 -0.38132200 0.00000000  C -1.96034300 2.69342900 0.00000000  H -1.97011500 3.75987700 0.00000000 | **2Nb + PhCCH-interm to Ph-C**  O 0.33915100 3.69249200 -1.22769700  P -2.45376500 0.86029600 0.25417500  P 2.58843400 0.40980500 0.25139200  C -2.35060600 1.13817800 2.09792200  C 2.54232900 0.71196200 2.09367300  H -2.37401100 0.14351900 2.55407400  H 2.39671000 -0.26922700 2.55632700  H -3.21286700 1.69083600 2.47627300  H 3.48844500 1.11021200 2.46569800  C -1.05601600 1.83472100 2.49350900  C 1.38843100 1.62311700 2.48894400  H -0.99723800 1.89983500 3.58897700  H 1.34446500 1.70100100 3.58428700  H -1.01729400 2.85336300 2.10194600  H 1.52547800 2.63180500 2.09360200  N 0.11047500 1.09662300 1.96973800  C 3.33094000 -1.31072000 0.16837200  C -3.49366400 -0.69747400 0.16063400  H 2.57120000 -1.89614800 0.69909500  H -2.84238100 -1.42031800 0.66529800  C 3.87140200 1.59095500 -0.44217400  C -3.50556300 2.25619600 -0.43052200  C 3.74843400 2.98838500 0.16108800  C -3.14617600 3.60404600 0.19059500  O 0.00821500 -0.06693400 -3.32959800  H -4.54112600 2.01376900 -0.16847700  H 4.84744800 1.17542300 -0.16942700  C -3.37185000 2.32219200 -1.95201700  C 3.75886500 1.65954000 -1.96516200  H -3.64048300 1.38601900 -2.44107000  H 3.86624100 0.68514600 -2.44150800  H -2.34652100 2.56444200 -2.23795200  H 2.79132900 2.06944300 -2.26110600  H -4.02727000 3.10470900 -2.34553100  H 4.54012700 2.31370900 -2.36315100  C 3.41771700 -1.84155000 -1.26072800  C -3.70041900 -1.17374500 -1.27528400  H 4.24332000 -1.38292300 -1.81013000  H -4.44106000 -0.56343300 -1.79774500  H 2.49596500 -1.67132900 -1.81904100  H -2.77355600 -1.15841500 -1.85064500  H 3.59850100 -2.91918000 -1.23992800  H -4.07016200 -2.20212500 -1.26959300  C 4.66179500 -1.45825500 0.90112900  C -4.81640600 -0.61935800 0.91859800  H 4.60850100 -1.13470800 1.94240400  H -4.68734400 -0.33946600 1.96579100  H 5.46106400 -0.89785700 0.40901300  H -5.50843300 0.09017800 0.45731600  H 4.96097100 -2.51027300 0.90389800  H -5.30233300 -1.59909500 0.90322200  H -0.08316900 -1.17315600 0.70216600  H 0.02669600 0.12812200 2.32323800  C -0.18277900 -2.11638600 1.40502500  C -0.32509200 -3.30742200 0.54067000  C -0.32690800 -3.21053600 -0.85034500  C -0.46088800 -4.33696200 -1.65394500  C -0.59666700 -5.59133100 -1.07598000  C -0.46307100 -4.58032000 1.11127200  C -0.59670500 -5.70347000 0.31342400  H -0.22117300 -2.23160900 -1.30979000  H -0.45843600 -4.23042100 -2.73362300  H -0.70138800 -6.47368700 -1.69798200  H -0.46037000 -4.64657600 2.19372100  H -0.70214800 -6.67935400 0.77645500  H 4.50874600 3.64015500 -0.27880400  H 2.77485900 3.43111900 -0.05966200  H 3.90198700 2.99756800 1.24189500  H -3.77858800 4.38296800 -0.24494700  H -3.30286300 3.62774600 1.27069900  H -2.10908000 3.87328100 -0.02052400  C -0.16716100 -2.09957500 2.72020000  H -0.05782800 -1.20488200 3.34256100  N 0.03443200 0.24780300 -2.19437900  Nb 0.07956500 0.77079600 -0.37015300  N 0.23856800 2.56101200 -0.88387300 |
| **2Nb + PhCCH-TS-HN transfer to C-H**  N -0.00014700 2.59510500 -0.85096300  O -0.00019000 3.73405000 -1.18976800  Nb -0.00006700 0.78200700 -0.36834000  P -2.52879500 0.64492600 0.23461800  P 2.52867600 0.64525200 0.23459900  C -2.46078700 0.80771000 2.09289100  C 2.46066500 0.80814500 2.09286600  H -2.41373200 -0.21425400 2.48122200  H 2.41378300 -0.21380400 2.48125400  H -3.36284600 1.27230000 2.49695100  H 3.36265400 1.27289800 2.49689300  C -1.22028200 1.56338000 2.54960400  C 1.22003900 1.56363200 2.54955400  H -1.16747700 1.53863400 3.64808300  H 1.16725700 1.53895400 3.64803600  H -1.26257600 2.61284500 2.24985700  H 1.26214200 2.61308400 2.24973400  N -0.00007100 0.96389900 1.97596800  C 3.45346600 -0.97590100 0.03493300  C -3.45338100 -0.97633500 0.03487900  H 2.77072300 -1.67002400 0.53803000  H -2.77064200 -1.67034300 0.53814200  C 3.68451300 2.00010200 -0.36063100  C -3.68480700 1.99969600 -0.36044700  C 3.39812200 3.33286200 0.32763900  C -3.39837500 3.33245700 0.32780400  N -0.00001900 0.24559100 -2.18899500  O 0.00001900 -0.09819600 -3.31942000  C -3.58389700 2.15588300 -1.87769400  C 3.58338100 2.15627500 -1.87786700  H -3.81236100 1.23473000 -2.41361600  H 3.81179700 1.23512600 -2.41381400  H -2.57825500 2.46787500 -2.16581900  H 2.57769100 2.46823700 -2.16585200  H -4.28697600 2.92239700 -2.21700200  H 4.28638900 2.92280800 -2.21727800  C 3.56528600 -1.41030700 -1.42472600  C -3.56490300 -1.41086900 -1.42476300  H 4.32766100 -0.83662300 -1.95692900  H -4.32725300 -0.83731500 -1.95714100  H 2.61965500 -1.30082900 -1.95791200  H -2.61919500 -1.30131500 -1.95779600  H 3.85728900 -2.46264100 -1.47363500  H -3.85677500 -2.46324000 -1.47364400  C 4.80621300 -1.02611400 0.73995900  C -4.80623900 -1.02666200 0.73968600  H 4.74004300 -0.76149800 1.79719300  H -4.74032200 -0.76170100 1.79685000  H 5.53433400 -0.36202600 0.26713000  H -5.53443100 -0.36289400 0.26651800  H 5.21210000 -2.04040200 0.68300600  H -5.21187200 -2.04106400 0.68297500  H -0.00001000 -1.18981900 0.57215200  H 0.00005400 -0.04535500 2.28433900  C 0.00015000 -2.12396500 1.38366700  C 0.00022700 -3.34959100 0.54665300  C 0.00017700 -3.28175700 -0.84402700  C 0.00026000 -4.43615100 -1.61772000  C 0.00039300 -5.68282800 -1.00669700  C 0.00036400 -4.61077800 1.15252700  C 0.00044600 -5.76303900 0.38436800  H 0.00008200 -2.30483400 -1.31914200  H 0.00022000 -4.35900700 -2.69976800  H 0.00045700 -6.58642600 -1.60665100  H 0.00040200 -4.65368300 2.23657900  H 0.00055100 -6.73323300 0.87037000  H 4.08362300 4.09374200 -0.05674400  H -4.08381000 4.09336800 -0.05663300  H 2.38244600 3.67509500 0.11862200  H -2.38267000 3.67463300 0.11884100  H 3.53849600 3.28811900 1.40938500  H -3.53881700 3.28773500 1.40954400  H 4.69776000 1.67923400 -0.09557400  H -4.69799400 1.67877000 -0.09523500  C 0.00025100 -1.96470300 2.65159500  H 0.00029400 -1.61904900 3.65929400 | **2Nb + PhCHCH2-TS-HM transfer**  O -2.32459100 2.73732800 -1.62446300  P 1.47093300 1.85851100 -0.05156200  P -2.54600500 -1.20470500 -0.10112600  C 2.29821000 0.70789800 -1.27067400  C -1.67776400 -2.25827600 -1.38154700  H 2.85914800 -0.02790800 -0.68758400  H -1.14353400 -3.03985100 -0.83451600  H 3.02020000 1.23740900 -1.89698000  H -2.39028200 -2.75844800 -2.04179200  C 1.28405800 -0.01166700 -2.14947800  C -0.68315000 -1.45079200 -2.20590000  H 1.80725300 -0.74570800 -2.77731100  H -0.11710700 -2.12961800 -2.85953500  H 0.77996700 0.69195900 -2.81608800  H -1.20413800 -0.73807200 -2.84939400  N 0.23960800 -0.68225400 -1.34873200  C -2.82446200 -2.45592500 1.27578800  C 2.68113900 1.82839000 1.38497200  H -1.82297000 -2.88969800 1.37016500  H 2.79911600 0.74920400 1.52526100  C -4.23621100 -0.86350500 -0.84266200  C 1.62047300 3.56169700 -0.82727900  C -4.12870700 -0.32514800 -2.26748100  C 1.14848900 3.56512800 -2.27955300  O -1.99479600 2.17618900 2.69189800  H 2.68568200 3.81553800 -0.80899900  H -4.75807100 -1.82580000 -0.87379100  C 0.84227900 4.59020700 -0.00833400  C -5.01766100 0.10682600 0.04133300  H 1.20818400 4.67406100 1.01561900  H -5.19413300 -0.28817000 1.04264000  H -0.21733000 4.32962800 0.03429600  H -4.48306800 1.05368200 0.14332700  H 0.92994500 5.57689300 -0.47272900  H -5.99291700 0.31474900 -0.40845200  C -3.15934300 -1.78913000 2.60795400  C 2.08014800 2.39218500 2.67013400  H -4.17242800 -1.38216200 2.61654100  H 1.98410100 3.47919700 2.63385000  H -2.46997600 -0.97349100 2.83208700  H 1.09237000 1.97306700 2.86714600  H -3.09847800 -2.52365100 3.41645100  H 2.72972200 2.15373500 3.51769900  C -3.79940200 -3.57970500 0.93644100  C 4.05118600 2.42664000 1.08086400  H -3.56302300 -4.06911400 -0.01157200  H 4.49672100 2.01225000 0.17359700  H -4.82848500 -3.21659000 0.88349200  H 4.00108800 3.51273600 0.97127500  H -3.76881400 -4.34586500 1.71688800  H 4.73799800 2.21931500 1.90702400  H 0.21216500 -0.57041500 1.33619900  H 0.70394700 -1.34703000 -0.71394100  C 0.92941400 -1.92033000 1.85254000  H -5.13328300 -0.14533900 -2.66167500  H -3.59036800 0.62319400 -2.29628800  H -3.63899400 -1.02731400 -2.94555500  H 1.24371700 4.57558900 -2.68804000  H 1.74223000 2.90447000 -2.91464100  H 0.09844000 3.27878700 -2.35808100  H 0.02404000 -2.19072600 2.37987700  C 1.42929400 -2.78628600 0.89996100  H 0.76080700 -3.54403800 0.49767400  N -1.56480300 1.64155900 1.73111800  N -1.75298300 1.94224500 -0.94965900  Nb -0.85686300 0.74802100 0.21711100  H 1.60735000 -1.32664600 2.45580800  C 2.77666200 -2.81395700 0.37466100  C 3.09543100 -3.67103700 -0.69898900  C 3.83386800 -2.03941200 0.89385200  C 4.37447800 -3.74061600 -1.22467400  H 2.31229900 -4.29822500 -1.11540700  C 5.11265600 -2.10909200 0.36382800  H 3.65653200 -1.39722000 1.74930400  C 5.39807800 -2.95407500 -0.70413900  H 4.57716800 -4.41679200 -2.04901300  H 5.90177500 -1.50391900 0.79870000  H 6.40027300 -3.00869100 -1.11302400 |
| **2Nb + Ph-CHCH2-interm**  O -2.37210900 2.79150000 -1.39968600  P 1.48644600 1.84113100 -0.08532200  P -2.59460300 -1.19003700 -0.10071900  C 2.30048100 0.65652600 -1.27304400  C -1.72473900 -2.27231300 -1.34872700  H 2.86391800 -0.06349700 -0.67161600  H -1.21668200 -3.05522300 -0.78020100  H 3.01926000 1.16485200 -1.92014300  H -2.43256100 -2.76650200 -2.01846500  C 1.27691800 -0.08688700 -2.11899800  C -0.69518100 -1.49463900 -2.15807400  H 1.79422300 -0.85528000 -2.70820100  H -0.11780500 -2.19900600 -2.77278000  H 0.78625200 0.59124100 -2.82121100  H -1.18657900 -0.79634100 -2.83955700  N 0.22236800 -0.72003200 -1.29392500  C -2.95012200 -2.42213000 1.27513700  C 2.71489500 1.87440400 1.33463000  H -1.95466100 -2.85140900 1.43452100  H 2.80035400 0.80517300 1.55385000  C -4.24909700 -0.77761800 -0.88285500  C 1.58130200 3.52205500 -0.91364900  C -4.08642300 -0.27952700 -2.31734100  C 1.10598900 3.46563900 -2.36373800  O -1.80847100 1.98456600 2.86916900  H 2.64070500 3.79976400 -0.90791200  H -4.81437500 -1.71533900 -0.90422000  C 0.78349100 4.56053700 -0.12653900  C -5.00464900 0.24731100 -0.03864000  H 1.14143800 4.67813800 0.89644500  H -5.20185000 -0.10647700 0.97375800  H -0.27288500 4.28917800 -0.08362200  H -4.44316500 1.18057500 0.03487100  H 0.86149700 5.53461700 -0.61831600  H -5.96886700 0.46951300 -0.50493400  C -3.37201800 -1.74857800 2.57896400  C 2.16667300 2.55911000 2.58447800  H -4.39358200 -1.36695400 2.52642400  H 2.14623300 3.64541600 2.47656300  H -2.71645700 -0.91573600 2.83765600  H 1.15598000 2.22498300 2.82358200  H -3.34025600 -2.47436100 3.39661600  H 2.81071800 2.33326800 3.43925200  C -3.89774100 -3.55321100 0.88504900  C 4.10011000 2.39312100 0.95997700  H -3.59954100 -4.05084100 -0.04060200  H 4.51499100 1.88386600 0.08777900  H -4.92285600 -3.19513600 0.76413600  H 4.08774000 3.46710800 0.75873400  H -3.91331000 -4.31134600 1.67353700  H 4.79168300 2.23052800 1.79185200  H 0.37687900 -0.81198700 1.40926000  H 0.71310800 -1.43685300 -0.67625000  C 0.85899600 -1.83337500 1.73281400  H -5.07217800 -0.05170800 -2.73315500  H -3.49565900 0.63690500 -2.35776600  H -3.62577600 -1.02357900 -2.97013300  H 1.17160400 4.46483300 -2.80406000  H 1.71573900 2.80113000 -2.97873200  H 0.06360100 3.14885400 -2.42954900  H 0.04778600 -2.30398100 2.28979300  C 1.39137200 -2.65882100 0.65242400  H 0.76312500 -3.47125200 0.29671600  N -1.44763900 1.51461100 1.84758500  N -1.76890100 1.96203600 -0.79848600  C 2.76974400 -2.74722400 0.29650200  C 3.19662800 -3.66213700 -0.70403900  C 3.79597000 -1.95981800 0.87841600  C 4.51631500 -3.76473600 -1.09315900  H 2.45225900 -4.30334100 -1.16849700  C 5.12030900 -2.07073900 0.48115000  H 3.55376200 -1.27626900 1.68514400  C 5.50281300 -2.96347800 -0.51353400  H 4.78858800 -4.48364600 -1.86016400  H 5.87003600 -1.45351600 0.96759600  H 6.53890400 -3.04711100 -0.81934700  H 1.60285600 -1.49648300 2.45857700  Nb -0.84317600 0.71612600 0.23702600 | **2Nb + Ph-CHCH2-TS-HN transfer**  O -2.42632500 2.79118200 -1.32476100  P 1.46321400 1.85285300 -0.10176000  P -2.60457400 -1.21244400 -0.09332500  C 2.29295300 0.65266800 -1.25676500  C -1.69894600 -2.32828300 -1.27892900  H 2.86935800 -0.03871100 -0.63546200  H -1.20519600 -3.08833400 -0.66902300  H 3.00124100 1.15526300 -1.91989300  H -2.38691400 -2.84822000 -1.95022200  C 1.27750000 -0.13571300 -2.07253300  C -0.64800700 -1.57133400 -2.08232900  H 1.80921000 -0.93356800 -2.60928600  H -0.02967400 -2.30338400 -2.62246500  H 0.80758700 0.50281400 -2.82674500  H -1.12372000 -0.93872200 -2.83760800  N 0.21808800 -0.73116800 -1.23067100  C -3.00953500 -2.39673500 1.31041600  C 2.68184200 1.93508800 1.32470900  H -2.02106600 -2.82276900 1.51593800  H 2.77349200 0.87267300 1.57432400  C -4.23007500 -0.81627800 -0.94072600  C 1.53676100 3.51344500 -0.97091400  C -4.01048300 -0.33548100 -2.37361500  C 1.04180400 3.41341500 -2.41228800  O -1.77863200 1.92298700 2.90455700  H 2.59546000 3.79382500 -0.98844900  H -4.78829200 -1.75798600 -0.97444000  C 0.74809700 4.57313100 -0.20339300  C -5.02656200 0.21259600 -0.14044200  H 1.12221800 4.72373700 0.80934500  H -5.27058500 -0.13527800 0.86371600  H -0.30701700 4.30218500 -0.13568800  H -4.47275200 1.14853800 -0.04729200  H 0.81563900 5.53165400 -0.72635000  H -5.96848300 0.42852800 -0.65299100  C -3.47213500 -1.68354100 2.57886000  C 2.12439900 2.65035300 2.55323300  H -4.49150600 -1.30484100 2.48268700  H 2.10304300 3.73339500 2.41709200  H -2.82520700 -0.84289200 2.83302800  H 1.11293300 2.32116500 2.79531400  H -3.46622600 -2.38406700 3.41885700  H 2.76352000 2.44792500 3.41751500  C -3.94689500 -3.53742900 0.92352000  C 4.06516200 2.45267900 0.94134400  H -3.61688200 -4.06569300 0.02613600  H 4.48776300 1.92037900 0.08686000  H -4.96531900 -3.18016100 0.75342300  H 4.04511600 3.51988900 0.70722600  H -3.99456300 -4.26911700 1.73539800  H 4.75396600 2.32112700 1.78100300  H 0.44212200 -0.81853700 1.47988900  H 0.78501700 -1.51432500 -0.55808300  C 0.89485400 -1.85282900 1.68902700  H -4.97814300 -0.10862400 -2.83038100  H -3.41382900 0.57766400 -2.40205600  H -3.52669500 -1.08887300 -2.99798500  H 1.09612900 4.39972500 -2.88219700  H 1.64557700 2.73317500 -3.01550300  H 0.00047000 3.08910300 -2.45474500  H 0.08749900 -2.39142900 2.18770600  C 1.41441600 -2.54654200 0.48558700  H 0.85630000 -3.43916400 0.20503900  N -1.43513900 1.47082200 1.87001900  N -1.81307700 1.96679200 -0.73034800  C 2.83389200 -2.67692100 0.23375600  C 3.29982600 -3.58347400 -0.74842200  C 3.82952700 -1.92079400 0.88959100  C 4.64016900 -3.70941400 -1.05781100  H 2.57282800 -4.20144200 -1.26852700  C 5.17672500 -2.05030500 0.57550200  H 3.54904600 -1.23725200 1.68398800  C 5.60166300 -2.93736400 -0.40439800  H 4.94611700 -4.42345800 -1.81642400  H 5.90543400 -1.45295900 1.11539200  H 6.65330700 -3.03802800 -0.64600500  H 1.64740600 -1.62962000 2.45005600  Nb -0.85186500 0.69620600 0.23597300 |
| **2Nb + PhCHO-TS-HM transfer**  O 2.15339500 3.27824000 -0.30343800  P -1.64661300 1.67694600 0.19244900  P 2.69945400 -0.91056600 0.18198500  C -1.79032800 1.25102100 2.00665900  C 2.57152200 -1.06877600 2.04115800  H -2.28761100 0.27744400 2.05204300  H 2.05290200 -2.01102800 2.23670100  H -2.42160100 1.96314200 2.54371900  H 3.55671200 -1.12489200 2.50968600  C -0.42578600 1.15293600 2.67750000  C 1.76322200 0.07163800 2.64743800  H -0.55658300 0.84347800 3.72444800  H 1.61972800 -0.11913600 3.72071300  H 0.06967800 2.12648300 2.68722700  H 2.29200600 1.02324500 2.55130000  N 0.45735000 0.20638000 1.97559600  C 2.73732700 -2.71753300 -0.33634600  C -3.22201400 0.93365900 -0.50029100  H 1.88100600 -3.10956200 0.22289500  H -3.09808600 -0.11517700 -0.21229800  C 4.42826100 -0.24517100 -0.12270000  C -1.86388500 3.54089900 0.09665900  C 4.72269800 0.98232900 0.73631100  C -1.05580600 4.27439500 1.16476500  O 0.66632000 0.65594700 -3.45165400  H -2.92726000 3.73715400 0.27093900  H 5.11860100 -1.04432900 0.16735700  C -1.47988500 4.04440100 -1.29493700  C 4.62199500 0.07545300 -1.60361900  H -2.06163100 3.57483100 -2.08830000  H 4.50611400 -0.80236200 -2.24073400  H -0.42472600 3.85117500 -1.49672000  H 3.90120300 0.82642900 -1.93439000  H -1.64440400 5.12447600 -1.35573700  H 5.62745900 0.47370400 -1.76899700  C 2.44589000 -2.90313400 -1.82361900  C -3.26566100 0.98364400 -2.02566700  H 3.28837300 -2.59364300 -2.44560000  H -3.48328800 1.98927300 -2.39285100  H 1.57220100 -2.32730300 -2.13438400  H -2.32355800 0.65385300 -2.46643800  H 2.25708600 -3.95957200 -2.03712800  H -4.05985800 0.32676200 -2.39100600  C 3.98013800 -3.48599100 0.10345600  C -4.51049400 1.46494900 0.12055800  H 4.19024100 -3.36640500 1.16897700  H -4.50591400 1.40819200 1.21131700  H 4.86588800 -3.17402900 -0.45525400  H -4.70111900 2.50266200 -0.16513300  H 3.84128700 -4.55493200 -0.08452500  H -5.35976100 0.87289200 -0.23269700  H -0.52404600 -1.01675200 -0.32514900  H 0.01305400 -0.72269500 1.99730000  C -0.90628000 -2.63302600 0.60256200  C -2.34553100 -2.72344400 0.23019700  C -2.71693600 -2.96274700 -1.09237100  C -4.05245700 -3.12658900 -1.42612700  C -5.02956600 -3.05868700 -0.43690200  C -3.32669500 -2.66658700 1.21871800  C -4.66435500 -2.83020900 0.88526500  H -1.95046100 -3.00212200 -1.86000300  H -4.33546300 -3.30929900 -2.45686400  H -6.07407700 -3.19170400 -0.69670000  H -3.01744700 -2.51543900 2.24686100  H -5.42424600 -2.79200400 1.65825600  H 5.74148300 1.32707300 0.53528200  H 4.04544900 1.80527700 0.50421000  H 4.66044000 0.77008300 1.80566200  H -1.20542100 5.35261500 1.05470000  H -1.35977300 4.00883700 2.17932400  H 0.01344200 4.08311800 1.05453900  O -0.53129700 -2.48685700 1.77138500  H -0.22795900 -3.03957000 -0.16213700  N 0.65958700 0.64349000 -2.27139300  N 1.59816200 2.22646000 -0.30761800  Nb 0.63565900 0.59123200 -0.37647200 | **2Nb + PhCHO-interm**  N -1.54561300 -2.21450800 -0.46986700  O -2.10745100 -3.25560500 -0.55308500  P 1.69366400 -1.66611400 0.22386500  P -2.71662300 0.88051800 0.20383300  C 1.87383000 -1.10886600 1.99209600  C -2.57626700 1.04424600 2.05423700  H 2.34960500 -0.12441600 1.94697800  H -2.08665700 2.00488900 2.22860200  H 2.53577700 -1.76711700 2.56054500  H -3.55701300 1.05942100 2.53439700  C 0.52573600 -0.98024500 2.68960500  C -1.70491600 -0.05786800 2.64239200  H 0.68399000 -0.52310200 3.67717200  H -1.51259600 0.17626200 3.69947900  H 0.08896800 -1.96813100 2.86537200  H -2.22031400 -1.02368800 2.61796400  N -0.42618600 -0.16985100 1.91627500  C -2.76555200 2.68150200 -0.32176300  C 3.25633500 -0.98495000 -0.55771900  H -1.86440500 3.05577500 0.17720000  H 3.16604000 0.08096500 -0.32124900  C -4.42144800 0.16733100 -0.11381000  C 1.87313900 -3.53368900 0.24444900  C -4.69374300 -1.05312600 0.76304700  C 1.02755400 -4.17712500 1.34097400  O -0.52259300 -0.44166200 -3.43205800  H 2.92846000 -3.73011500 0.46175800  H -5.13153900 0.95541700 0.15868300  C 1.52177800 -4.12771800 -1.11929800  C -4.59839100 -0.18062900 -1.59073100  H 2.13502800 -3.72507900 -1.92532500  H -4.48089200 0.68516400 -2.24312000  H 0.47569300 -3.94094500 -1.36770100  H -3.87233900 -0.93472000 -1.90163600  H 1.67331100 -5.21099900 -1.09720000  H -5.60003000 -0.58763500 -1.75749100  C -2.59469000 2.87530500 -1.82644400  C 3.26798200 -1.11442100 -2.07915400  H -3.50031500 2.60992300 -2.37621600  H 3.48518400 -2.13625300 -2.39766200  H -1.77361300 2.27749400 -2.22574000  H 2.31759700 -0.81458500 -2.52353700  H -2.38302100 3.92666800 -2.04116300  H 4.05101600 -0.47315500 -2.49253200  C -3.96637900 3.45580600 0.21507500  C 4.55032700 -1.50390100 0.06328400  H -4.08900600 3.34129100 1.29422700  H 4.57225500 -1.38380500 1.14830700  H -4.89637600 3.14819200 -0.26978900  H 4.71719100 -2.55895500 -0.16860400  H -3.83569700 4.52309200 0.01351700  H 5.39882200 -0.94580200 -0.34237200  H 0.73410400 1.16677500 -0.24333100  H -0.03294600 0.88049800 1.83746700  C 0.79462200 2.22687400 0.27299700  C 2.25933000 2.60643900 0.08490000  C 2.81221300 2.74967300 -1.18737600  C 4.14148600 3.11785200 -1.34338000  C 4.93584700 3.35124100 -0.22419400  C 3.05466300 2.85123400 1.19839100  C 4.38746500 3.21997300 1.04535000  H 2.19422300 2.57296700 -2.06402300  H 4.55944900 3.22966700 -2.33837200  H 5.97324800 3.64409300 -0.34435800  H 2.59198000 2.76759800 2.17550400  H 4.99779800 3.41521600 1.92115000  H -5.70260300 -1.42497600 0.56118800  H -3.99730300 -1.86448400 0.54606200  H -4.64035500 -0.82430500 1.82900500  H 1.14213200 -5.26401700 1.29508500  H 1.32858600 -3.86081600 2.34116900  H -0.03350400 -3.95622900 1.20733900  O 0.34040300 2.22669600 1.52556400  H 0.20796200 2.84400500 -0.43691300  N -0.57056800 -0.52187600 -2.25769200  Nb -0.61964200 -0.59950000 -0.35944600 |
| **2Nb +PhCHO-TS-HN transfer**  N 1.56078600 -2.19359900 0.55291900  O 2.13337700 -3.22430500 0.67894900  P -1.67395300 -1.67924400 -0.20739100  P 2.73048900 0.88168500 -0.20304300  C -1.84604600 -1.16632400 -1.98852400  C 2.56685700 1.06513500 -2.04855400  H -2.33981000 -0.19009400 -1.97156100  H 2.06209000 2.02048600 -2.21045400  H -2.48856200 -1.85054300 -2.54856200  H 3.54193100 1.10041000 -2.53964300  C -0.49143600 -1.02570400 -2.67123500  C 1.70324800 -0.04320300 -2.63786500  H -0.64859700 -0.58184100 -3.66555300  H 1.49288700 0.20520000 -3.68865400  H -0.04073200 -2.01050900 -2.83523800  H 2.23970600 -0.99878700 -2.64044600  N 0.43692400 -0.18843700 -1.89873700  C 2.79907600 2.67597900 0.34681700  C -3.24612600 -0.99167400 0.54990000  H 1.90461700 3.07237300 -0.14664500  H -3.16652500 0.06744500 0.28091900  C 4.43567000 0.15683000 0.08365800  C -1.83781700 -3.54792800 -0.18686700  C 4.68104500 -1.06468300 -0.79964800  C -0.96458700 -4.20664100 -1.25228700  O 0.47353800 -0.31231200 3.42737500  H -2.88687000 -3.75814000 -0.42118500  H 5.14621200 0.93942800 -0.20301500  C -1.50941500 -4.10884200 1.19626600  C 4.63894700 -0.19268800 1.55669000  H -2.14714900 -3.69917600 1.97944100  H 4.55035000 0.67585500 2.21003900  H -0.47215400 -3.90149800 1.46465900  H 3.90822300 -0.93485400 1.88463200  H -1.64471100 -5.19448800 1.19313800  H 5.63740200 -0.61541500 1.70189400  C 2.62226800 2.85311300 1.85287400  C -3.26321100 -1.07436200 2.07454400  H 3.51774700 2.56034700 2.40493400  H -3.47138300 -2.08801300 2.42363400  H 1.78611500 2.26745000 2.23812100  H -2.31804600 -0.75152000 2.51368900  H 2.43220500 3.90589800 2.08061800  H -4.05447500 -0.42867500 2.46471600  C 4.01004600 3.44361200 -0.17660500  C -4.53172400 -1.54324100 -0.06040500  H 4.13538600 3.33981800 -1.25657600  H -4.54908000 -1.45778900 -1.14881800  H 4.93422400 3.11891800 0.30797300  H -4.68832400 -2.59224800 0.20382700  H 3.89147300 4.50985300 0.03751000  H -5.38815700 -0.98186000 0.32348600  H -0.71695200 1.23494800 0.19931700  H -0.01344300 0.90303600 -1.84970700  C -0.84211000 2.23743000 -0.38666600  C -2.30410300 2.60108100 -0.16546400  C -2.81224200 2.79492500 1.11891200  C -4.14096900 3.14880700 1.30768200  C -4.98002100 3.31786500 0.20981300  C -3.14447300 2.78067000 -1.25820700  C -4.47684500 3.13560200 -1.07189300  H -2.16044200 2.66739000 1.97933600  H -4.52392200 3.29855000 2.31168300  H -6.01733300 3.59912400 0.35549300  H -2.71973000 2.65495100 -2.24774800  H -5.12236700 3.27917800 -1.93226000  H 5.68983100 -1.44606600 -0.61619100  H 3.98101000 -1.86986100 -0.57152900  H 4.61042100 -0.83286300 -1.86387300  H -1.07045400 -5.29335700 -1.18570500  H -1.24776900 -3.91366100 -2.26465000  H 0.09143200 -3.97259800 -1.10249000  O -0.44741100 2.14451700 -1.66483000  H -0.23857100 2.93326200 0.22816400  N 0.54702800 -0.44071800 2.25816600  Nb 0.63157400 -0.58881500 0.36404300 | **2Nb + Ph-COCH3-TS**  O 2.09925800 3.15858500 -0.69243100  P -1.63476300 1.70367100 0.23400800  P 2.81326400 -0.78636400 0.13446700  C -1.66099500 1.43171500 2.07941200  C 2.65936500 -1.00088300 1.98460200  H -2.16933400 0.47544900 2.23522900  H 2.14005700 -1.95001200 2.14545000  H -2.23294100 2.20362200 2.59968100  H 3.63572100 -1.08112100 2.46886000  C -0.25648600 1.33603400 2.66187900  C 1.85247700 0.12384800 2.62375100  H -0.32837800 1.11263700 3.73583400  H 1.72629700 -0.08958800 3.69475500  H 0.27609100 2.28469000 2.56187200  H 2.38766400 1.07294700 2.54443700  N 0.53626500 0.29302500 1.98398300  C 3.11234300 -2.54845600 -0.44338600  C -3.30937900 1.04505000 -0.28674100  H 2.20058400 -3.03969300 -0.09621700  H -3.21946500 -0.01176400 -0.02081000  C 4.45582600 0.09204400 -0.12809300  C -1.74700000 3.56581500 -0.01156900  C 4.68031500 1.23271800 0.86181500  C -0.88492000 4.34751200 0.97684500  O 0.40602800 0.25357700 -3.45035900  H -2.79593100 3.82437700 0.16936200  H 5.22883800 -0.66493400 0.04188300  C -1.38137800 3.94586000 -1.44694800  C 4.56761900 0.60582900 -1.56382100  H -1.98338500 3.42225900 -2.18920300  H 4.44554100 -0.18313200 -2.30583800  H -0.33340800 3.72410300 -1.65107600  H 3.81478600 1.36964100 -1.76165900  H -1.53323600 5.01994300 -1.59201100  H 5.55326100 1.05592400 -1.71654500  C 3.13390200 -2.66321700 -1.96648600  C -3.51282600 1.12374300 -1.79826200  H 4.07246700 -2.29465300 -2.38590800  H -3.72016000 2.14560100 -2.12493600  H 2.31356000 -2.10945200 -2.42661200  H -2.64179000 0.75739800 -2.34477400  H 3.04219600 -3.71324300 -2.25940500  H -4.37142300 0.51056200 -2.08372100  C 4.30969600 -3.24808600 0.19367100  C -4.49581300 1.63463500 0.47054400  H 4.29030000 -3.20457400 1.28479500  H -4.39221000 1.53716300 1.55300900  H 5.25714800 -2.82263400 -0.14597900  H -4.64650300 2.69181300 0.23638900  H 4.31443800 -4.30471700 -0.09108800  H -5.41033600 1.10802300 0.18247100  H -0.38690700 -1.26796000 -0.10032200  H 0.01158400 -0.59196000 2.09776200  C -1.19948600 -2.46337800 0.99880600  C -2.52857400 -2.49098200 0.28255900  C -2.64814700 -2.67666000 -1.09470500  C -3.89809400 -2.80582400 -1.68094100  C -5.04764400 -2.76064600 -0.89710200  C -3.68410000 -2.44326200 1.06112000  C -4.93735500 -2.57791700 0.47507200  H -1.75703400 -2.67905800 -1.71195200  H -3.97841000 -2.93662300 -2.75457200  H -6.02409900 -2.86711300 -1.35698100  H -3.57912200 -2.30919000 2.13159000  H -5.82841500 -2.54603900 1.09291800  H 5.64730500 1.70160300 0.65668300  H 3.91788400 2.00636100 0.75785500  H 4.70115500 0.89214600 1.89887900  H -0.99696000 5.41885300 0.78491800  H -1.17181100 4.17373200 2.01577900  H 0.17309400 4.10753900 0.85696600  O -1.13090400 -1.96986900 2.14099800  N 0.48538600 0.35784000 -2.27807900  C -0.28704600 -3.62077400 0.64106100  H -0.77445600 -4.53634800 0.99649600  H -0.11589200 -3.72033200 -0.42930200  H 0.65885400 -3.51981900 1.16966600  Nb 0.59468400 0.48665200 -0.38867400  N 1.51754700 2.13036000 -0.54880300 |
| **1Ta + H2-TS**  N -0.64237800 1.81362000 0.00000000  O -1.17494200 2.87927300 0.00000000  P -0.09736900 -0.40309100 -2.50193400  P -0.09736900 -0.40309100 2.50193400  C -1.36836300 -1.76532300 -2.45214000  C -1.36836300 -1.76532300 2.45214000  H -0.80439400 -2.70262700 -2.43259800  H -0.80439400 -2.70262700 2.43259800  H -1.98587400 -1.77313800 -3.35363800  H -1.98587400 -1.77313800 3.35363800  C -2.23388700 -1.66775800 -1.19774600  C -2.23388700 -1.66775800 1.19774600  H -2.81614300 -2.60095400 -1.11612600  H -2.81614300 -2.60095400 1.11612600  H -2.97571300 -0.86123700 -1.32668100  H -2.97571300 -0.86123700 1.32668100  N -1.44404500 -1.45978000 0.00000000  C 1.32469800 -1.24809400 3.39441200  C 1.32469800 -1.24809400 -3.39441200  H 1.45836700 -2.13682800 2.76565300  H 1.45836700 -2.13682800 -2.76565300  C -0.78759700 0.90123400 3.65618200  C -0.78759700 0.90123400 -3.65618200  C -2.21476300 1.27774600 3.26339200  C -2.21476300 1.27774600 -3.26339200  N 1.86920900 1.00357900 0.00000000  O 2.94417500 1.51009600 0.00000000  H -0.80638800 0.44872800 -4.65379700  H -0.80638800 0.44872800 4.65379700  C 0.10714700 2.13932100 -3.67529000  C 0.10714700 2.13932100 3.67529000  H 1.11572000 1.92441700 -4.02903800  H 1.11572000 1.92441700 4.02903800  H 0.18601000 2.57536400 -2.67751700  H 0.18601000 2.57536400 2.67751700  H -0.32367000 2.89338800 -4.34051000  H -0.32367000 2.89338800 4.34051000  C 2.62867300 -0.45509500 3.34526600  C 2.62867300 -0.45509500 -3.34526600  H 2.60968600 0.39704200 4.02750500  H 2.60968600 0.39704200 -4.02750500  H 2.84232600 -0.07976700 2.34401000  H 2.84232600 -0.07976700 -2.34401000  H 3.45988700 -1.09584200 3.65406800  H 3.45988700 -1.09584200 -3.65406800  C 0.99071900 -1.70249400 4.81276900  C 0.99071900 -1.70249400 -4.81276900  H 0.07570600 -2.29715600 4.85893900  H 0.07570600 -2.29715600 -4.85893900  H 0.87732700 -0.85176000 5.48927300  H 0.87732700 -0.85176000 -5.48927300  H 1.80399300 -2.31953800 5.20646000  H 1.80399300 -2.31953800 -5.20646000  H 0.91042400 -1.80538800 0.00000000  H -0.01960100 -1.91699800 0.00000000  H -2.58773700 2.04486200 3.94827200  H -2.58773700 2.04486200 -3.94827200  H -2.25033800 1.69140800 2.25380500  H -2.25033800 1.69140800 -2.25380500  H -2.90119900 0.43079200 3.31568000  H -2.90119900 0.43079200 -3.31568000  Ta 0.19290700 0.13793800 0.00000000 | **2Ta +PhCN-TS-HM transfer**  N -2.56911600 -0.64270900 0.00000000  O -3.74767000 -0.84620300 0.00000000  P -0.57539000 0.26805000 2.50584100  P -0.57539000 0.26805000 -2.50584100  C -0.70896000 2.12989200 2.46167700  C -0.70896000 2.12989200 -2.46167700  H 0.31479600 2.51316900 2.42666100  H 0.31479600 2.51316900 -2.42666100  H -1.17819900 2.52779900 3.36387700  H -1.17819900 2.52779900 -3.36387700  C -1.45614000 2.59869800 1.22037700  C -1.45614000 2.59869800 -1.22037700  H -1.42989800 3.69609200 1.17348900  H -1.42989800 3.69609200 -1.17348900  H -2.50506400 2.29540000 1.25517400  H -2.50506400 2.29540000 -1.25517400  N -0.85216800 2.02912000 0.00000000  C 1.04170500 0.02562700 -3.42692000  C 1.04170500 0.02562700 3.42692000  H 1.74393800 0.52231300 -2.74837900  H 1.74393800 0.52231300 2.74837900  C -1.93688200 -0.32436200 -3.65498000  C -1.93688200 -0.32436200 3.65498000  C -3.25732700 0.39785900 -3.39481700  C -3.25732700 0.39785900 3.39481700  N -0.32433200 -2.15998400 0.00000000  O -0.04150000 -3.31503900 0.00000000  C -2.12664700 -1.83502700 3.51704000  C -2.12664700 -1.83502700 -3.51704000  H -1.21695100 -2.39734000 3.72756700  H -1.21695100 -2.39734000 -3.72756700  H -2.44766700 -2.08944700 2.50531900  H -2.44766700 -2.08944700 -2.50531900  H -2.89805900 -2.17400300 4.21496100  H -2.89805900 -2.17400300 -4.21496100  C 1.44523800 -1.44416100 -3.51924800  C 1.44523800 -1.44416100 3.51924800  H 0.85978300 -1.97301000 -4.27483000  H 0.85978300 -1.97301000 4.27483000  H 1.32003600 -1.96216700 -2.56708700  H 1.32003600 -1.96216700 2.56708700  H 2.49609600 -1.52110300 -3.81172200  H 2.49609600 -1.52110300 3.81172200  C 1.10908200 0.71284800 -4.78800900  C 1.10908200 0.71284800 4.78800900  H 0.86605300 1.77599400 -4.73494400  H 0.86605300 1.77599400 4.73494400  H 0.43560500 0.24537100 -5.51081700  H 0.43560500 0.24537100 5.51081700  H 2.12207200 0.62957900 -5.19299200  H 2.12207200 0.62957900 5.19299200  H 1.17537000 0.25270200 0.00000000  H 0.14786800 2.31863800 0.00000000  N 1.98016000 2.53974300 0.00000000  C 2.36019800 1.42064800 0.00000000  C 3.54109200 0.55890800 0.00000000  C 3.47501000 -0.83038800 0.00000000  C 4.64141700 -1.58357100 0.00000000  C 5.87979900 -0.95507300 0.00000000  C 4.79094200 1.19185800 0.00000000  C 5.95091200 0.43495700 0.00000000  H 2.49895500 -1.30145600 0.00000000  H 4.57951300 -2.66595700 0.00000000  H 6.78956800 -1.54531100 0.00000000  H 4.83126500 2.27459300 0.00000000  H 6.91540200 0.93054400 0.00000000  H -4.01660500 0.02015800 -4.08594900  H -4.01660500 0.02015800 4.08594900  H -3.61759000 0.20992800 -2.38149900  H -3.61759000 0.20992800 2.38149900  H -3.18733800 1.47619800 -3.55087100  H -3.18733800 1.47619800 3.55087100  H -1.60384300 -0.09116100 -4.67228800  H -1.60384300 -0.09116100 4.67228800  Ta -0.71611000 -0.31981600 0.00000000 |
| **2Ta + PhCN-interm**  N 0.00164500 -2.53913800 -0.71841200  O 0.00231100 -3.70449500 -0.98006300  P 2.51384100 -0.56769600 0.27321700  P -2.51297800 -0.57109100 0.27327300  C 2.46390600 -0.63577100 2.13475100  C -2.46290900 -0.63865300 2.13480800  H 2.42890000 0.40141000 2.47922600  H -2.42915200 0.39865900 2.47901900  H 3.36291600 -1.09424200 2.55201300  H -3.36136000 -1.09808400 2.55221900  C 1.21486800 -1.35758500 2.62280300  C -1.21298900 -1.35883700 2.62300500  H 1.15223400 -1.26214300 3.71556900  H -1.15042300 -1.26300700 3.71573700  H 1.26097800 -2.42482000 2.39065100  H -1.25784600 -2.42618700 2.39113100  N 0.00058800 -0.78680000 2.00597500  C -3.43784700 1.03281800 -0.03273900  C 3.43668900 1.03744000 -0.03240300  H -2.77057000 1.75675700 0.44821300  H 2.76860200 1.76037500 0.44894400  C -3.64444300 -1.96300400 -0.27693900  C 3.64707400 -1.95809200 -0.27727600  C -3.35713400 -3.25902000 0.47844700  C 3.36142200 -3.25462900 0.47782600  N 0.00015900 -0.25557800 -2.13218200  O -0.00008100 0.07834300 -3.27194500  H 4.66504700 -1.63092400 -0.03893200  H -4.66283600 -1.63708900 -0.03868400  C 3.52798100 -2.18549100 -1.78413800  C -3.52498700 -2.19055700 -1.78375500  H 3.74938900 -1.29117800 -2.36639200  H -3.74744900 -1.29662700 -2.36619600  H 2.52015300 -2.51267900 -2.04530900  H -2.51673700 -2.51655500 -2.04479900  H 4.22870800 -2.96677800 -2.09312500  H -4.22473400 -2.97276400 -2.09262900  C -3.52388300 1.39075100 -1.51477900  C 3.52198700 1.39602000 -1.51432100  H -4.27590000 0.78812700 -2.02904100  H 4.27455300 0.79443500 -2.02899200  H -2.56989800 1.25410000 -2.02636800  H 2.56803000 1.25848600 -2.02573200  H -3.81823900 2.43806300 -1.62352400  H 3.81513700 2.44370400 -1.62275300  C -4.80355500 1.11114500 0.64459200  C 4.80241700 1.11722200 0.64471800  H -4.75438900 0.90288100 1.71519800  H 4.75372700 0.90842100 1.71524100  H -5.51870800 0.41814800 0.19419000  H 5.51839200 0.42536900 0.19386900  H -5.21418000 2.11822600 0.52684200  H 5.21170400 2.12489300 0.52735000  H -0.00087100 1.28514600 0.35810100  H 0.00008900 0.26788300 2.28576800  N -0.00093300 1.88602400 2.43371300  C -0.00135400 2.17607700 1.25162100  C -0.00240500 3.46179300 0.51249500  C -0.00241500 3.49711800 -0.87811700  C -0.00339600 4.71217000 -1.55198500  C -0.00437900 5.90216700 -0.83584900  C -0.00337800 4.66136200 1.22955600  C -0.00436500 5.87248500 0.55680700  H -0.00163400 2.56153800 -1.42947200  H -0.00338800 4.72838900 -2.63632200  H -0.00515300 6.85203500 -1.35933500  H -0.00333700 4.61460900 2.31264300  H -0.00512200 6.80077300 1.11800500  H -4.03761600 -4.03960100 0.12599900  H 4.04304700 -4.03420400 0.12536000  H -2.33911600 -3.60727500 0.29328400  H 2.34391800 -3.60424200 0.29241700  H -3.50642500 -3.16187200 1.55545700  H 3.51038800 -3.15747400 1.55487800  Ta 0.00050300 -0.72255900 -0.30793700 | **2Ta + PhCN-TS-HN transfer**  N 0.00371600 -2.55714900 -0.73393700  O 0.00543900 -3.72059400 -1.00221400  P 2.51725900 -0.58001500 0.26947600  P -2.51552600 -0.58731500 0.26944600  C 2.46961100 -0.53661600 2.12978300  C -2.46803600 -0.54388900 2.12975700  H 2.45690600 0.51935200 2.41217400  H -2.45843300 0.51209800 2.41220200  H 3.36076200 -0.98704900 2.57238100  H -3.35786800 -0.99695800 2.57231700  C 1.20609800 -1.20513400 2.65765300  C -1.20257400 -1.20872500 2.65760300  H 1.13243200 -1.00852200 3.73707900  H -1.12950500 -1.01197500 3.73704400  H 1.26079000 -2.29171800 2.53429000  H -1.25406700 -2.29545400 2.53415300  N 0.00100700 -0.69104900 1.98065600  C -3.44824100 0.99024100 -0.13622000  C 3.44529400 1.00027900 -0.13628200  H -2.80248400 1.74171100 0.33219300  H 2.79723400 1.74986500 0.33196900  C -3.63229600 -2.02024800 -0.19559600  C 3.63828500 -2.00963800 -0.19545300  C -3.29842300 -3.27486800 0.60915900  C 3.30809800 -3.26520400 0.60934600  N 0.00043200 -0.26235600 -2.11660100  O -0.00004600 0.09855700 -3.24868900  C 3.55450600 -2.30092200 -1.69345400  C -3.54760300 -2.31122200 -1.69360700  H 3.82030500 -1.44043000 -2.30729600  H -3.81584600 -1.45147600 -2.30743500  H 2.54554500 -2.61106900 -1.97061600  H -2.53774100 -2.61845600 -1.97073100  H 4.24005300 -3.11498400 -1.94680500  H -4.23079000 -3.12724500 -1.94702500  C -3.49616000 1.28740200 -1.63351800  C 3.49251900 1.29742900 -1.63360700  H -4.23033900 0.65983200 -2.14333200  H 4.22865400 0.67202100 -2.14325600  H -2.52864200 1.13659100 -2.11475700  H 2.52553100 1.14368100 -2.11498600  H -3.79457900 2.32730700 -1.79207900  H 3.78784300 2.33821000 -1.79222100  C -4.83235700 1.08217600 0.50104200  C 4.82905800 1.09642300 0.50113500  H -4.81048800 0.91261100 1.57947500  H 4.80754400 0.92710800 1.57961500  H -5.52915300 0.36690000 0.05690300  H 5.52799600 0.38304600 0.05729800  H -5.24763900 2.08063900 0.33574200  H 5.24145400 2.09604300 0.33560400  H -0.00161500 1.35727200 0.28574100  H -0.00076000 0.48466300 2.23690900  N -0.00288000 1.88081600 2.34166500  C -0.00315400 2.19528300 1.15274400  C -0.00515100 3.51702200 0.48487700  C -0.00512700 3.61494300 -0.90405600  C -0.00703800 4.85930000 -1.52205800  C -0.00898700 6.01522300 -0.75207800  C -0.00711400 4.68280100 1.25517600  C -0.00901900 5.92295500 0.63793900  H -0.00360800 2.70722300 -1.50034600  H -0.00700800 4.92532000 -2.60445300  H -0.01048500 6.98784300 -1.23191800  H -0.00710400 4.58669700 2.33502900  H -0.01054300 6.82523500 1.23999700  H -3.96751900 -4.08561100 0.30654900  H 3.97960800 -4.07397600 0.30681400  H -2.27632500 -3.60737100 0.41796800  H 2.28699700 -3.60073500 0.41811200  H -3.42661400 -3.13247600 1.68374000  H 3.43580300 -3.12237800 1.68392600  H -4.65051400 -1.70392100 0.05594500  H 4.65554400 -1.69026600 0.05611300  Ta 0.00110200 -0.75184700 -0.29617600 |
| **2Ta + Ph-CHNH-TS**  O -2.17803900 -2.98754000 -0.81962000  P 1.62125300 -1.78852900 0.25284200  P -2.55013000 1.03251300 0.24573600  C 1.58729200 -1.74491500 2.11826100  C -2.50720600 1.02755600 2.11089700  H 2.17401000 -0.87039000 2.41311500  H -1.90605100 1.89016800 2.41336200  H 2.06769100 -2.62135000 2.55869700  H -3.50240400 1.14960800 2.54430700  C 0.16604800 -1.59679600 2.64596600  C -1.84825300 -0.23988200 2.64115200  H 0.19791000 -1.46718600 3.73705000  H -1.74248700 -0.15822300 3.73176600  H -0.41709200 -2.49847600 2.44252400  H -2.46628100 -1.11742900 2.43627000  N -0.52240700 -0.44816900 2.02625300  C -2.55255800 2.87299900 -0.13712800  C 3.29916500 -1.04339200 -0.12459100  H -1.64199800 3.20119300 0.37559300  H 3.18542600 -0.03759700 0.29468000  C -4.25607900 0.41085900 -0.23443800  C 1.72954100 -3.60246600 -0.22075200  C -4.67602200 -0.81004300 0.58122100  C 0.78987400 -4.47145700 0.61279300  O -0.16865400 0.04659400 -3.32244700  H 2.76165400 -3.90801300 -0.01651000  H -4.94804600 1.22993200 -0.01156100  C 1.43415300 -3.78489800 -1.70990700  C -4.31035500 0.09727500 -1.72933300  H 2.09587600 -3.19929900 -2.34789800  H -4.06250600 0.95790800 -2.35091700  H 0.40757800 -3.49297400 -1.93670600  H -3.61575100 -0.70611700 -1.97953300  H 1.55480400 -4.83806200 -1.98101200  H -5.31918100 -0.22878000 -1.99937100  C -2.37319100 3.16246100 -1.62587200  C 3.53934500 -0.88707100 -1.62443900  H -3.29308600 2.97669200 -2.18426700  H 3.77693200 -1.84418800 -2.09465800  H -1.58214300 2.55381800 -2.06729600  H 2.67312200 -0.45980500 -2.13198800  H -2.11565800 4.21559100 -1.77037000  H 4.39010900 -0.22151400 -1.79188600  C -3.72714100 3.64757500 0.45460100  C 4.47344800 -1.73306300 0.56433500  H -3.85064400 3.46885300 1.52485300  H 4.33785700 -1.81885200 1.64460000  H -4.66725600 3.39887100 -0.04352300  H 4.64626500 -2.73521900 0.16371100  H -3.56679200 4.72128200 0.31872600  H 5.38796800 -1.15720900 0.39473600  H 0.72183400 1.06289800 0.17269700  H 0.04792800 0.41729700 2.26858800  C 1.11248200 2.19802400 1.14596600  C 2.37378300 2.63168200 0.45228000  C 2.39477100 2.82468300 -0.93020500  C 3.53384400 3.29319600 -1.56540800  C 4.67993000 3.57540600 -0.82731100  C 3.52144200 2.93065700 1.18379100  C 4.66946900 3.39250100 0.54814200  H 1.51151600 2.57600400 -1.50947200  H 3.53182200 3.43289600 -2.64091400  H 5.57249300 3.94043600 -1.32338700  H 3.50912300 2.83322500 2.26393100  H 5.55218800 3.62397000 1.13451000  H -5.67520100 -1.12483500 0.26591500  H -4.00213200 -1.65181600 0.41361400  H -4.72633100 -0.60331800 1.65209000  H 0.89152700 -5.51466700 0.29937300  H 1.01334800 -4.43263500 1.68080200  H -0.25266000 -4.18694600 0.45837100  H 0.25208800 2.77203300 0.80103900  N -0.31180500 -0.16874300 -2.16355000  N -1.54682700 -1.99230000 -0.61349500  Ta -0.50971900 -0.45971600 -0.31388900  N 1.05479800 1.82282400 2.41385900  H 1.96981400 1.49865300 2.72653900 | **2Ta + Ph-CHNCH2Ph-TS**  O -2.69199000 0.21948200 2.94272400  P 0.50712100 2.29991600 0.76054100  P -2.34379500 -1.41401700 -1.14427000  C 1.56340900 2.22971900 -0.77602000  C -1.18331100 -1.48876800 -2.60579400  H 2.39503200 1.55522200 -0.56221900  H -0.40665400 -2.21807600 -2.35671800  H 1.99811500 3.20181800 -1.01708800  H -1.68478100 -1.84463800 -3.50889700  C 0.77958300 1.69625300 -1.96764000  C -0.53346000 -0.13495400 -2.86769700  H 1.46267900 1.57225500 -2.81832400  H 0.20419800 -0.23993900 -3.67466200  H 0.00350000 2.40496700 -2.26726100  H -1.27892500 0.59114000 -3.19940900  N 0.12317500 0.40726300 -1.65994900  C -2.37303900 -3.20265400 -0.56036200  C 1.76554100 2.05230400 2.13116500  H -1.31556600 -3.38937300 -0.34858300  H 2.10326600 1.02991400 1.93127200  C -4.05585600 -1.10811300 -1.85754400  C -0.06172700 4.08417200 0.92169200  C -4.05077100 -0.06754500 -2.97509300  C -0.45451600 4.69591400 -0.42164400  O -3.28247200 2.57542500 -0.71653500  C -1.22382800 4.19201800 1.90989200  C -5.03249600 -0.69962000 -0.75447600  H -0.98756700 3.77800500 2.88989200  H -5.09021200 -1.43078600 0.05184900  H -2.10198400 3.66849200 1.53012600  H -4.74365600 0.25704200 -0.31768900  H -1.48988700 5.24447700 2.04724200  H -6.03570700 -0.59034200 -1.17729000  C -3.13360400 -3.37154500 0.75352600  C 1.11963300 2.06041000 3.51511500  H -4.21387500 -3.32240300 0.60129500  H 0.86518800 3.07468100 3.83108600  H -2.85642600 -2.61064800 1.48498300  H 0.21118100 1.45600800 3.54716600  H -2.91245400 -4.35220900 1.18401300  H 1.82091500 1.65849000 4.25164400  C -2.82370900 -4.21285800 -1.61217900  C 2.97021400 2.98732700 2.07018100  H -2.27041800 -4.11922500 -2.54912500  H 3.47861300 2.95645200 1.10455900  H -3.88916300 -4.11881800 -1.83491200  H 2.68891900 4.02392600 2.27229700  H -2.66393600 -5.22850300 -1.23807000  H 3.69917400 2.69899900 2.83358600  H 0.22723400 -0.78955100 0.76856200  H 0.88039400 -0.27422800 -1.40201600  N 2.03248700 -1.53830000 -0.66535900  H 0.79816400 4.63657400 1.31652800  H -4.37414200 -2.06595300 -2.28214900  H -5.06980400 0.05403400 -3.35416500  H -0.76261500 5.73411200 -0.26629900  H -3.72306600 0.90721000 -2.61053800  H -1.30262700 4.16993000 -0.86317500  H -3.42582900 -0.36055700 -3.82109700  H 0.36828800 4.70821900 -1.13895400  C 3.31089900 -1.03158000 -0.22255300  H 3.19716700 -0.19548400 0.48839500  H 3.87084500 -1.79136500 0.34297100  C 4.18499900 -0.57044200 -1.36596900  C 3.95482300 -0.98979700 -2.67393800  C 5.27659500 0.26315200 -1.11727000  C 4.79396000 -0.58598400 -3.70685000  H 3.10809700 -1.63870300 -2.86266000  C 6.11570100 0.66869900 -2.14623900  H 5.47333900 0.59638400 -0.10189500  C 5.87656600 0.24481700 -3.44880300  H 4.60215000 -0.92569900 -4.71946300  H 6.95841700 1.31730800 -1.93177300  H 6.53024100 0.55994500 -4.25469100  C 1.19028400 -1.95795700 0.25529800  H 0.32895700 -2.48048400 -0.15625100  C 1.59642800 -2.51694500 1.59651600  C 2.43278100 -3.63899000 1.59133800  C 1.13930800 -2.03579200 2.81954300  C 2.80691900 -4.25269500 2.77812100  H 2.78464100 -4.03290700 0.64345400  C 1.51085500 -2.65240500 4.00939800  H 0.48130100 -1.17506100 2.82823500  C 2.34760300 -3.75960800 3.99425800  H 3.45539600 -5.12187900 2.75272500  H 1.14054900 -2.26328500 4.95170000  H 2.63878400 -4.23834900 4.92273000  N -2.14788300 0.33236200 1.89433700  N -2.49208800 1.75053200 -0.35893900  Ta -1.25066000 0.48319100 0.24574000 |
| **2Ta + Ph-CHNPh-TS**  O -1.77326100 0.07877900 3.32107000  P 0.44436000 2.45352100 0.33501500  P -2.31015300 -1.66629100 -0.68689300  C 1.10252400 2.38945000 -1.40958400  C -1.62538100 -1.63597900 -2.42477300  H 2.01630300 1.78960500 -1.37678000  H -0.72493900 -2.25811100 -2.42086100  H 1.37940000 3.37955800 -1.77851600  H -2.31886300 -2.07389400 -3.14607500  C 0.09978500 1.74286600 -2.35715800  C -1.24956500 -0.22125500 -2.84937000  H 0.55085300 1.65257700 -3.35451300  H -0.77865200 -0.25644100 -3.84120600  H -0.79287500 2.36498300 -2.45669200  H -2.13875900 0.40761700 -2.93098100  N -0.33102400 0.41113800 -1.88045800  C -1.95742300 -3.43586700 -0.14914200  C 2.01307300 2.43316300 1.36003100  H -0.86433600 -3.47881200 -0.18318100  H 2.44423500 1.47681700 1.05115600  C -4.18200600 -1.59252900 -0.85729500  C -0.28422200 4.17177600 0.55108400  C -4.63923900 -0.62479800 -1.94628300  C -1.08723200 4.62644400 -0.66590900  O -3.58999700 2.19680900 -0.06139600  C -1.14880100 4.23462200 1.81073700  C -4.83138400 -1.23270500 0.47947000  H -0.60831300 3.93899900 2.70989600  H -4.54250700 -1.90634100 1.28603400  H -2.01876800 3.58374600 1.71477400  H -4.56234000 -0.21957700 0.77929400  H -1.50668500 5.25807000 1.95844300  H -5.92000400 -1.27921400 0.37941300  C -2.37709600 -3.69159800 1.29733400  C 1.72856300 2.35166000 2.85812500  H -3.46067100 -3.79548900 1.38671200  H 1.39956200 3.31332700 3.25832200  H -2.05405700 -2.89080700 1.96496400  H 0.96485400 1.60670500 3.08773800  H -1.93264400 -4.62624400 1.65037700  H 2.64259700 2.07637600 3.39199800  C -2.49450000 -4.51068500 -1.09089100  C 3.00744300 3.54234000 1.03081100  H -2.16414000 -4.36926900 -2.12188100  H 3.26074800 3.57600500 -0.03050600  H -3.58644200 -4.54824200 -1.08517900  H 2.63247400 4.52558500 1.32617400  H -2.13907700 -5.49314600 -0.76610600  H 3.93806200 3.37674600 1.58185400  H 0.62692900 -0.56305200 0.49620300  H 0.51682200 -0.19274500 -1.84151700  N 1.98903800 -1.33858900 -1.46356500  H 0.57237400 4.84415100 0.66963500  H -4.49072000 -2.60339400 -1.14396400  H -5.73157700 -0.64296200 -2.00428900  H -1.47165000 5.63480900 -0.48572200  H -4.34524800 0.40030500 -1.71576500  H -1.94842200 3.97867500 -0.83837000  H -4.26018100 -0.89123300 -2.93493700  H -0.48593200 4.66938200 -1.57620400  C 1.53460700 -1.78319400 -0.31475800  H 0.58787700 -2.30601900 -0.41002200  C 2.33446800 -2.30965500 0.84139000  C 3.43416900 -3.12777500 0.56680400  C 1.94042800 -2.14045100 2.16781300  C 4.12916500 -3.74698000 1.59599600  H 3.74135600 -3.27717000 -0.46174500  C 2.63650700 -2.76142900 3.19696000  H 1.09180300 -1.50186100 2.38376700  C 3.73491800 -3.56424800 2.91605700  H 4.98135700 -4.37657800 1.36418400  H 2.31906500 -2.61256900 4.22331900  H 4.28032600 -4.04538200 3.72046900  C 3.22561100 -0.71695600 -1.62233700  C 3.70002500 -0.60393700 -2.94071300  C 4.00718500 -0.14867800 -0.60202800  C 4.90000100 0.02525900 -3.22551900  H 3.09812300 -1.03607000 -3.73269400  C 5.20629600 0.48788100 -0.89485400  H 3.68133100 -0.22195000 0.42685400  C 5.66502700 0.57912700 -2.20303100  H 5.24174700 0.08692100 -4.25347000  H 5.79145200 0.91335500 -0.08608600  H 6.60395000 1.07398400 -2.42346000  N -1.53597000 0.21809700 2.16662900  Ta -1.12506300 0.40707400 0.33972600  N -2.64074000 1.47985700 0.07398000 | **2Ta + Ph-CCH-TS-HM transfer to C-H**  N -2.56307200 -0.68665400 0.00000000  O -3.74004600 -0.90262100 0.00000000  P -0.57334200 0.26314100 2.50200600  P -0.57334200 0.26314100 -2.50200600  C -0.72894400 2.12373200 2.45949800  C -0.72894400 2.12373200 -2.45949800  H 0.29307700 2.51210300 2.41888800  H 0.29307700 2.51210300 -2.41888800  H -1.19628100 2.51873200 3.36399100  H -1.19628100 2.51873200 -3.36399100  C -1.48433500 2.58815700 1.22158700  C -1.48433500 2.58815700 -1.22158700  H -1.45970000 3.68621600 1.17012300  H -1.45970000 3.68621600 -1.17012300  H -2.53301300 2.28539000 1.26324100  H -2.53301300 2.28539000 -1.26324100  N -0.88889200 2.01384700 0.00000000  C 1.05312400 0.04193500 -3.41029400  C 1.05312400 0.04193500 3.41029400  H 1.74343400 0.53907600 -2.71972600  H 1.74343400 0.53907600 2.71972600  C -1.92136600 -0.34262600 -3.66027900  C -1.92136600 -0.34262600 3.66027900  C -3.25157200 0.36185300 -3.40123900  C -3.25157200 0.36185300 3.40123900  N -0.26284700 -2.14675800 0.00000000  O 0.06125400 -3.29157700 0.00000000  C -2.09299700 -1.85587900 3.52654500  C -2.09299700 -1.85587900 -3.52654500  H -1.17598800 -2.40629600 3.73655700  H -1.17598800 -2.40629600 -3.73655700  H -2.41275700 -2.11645500 2.51590900  H -2.41275700 -2.11645500 -2.51590900  H -2.85889200 -2.20262700 4.22678000  H -2.85889200 -2.20262700 -4.22678000  C 1.46973100 -1.42384200 -3.50938400  C 1.46973100 -1.42384200 3.50938400  H 0.89763700 -1.95162300 -4.27604500  H 0.89763700 -1.95162300 4.27604500  H 1.33927500 -1.95020900 -2.56267400  H 1.33927500 -1.95020900 2.56267400  H 2.52466500 -1.48913600 -3.78943500  H 2.52466500 -1.48913600 3.78943500  C 1.12664700 0.73790600 -4.76657900  C 1.12664700 0.73790600 4.76657900  H 0.87467300 1.79892000 -4.71006900  H 0.87467300 1.79892000 4.71006900  H 0.46315700 0.26963000 -5.49818700  H 0.46315700 0.26963000 5.49818700  H 2.14380000 0.66495500 -5.16309700  H 2.14380000 0.66495500 5.16309700  H 1.13847900 0.37725200 0.00000000  H 0.11928600 2.28892400 0.00000000  C 2.40287700 1.53682300 0.00000000  C 3.51228900 0.59351500 0.00000000  C 3.37546500 -0.79306600 0.00000000  C 4.49402400 -1.61601400 0.00000000  C 5.76967300 -1.06850200 0.00000000  C 4.80681000 1.13838900 0.00000000  C 5.92020100 0.31514400 0.00000000  H 2.37569700 -1.21034200 0.00000000  H 4.36279500 -2.69246100 0.00000000  H 6.64204000 -1.71270200 0.00000000  H 4.92004400 2.21631600 0.00000000  H 6.91169100 0.75499500 0.00000000  H -4.00563000 -0.02499500 -4.09305200  H -4.00563000 -0.02499500 4.09305200  H -3.60963100 0.16815500 -2.38809000  H -3.60963100 0.16815500 2.38809000  H -3.19568900 1.44128600 -3.55627300  H -3.19568900 1.44128600 3.55627300  H -1.58782400 -0.10259000 -4.67591600  H -1.58782400 -0.10259000 4.67591600  Ta -0.71702500 -0.32057800 0.00000000  C 2.03042300 2.71684800 0.00000000  H 2.10439400 3.78182500 0.00000000 |
| **2Ta + PhCCH-TS-HM transfer to Ph-C**  N -2.56307200 -0.68665400 0.00000000  O -3.74004600 -0.90262100 0.00000000  P -0.57334200 0.26314100 2.50200600  P -0.57334200 0.26314100 -2.50200600  C -0.72894400 2.12373200 2.45949800  C -0.72894400 2.12373200 -2.45949800  H 0.29307700 2.51210300 2.41888800  H 0.29307700 2.51210300 -2.41888800  H -1.19628100 2.51873200 3.36399100  H -1.19628100 2.51873200 -3.36399100  C -1.48433500 2.58815700 1.22158700  C -1.48433500 2.58815700 -1.22158700  H -1.45970000 3.68621600 1.17012300  H -1.45970000 3.68621600 -1.17012300  H -2.53301300 2.28539000 1.26324100  H -2.53301300 2.28539000 -1.26324100  N -0.88889200 2.01384700 0.00000000  C 1.05312400 0.04193500 -3.41029400  C 1.05312400 0.04193500 3.41029400  H 1.74343400 0.53907600 -2.71972600  H 1.74343400 0.53907600 2.71972600  C -1.92136600 -0.34262600 -3.66027900  C -1.92136600 -0.34262600 3.66027900  C -3.25157200 0.36185300 -3.40123900  C -3.25157200 0.36185300 3.40123900  N -0.26284700 -2.14675800 0.00000000  O 0.06125400 -3.29157700 0.00000000  C -2.09299700 -1.85587900 3.52654500  C -2.09299700 -1.85587900 -3.52654500  H -1.17598800 -2.40629600 3.73655700  H -1.17598800 -2.40629600 -3.73655700  H -2.41275700 -2.11645500 2.51590900  H -2.41275700 -2.11645500 -2.51590900  H -2.85889200 -2.20262700 4.22678000  H -2.85889200 -2.20262700 -4.22678000  C 1.46973100 -1.42384200 -3.50938400  C 1.46973100 -1.42384200 3.50938400  H 0.89763700 -1.95162300 -4.27604500  H 0.89763700 -1.95162300 4.27604500  H 1.33927500 -1.95020900 -2.56267400  H 1.33927500 -1.95020900 2.56267400  H 2.52466500 -1.48913600 -3.78943500  H 2.52466500 -1.48913600 3.78943500  C 1.12664700 0.73790600 -4.76657900  C 1.12664700 0.73790600 4.76657900  H 0.87467300 1.79892000 -4.71006900  H 0.87467300 1.79892000 4.71006900  H 0.46315700 0.26963000 -5.49818700  H 0.46315700 0.26963000 5.49818700  H 2.14380000 0.66495500 -5.16309700  H 2.14380000 0.66495500 5.16309700  H 1.13847900 0.37725200 0.00000000  H 0.11928600 2.28892400 0.00000000  C 2.40287700 1.53682300 0.00000000  C 3.51228900 0.59351500 0.00000000  C 3.37546500 -0.79306600 0.00000000  C 4.49402400 -1.61601400 0.00000000  C 5.76967300 -1.06850200 0.00000000  C 4.80681000 1.13838900 0.00000000  C 5.92020100 0.31514400 0.00000000  H 2.37569700 -1.21034200 0.00000000  H 4.36279500 -2.69246100 0.00000000  H 6.64204000 -1.71270200 0.00000000  H 4.92004400 2.21631600 0.00000000  H 6.91169100 0.75499500 0.00000000  H -4.00563000 -0.02499500 -4.09305200  H -4.00563000 -0.02499500 4.09305200  H -3.60963100 0.16815500 -2.38809000  H -3.60963100 0.16815500 2.38809000  H -3.19568900 1.44128600 -3.55627300  H -3.19568900 1.44128600 3.55627300  H -1.58782400 -0.10259000 -4.67591600  H -1.58782400 -0.10259000 4.67591600  Ta -0.71702500 -0.32057800 0.00000000  C 2.03042300 2.71684800 0.00000000  H 2.10439400 3.78182500 0.00000000 | **2Ta + PhCCH-interm to Ph-C**  O -0.33162000 3.63669100 1.09125100  P 2.44339000 0.77819100 -0.28835300  P -2.55617100 0.33149100 -0.28552200  C 2.36554300 1.04620800 -2.13398500  C -2.53132500 0.61680200 -2.13009000  H 2.40079600 0.05067400 -2.58717000  H -2.39448900 -0.36798000 -2.58750600  H 3.22663800 1.60546900 -2.50464300  H -3.47761200 1.01909000 -2.49670100  C 1.06885600 1.73313400 -2.53844500  C -1.37476600 1.52016800 -2.53427000  H 1.00637900 1.78305300 -3.63396000  H -1.32441200 1.58362600 -3.62971300  H 1.02560800 2.75563200 -2.15822700  H -1.50919200 2.53329900 -2.15025100  N -0.09707500 0.99617300 -2.00452900  C -3.29773900 -1.38671100 -0.16911900  C 3.47901700 -0.77949900 -0.16415200  H -2.54146100 -1.98291000 -0.69246300  H 2.83551200 -1.50674500 -0.67218200  C -3.82148600 1.52227800 0.42283800  C 3.47846900 2.17853200 0.41096200  C -3.71542500 2.91109400 -0.20338100  C 3.12986500 3.52297900 -0.22389100  O 0.00681900 -0.16133100 3.25331900  H 4.51845800 1.93386800 0.16885400  H -4.80229800 1.09982600 0.17880100  C 3.31615800 2.25245300 1.92930500  C -3.67335900 1.61381900 1.94169400  H 3.57487600 1.31920700 2.42900300  H -3.75948200 0.64586200 2.43498400  H 2.28598200 2.49715100 2.19382500  H -2.70371300 2.03811200 2.20816100  H 3.96523100 3.03700300 2.32916100  H -4.45248400 2.26612300 2.34685400  C -3.38036700 -1.88999800 1.27020600  C 3.66438900 -1.24197400 1.27934200  H -4.20421800 -1.42001400 1.81255400  H 4.39970200 -0.62829600 1.80523100  H -2.45727100 -1.70968900 1.82288200  H 2.73037200 -1.21849100 1.84266300  H -3.56237600 -2.96761600 1.26998500  H 4.03181300 -2.27117000 1.28823700  C -4.63197600 -1.54402000 -0.89381400  C 4.81281100 -0.70715400 -0.90319100  H -4.58184500 -1.24249600 -1.94185000  H 4.69951900 -0.43673300 -1.95474800  H -5.42733600 -0.97070800 -0.41036100  H 5.49756600 0.00679100 -0.43798600  H -4.93469300 -2.59479000 -0.87345500  H 5.29868700 -1.68647800 -0.87159500  H 0.09569100 -1.23696300 -0.71701800  H -0.01254600 0.02619100 -2.35800000  C 0.19137900 -2.19074100 -1.43419600  C 0.32300700 -3.37592800 -0.56065700  C 0.32102900 -3.27036600 0.82939500  C 0.44547700 -4.39344300 1.63911600  C 0.57519800 -5.65166500 1.06830100  C 0.45469900 -4.65237000 -1.12476300  C 0.57883900 -5.77190800 -0.32029700  H 0.22013300 -2.28868700 1.28304600  H 0.44041700 -4.28052200 2.71802200  H 0.67257600 -6.53118300 1.69546400  H 0.45514000 -4.72548200 -2.20662000  H 0.67968100 -6.75087500 -0.77766800  H -4.47200300 3.56453100 0.24045000  H -2.74088600 3.36163800 -0.00423500  H -3.88852700 2.90418500 -1.28135200  H 3.76007100 4.30204300 0.21457500  H 3.30080600 3.53965900 -1.30207800  H 2.09149600 3.79660600 -0.02585300  C 0.17873200 -2.17049000 -2.74464700  H 0.07944500 -1.29559100 -3.39228000  N -0.02290600 0.17676000 2.11740900  Ta -0.06928200 0.69917500 0.31026800  N -0.22861700 2.48545500 0.78906600 |
| **2Ta + PhCCH-TS-HN transfer to C-H**  N -0.00064300 -2.51194500 -0.75432700  O -0.00092500 -3.67239100 -1.04323100  Ta -0.00019400 -0.70236100 -0.31038200  P 2.50800600 -0.56362200 0.27019100  P -2.50836600 -0.56237700 0.27011200  C 2.46186500 -0.72943600 2.12806600  C -2.46243100 -0.72869300 2.12795800  H 2.42382400 0.29107600 2.52086900  H -2.42414300 0.29169500 2.52105700  H 3.36366000 -1.20192800 2.52280800  H -3.36439900 -1.20104200 2.52247500  C 1.21978600 -1.48162200 2.58510500  C -1.22062300 -1.48139100 2.58489000  H 1.16199600 -1.45418500 3.68265500  H -1.16289000 -1.45426100 3.68245100  H 1.25920300 -2.53091300 2.28522400  H -1.26036400 -2.53058800 2.28472600  N -0.00031100 -0.87996600 2.00746900  C -3.42641400 1.05953600 0.05423300  C 3.42705200 1.05767400 0.05392800  H -2.74417900 1.75652600 0.55383400  H 2.74527800 1.75520700 0.55339700  C -3.65030100 -1.91640400 -0.35157600  C 3.64920000 -1.91846100 -0.35109400  C -3.38440500 -3.24888000 0.34571600  C 3.38248800 -3.25062400 0.34647800  N -0.00005700 -0.17723000 -2.11778500  O 0.00002700 0.18097400 -3.25088500  C 3.51197900 -2.07820100 -1.86524200  C -3.51305000 -2.07591100 -1.86574500  H 3.72247900 -1.15743500 -2.40894400  H -3.72246200 -1.15478900 -2.40926300  H 2.50147700 -2.39632000 -2.12764400  H -2.50285600 -2.39506100 -2.12807800  H 4.21127100 -2.84195800 -2.21824300  H -4.21312000 -2.83882500 -2.21902800  C -3.53383800 1.48049700 -1.40976300  C 3.53470300 1.47825800 -1.41016400  H -4.29754800 0.90415200 -1.93713100  H 4.29835000 0.90161900 -1.93730100  H -2.58822000 1.36308800 -1.94105400  H 2.58912200 1.36091600 -1.94153500  H -3.82275200 2.53316700 -1.46833500  H 3.82384100 2.53085300 -1.46897300  C -4.78148100 1.11674000 0.75445100  C 4.78217100 1.11418400 0.75410300  H -4.71921100 0.86412700 1.81485600  H 4.71982900 0.86149700 1.81448700  H -5.50799700 0.44742700 0.28657200  H 5.50835000 0.44457500 0.28612400  H -5.18698800 2.13032200 0.68467800  H 5.18814900 2.12758300 0.68441400  H 0.00031600 1.24260300 0.59423200  H -0.00024100 0.12737200 2.31982400  C 0.00045900 2.20346500 1.42506000  C 0.00093400 3.41227500 0.56826800  C 0.00108500 3.32676600 -0.82141800  C 0.00152200 4.47174000 -1.60890300  C 0.00181800 5.72589400 -1.01363600  C 0.00124200 4.68129200 1.15881100  C 0.00167800 5.82371900 0.37619000  H 0.00085700 2.34467600 -1.28459300  H 0.00162500 4.38042500 -2.68974100  H 0.00215800 6.62186200 -1.62488600  H 0.00112200 4.73907900 2.24192700  H 0.00191100 6.79974200 0.85023900  H -4.06987900 -4.00492100 -0.04813800  H 4.06762100 -4.00712300 -0.04708700  H -2.36850200 -3.59942100 0.15282500  H 2.36642800 -3.60067600 0.15352300  H -3.54321100 -3.20054400 1.42486900  H 3.54116100 -3.20210300 1.42564300  H -4.66832200 -1.59069700 -0.11131900  H 4.66738400 -1.59327800 -0.11082400  C 0.00019800 2.04587600 2.68863900  H -0.00010000 1.68436200 3.69101300 | **2Ta + PhCHCH2-TS-HM transfer**  O -2.26482900 2.47959700 -1.77037400  P 1.47281000 1.83421100 -0.06870500  P -2.40193500 -1.35462100 -0.11525500  C 2.36453500 0.71798000 -1.27166600  C -1.50553200 -2.39653000 -1.38367600  H 2.95795300 0.01495400 -0.68048700  H -0.95579100 -3.16246300 -0.83012600  H 3.06110300 1.27547900 -1.90193200  H -2.20053800 -2.91529500 -2.04775200  C 1.38346300 -0.05327600 -2.14336000  C -0.52793300 -1.56234600 -2.20099400  H 1.93482200 -0.77797200 -2.75640700  H 0.07293100 -2.22453600 -2.83915800  H 0.85447700 0.62064800 -2.82086300  H -1.06346600 -0.87202200 -2.85639500  N 0.35941400 -0.75475700 -1.33618400  C -2.64881000 -2.59511100 1.27622800  C 2.66315900 1.87057800 1.38311300  H -1.63202000 -2.98649800 1.38988900  H 2.80415400 0.79849000 1.55371500  C -4.10037200 -1.04401900 -0.85015900  C 1.52795800 3.54245200 -0.84399500  C -4.01276500 -0.55552300 -2.29438700  C 1.11128600 3.51402100 -2.31306200  O -2.00104000 2.04633000 2.62081200  H 2.57183300 3.86879600 -0.78538400  H -4.61658800 -2.00984900 -0.84038800  C 0.64908100 4.51405800 -0.05758800  C -4.87650600 -0.04661500 0.00840000  H 0.96080600 4.61578300 0.98234100  H -5.02876700 -0.39982800 1.02897600  H -0.39185100 4.18532400 -0.06471200  H -4.35170700 0.90941100 0.05925900  H 0.69499500 5.50627300 -0.51608200  H -5.86237700 0.12955700 -0.43160800  C -3.03219400 -1.92675900 2.59443100  C 2.03579200 2.45737500 2.64520000  H -4.06433200 -1.57107600 2.58408100  H 1.93075100 3.54221200 2.58030400  H -2.38766900 -1.07491800 2.81718800  H 1.04928600 2.03400900 2.83954800  H -2.94635400 -2.64689000 3.41347300  H 2.67558900 2.24670800 3.50732800  C -3.57181100 -3.76213100 0.93692900  C 4.02301300 2.49099400 1.07699700  H -3.30394900 -4.25117400 -0.00280900  H 4.48731000 2.06380600 0.18533700  H -4.61447500 -3.44318100 0.86834300  H 3.95051700 3.57259500 0.93982900  H -3.51847300 -4.51803900 1.72602100  H 4.70507400 2.31964100 1.91517000  H 0.32215000 -0.64257300 1.31483300  H 0.85123500 -1.40945800 -0.70627800  C 1.06288100 -1.90936700 1.83092100  H -5.02410600 -0.40502700 -2.68354600  H -3.49020300 0.39959300 -2.36209400  H -3.52046600 -1.27482300 -2.95243000  H 1.16303200 4.52797300 -2.72067500  H 1.76629600 2.88906000 -2.92364200  H 0.08277900 3.16842800 -2.42873800  H 0.17964300 -2.22391500 2.37255900  C 1.59897000 -2.76886700 0.88454200  H 0.96210800 -3.55998100 0.49579300  N -1.54048500 1.51363100 1.66522500  N -1.68832000 1.74218700 -1.02441000  Ta -0.78572900 0.62971400 0.18584200  H 1.72450300 -1.29975600 2.43769000  C 2.95054600 -2.75918500 0.37262200  C 3.30897500 -3.62274600 -0.68422000  C 3.97748700 -1.94103300 0.88703000  C 4.59408400 -3.65760200 -1.19757500  H 2.55152900 -4.28329900 -1.09666600  C 5.26270300 -1.97635200 0.36886900  H 3.77234500 -1.29137600 1.73062300  C 5.58644000 -2.82813600 -0.68245200  H 4.82658500 -4.34038400 -2.00854600  H 6.02695500 -1.33787500 0.80064200  H 6.59342100 -2.85549000 -1.08209700 |
| **2Ta + Ph-CHCH2-interm**  O -2.37387500 2.57242900 -1.51351900  P 1.46979600 1.83037500 -0.10258300  P -2.43872000 -1.35484900 -0.11880400  C 2.36119900 0.68483700 -1.26976200  C -1.53442000 -2.41698100 -1.35727500  H 2.95340300 -0.00208000 -0.65764600  H -1.00291500 -3.18090500 -0.78464100  H 3.05894900 1.22356400 -1.91473000  H -2.22238400 -2.93471200 -2.02942800  C 1.37915300 -0.11216500 -2.11535900  C -0.53013500 -1.60140200 -2.16042500  H 1.93157200 -0.87128000 -2.68323600  H 0.09137200 -2.28315400 -2.75626500  H 0.87019900 0.53396700 -2.83433000  H -1.04261900 -0.93345300 -2.85642900  N 0.34006400 -0.77587300 -1.28972800  C -2.74175000 -2.57619600 1.27746100  C 2.66193800 1.93643000 1.34281300  H -1.72727500 -2.95262400 1.44966300  H 2.75680500 0.87818100 1.60714200  C -4.11008500 -0.99802000 -0.89166400  C 1.47411300 3.51362600 -0.93149800  C -3.97369600 -0.52754200 -2.33830000  C 1.06135500 3.42308300 -2.39918700  O -1.78777100 1.81580500 2.82682700  H 2.51043800 3.86523200 -0.88363000  H -4.65064900 -1.95055400 -0.88594200  C 0.57260400 4.49427000 -0.18251500  C -4.88283900 0.02651400 -0.06252500  H 0.86180900 4.62133800 0.86060700  H -5.05568800 -0.30533000 0.96156900  H -0.46617000 4.16134400 -0.20547300  H -4.34760400 0.97672800 -0.02261100  H 0.62270000 5.47603200 -0.66256400  H -5.85918600 0.20751200 -0.52127100  C -3.20698000 -1.90237300 2.56638000  C 2.07512200 2.66438600 2.55022000  H -4.24900900 -1.58300300 2.50232800  H 2.06044200 3.74586300 2.40065300  H -2.60300300 -1.02771800 2.81197300  H 1.05783700 2.33889900 2.77267500  H -3.13720000 -2.60983500 3.39759300  H 2.69417500 2.47088400 3.43091200  C -3.62914100 -3.75928700 0.90003400  C 4.04766300 2.46122200 0.97815400  H -3.29990700 -4.25732700 -0.01482700  H 4.49513100 1.91661700 0.14444600  H -4.66980500 -3.45473000 0.76649300  H 4.02257700 3.52337600 0.72268400  H -3.61274800 -4.50352500 1.70155700  H 4.71859900 2.35353200 1.83544100  H 0.48021100 -0.82485500 1.36883800  H 0.86439800 -1.47878000 -0.66614000  C 1.02072400 -1.82572800 1.70277800  H -4.96993400 -0.34152800 -2.74987700  H -3.41457300 0.40701000 -2.40291700  H -3.49494700 -1.27099400 -2.97876100  H 1.07914600 4.42412800 -2.83973700  H 1.73651500 2.79933000 -2.98805700  H 0.04429000 3.04071300 -2.50310500  H 0.23334400 -2.32049100 2.27209600  C 1.58237700 -2.63324800 0.62785400  H 0.99455100 -3.48616300 0.29825400  N -1.41765400 1.37169300 1.78965900  N -1.74955100 1.78950900 -0.85945000  C 2.97109500 -2.68242800 0.28594900  C 3.43490600 -3.60188700 -0.69128600  C 3.96419100 -1.85083400 0.85967300  C 4.76102100 -3.66967800 -1.06808300  H 2.71580200 -4.27619600 -1.14860500  C 5.29541400 -1.92568200 0.47564600  H 3.69294000 -1.15729800 1.64851700  C 5.71521300 -2.82545100 -0.49691200  H 5.06299800 -4.39467100 -1.81797600  H 6.02002000 -1.27408800 0.95513800  H 6.75615000 -2.88124500 -0.79253400  H 1.74927000 -1.43429900 2.41604100  Ta -0.78503100 0.60709200 0.19170000 | **2Ta + Ph-CHCH2-TS-HN transfer**  O -2.42696000 2.58030200 -1.44610600  P 1.45333600 1.84160700 -0.11578500  P -2.44311400 -1.37027300 -0.11250300  C 2.35672000 0.68733600 -1.26091700  C -1.51085500 -2.45475000 -1.30575900  H 2.96001900 0.02283400 -0.63583500  H -0.98784400 -3.20072500 -0.70305000  H 3.04481500 1.22318500 -1.91869500  H -2.18289000 -2.99286600 -1.97822300  C 1.38262100 -0.14408100 -2.08351800  C -0.49335400 -1.65148400 -2.10611700  H 1.94704900 -0.92437100 -2.61083400  H 0.15759300 -2.35024200 -2.65005200  H 0.89080500 0.47177200 -2.84168600  H -0.99524200 -1.03040100 -2.85305100  N 0.33808200 -0.77938300 -1.24626700  C -2.77744100 -2.55659800 1.30646000  C 2.63778000 1.98091300 1.33329900  H -1.76556300 -2.92179200 1.51507300  H 2.74728200 0.92665700 1.60887100  C -4.09540200 -1.02896000 -0.93118600  C 1.44216300 3.50952800 -0.97364800  C -3.91997100 -0.57172500 -2.37797900  C 1.00524300 3.38739800 -2.43216000  O -1.75391300 1.75965100 2.85935100  H 2.47949200 3.86092300 -0.95098300  H -4.62987300 -1.98506000 -0.93238000  C 0.55456500 4.50657800 -0.23019200  C -4.89837300 -0.00236900 -0.13419100  H 0.86798700 4.66220900 0.80199200  H -5.10328600 -0.32893700 0.88558700  H -0.48355900 4.17100600 -0.22039700  H -4.36937900 0.95066800 -0.08326600  H 0.59024400 5.47552400 -0.73680900  H -5.86009200 0.17146100 -0.62548200  C -3.28159400 -1.85637900 2.56639500  C 2.03938700 2.71206300 2.53311800  H -4.32513500 -1.55090000 2.46882200  H 2.01099800 3.79183300 2.37406100  H -2.69342200 -0.96963800 2.80609400  H 1.02614500 2.37596900 2.75750600  H -3.22521700 -2.54286900 3.41602400  H 2.65957100 2.53442200 3.41637700  C -3.64712400 -3.75403400 0.93310300  C 4.01657500 2.52169100 0.96544100  H -3.28833800 -4.27243400 0.04102700  H 4.47257500 1.97581000 0.13719500  H -4.68484800 -3.45862800 0.76136000  H 3.97607800 3.58084600 0.69963800  H -3.65089200 -4.47793100 1.75322300  H 4.68803400 2.43204100 1.82440300  H 0.52337300 -0.82597300 1.42252500  H 0.92038700 -1.52781800 -0.58184900  C 1.05262800 -1.82689100 1.67425700  H -4.90441500 -0.38952700 -2.81855800  H -3.35885800 0.36215800 -2.43618100  H -3.42289200 -1.32075300 -2.99738700  H 1.01401100 4.37870700 -2.89443800  H 1.67126800 2.75120700 -3.01787500  H -0.01236100 3.00060500 -2.51133100  H 0.28320300 -2.37974600 2.21496800  C 1.59723800 -2.54338500 0.50467600  H 1.05943600 -3.45114900 0.23517000  N -1.40152600 1.33502900 1.80828900  N -1.78947900 1.79920800 -0.80491900  C 3.01621000 -2.62833700 0.23899200  C 3.50265600 -3.54611500 -0.72287200  C 3.99287100 -1.82157900 0.86286600  C 4.84329800 -3.63597100 -1.04339000  H 2.79180100 -4.20246600 -1.21765400  C 5.34011700 -1.91515900 0.53748300  H 3.69872500 -1.12551100 1.64130800  C 5.78490500 -2.81451100 -0.42241900  H 5.16511000 -4.36033600 -1.78545100  H 6.05372900 -1.27924700 1.05288700  H 6.83681200 -2.88677600 -0.67269700  H 1.79711000 -1.50740300 2.40747900  Ta -0.79137800 0.59658900 0.18713400 |
| **2Ta + PhCHO-TS-HM transfer**  O -2.12389500 -3.15209300 -0.17313600  P 1.67974800 -1.62814500 0.23007000  P -2.60840800 0.99371300 0.21759700  C 1.84302400 -1.21786300 2.04485700  C -2.49809400 1.15456500 2.07614200  H 2.36242800 -0.25618400 2.09479400  H -1.97787100 2.09497800 2.27579300  H 2.45708000 -1.94771100 2.57759800  H -3.48589200 1.21114400 2.53841700  C 0.47928600 -1.09418800 2.71227900  C -1.69644700 0.00869700 2.67985900  H 0.61052100 -0.78074100 3.75719800  H -1.54625400 0.19684000 3.75195300  H -0.03258700 -2.05894100 2.72325800  H -2.23048200 -0.93952200 2.58241400  N -0.38938700 -0.13374000 2.00498500  C -2.63577700 2.79780900 -0.30884700  C 3.26485700 -0.92010000 -0.47512800  H -1.77290500 3.18627000 0.24263700  H 3.16359300 0.13425700 -0.19890600  C -4.32820800 0.32265400 -0.12006200  C 1.83916500 -3.49542400 0.10543400  C -4.65511800 -0.88001200 0.76233400  C 1.04428000 -4.22161400 1.18857300  O -0.59801600 -0.56361800 -3.38741200  H 2.90215500 -3.71960400 0.24549800  H -5.02171800 1.13323100 0.12776900  C 1.40131300 -3.97220900 -1.27987400  C -4.47977100 -0.03696100 -1.59716100  H 1.96382400 -3.50152900 -2.08621800  H -4.32896100 0.81942700 -2.25557100  H 0.34355500 -3.75964700 -1.44284900  H -3.76166900 -0.80826800 -1.88270000  H 1.54653700 -5.05385300 -1.35886800  H -5.48635100 -0.42371800 -1.78171400  C -2.35746800 2.97629700 -1.79950200  C 3.30294000 -0.99135300 -1.99990600  H -3.21287000 2.68053300 -2.41032900  H 3.50371100 -2.00558700 -2.35272700  H -1.49775400 2.38590600 -2.12160900  H 2.36545200 -0.65305200 -2.44421700  H -2.15405900 4.02926700 -2.01632300  H 4.10699500 -0.35267400 -2.37561400  C -3.87007000 3.57572700 0.13886600  C 4.54411000 -1.46948800 0.14935700  H -4.07445100 3.45874100 1.20574200  H 4.54603600 -1.39439900 1.23895800  H -4.76167700 3.27071400 -0.41421000  H 4.71113000 -2.51560700 -0.11990200  H -3.72371100 4.64331400 -0.05076700  H 5.40399400 -0.90158000 -0.21739600  H 0.58759300 1.09429600 -0.25033200  H 0.06376900 0.79376200 2.04394800  C 0.97816600 2.64049400 0.62546700  C 2.41834700 2.71501100 0.24325700  C 2.78594700 2.93846600 -1.08299300  C 4.12138400 3.08794900 -1.42408900  C 5.10241100 3.02159100 -0.43859800  C 3.40301100 2.66031800 1.22783800  C 4.74083400 2.80958300 0.88711700  H 2.01686700 2.97768000 -1.84815400  H 4.40112500 3.25841500 -2.45781800  H 6.14678900 3.14370600 -0.70416800  H 3.09651500 2.52344800 2.25879800  H 5.50348500 2.77348700 1.65751100  H -5.67286200 -1.21777600 0.54478600  H -3.98276300 -1.71607700 0.56576700  H -4.61733600 -0.64172400 1.82739500  H 1.17426800 -5.30116600 1.06738400  H 1.37707500 -3.96884800 2.19743500  H -0.02392000 -4.01303300 1.10318000  O 0.61403700 2.51435100 1.80396300  H 0.30693400 3.08286300 -0.12598500  N -0.59218400 -0.55424900 -2.20059200  N -1.54053100 -2.10804000 -0.22425900  Ta -0.56625300 -0.50302900 -0.31954100 | **2Ta + PhCHO-interm**  O -2.12586800 -3.13580700 -0.39654200  P 1.70426900 -1.60941700 0.24306500  P -2.62007100 0.99817200 0.24160700  C 1.87867500 -1.16235600 2.04254100  C -2.49661700 1.15730200 2.09359400  H 2.39473500 -0.19787800 2.06416100  H -1.98386300 2.10349900 2.28181800  H 2.49767500 -1.88080100 2.58506800  H -3.48055300 1.19526100 2.56569000  C 0.51849500 -1.01653100 2.71304400  C -1.66210700 0.02278600 2.67718600  H 0.66660100 -0.61366300 3.72482800  H -1.46634100 0.24046100 3.73639900  H 0.03960000 -1.99403200 2.82669900  H -2.20966600 -0.92460500 2.63821300  N -0.38101200 -0.12720100 1.95699200  C -2.63111800 2.79364900 -0.30517800  C 3.27889500 -0.91667100 -0.49929200  H -1.75771600 3.17841900 0.23242500  H 3.18854500 0.14587700 -0.25020300  C -4.32655500 0.31060200 -0.11628300  C 1.83812600 -3.47726900 0.12827200  C -4.65015800 -0.89140600 0.76862600  C 1.02103200 -4.17741000 1.21127900  O -0.47405800 -0.35902200 -3.35469200  H 2.89694400 -3.70811800 0.28745000  H -5.02888400 1.11621100 0.12313400  C 1.41889300 -3.96698700 -1.25800000  C -4.46242200 -0.05525000 -1.59349500  H 1.98768000 -3.50030400 -2.06181900  H -4.31302500 0.79928700 -2.25438100  H 0.36155700 -3.76707900 -1.43664800  H -3.73747000 -0.82332400 -1.87022800  H 1.57345500 -5.04804200 -1.32507900  H -5.46456700 -0.45003700 -1.78432300  C -2.37473000 2.96028900 -1.80073200  C 3.31931800 -1.02925600 -2.02161800  H -3.24235700 2.67008100 -2.39663900  H 3.54966600 -2.04681100 -2.34454700  H -1.52547000 2.36235400 -2.13584900  H 2.37636600 -0.73027600 -2.48245200  H -2.16292100 4.00962900 -2.02482100  H 4.10655400 -0.37902500 -2.41201600  C -3.85679600 3.57789400 0.15513600  C 4.55837500 -1.44917300 0.14023400  H -4.04129800 3.47350000 1.22669700  H 4.56048500 -1.33949700 1.22640100  H -4.75836100 3.26793500 -0.37902900  H 4.72495600 -2.50272000 -0.09865700  H -3.71080600 4.64254700 -0.04940900  H 5.41628000 -0.89084800 -0.24449100  H 0.73774200 1.25903000 -0.12651000  H 0.08104000 0.91449100 1.94551500  C 0.91319900 2.28006900 0.46097600  C 2.37627900 2.58675100 0.17086300  C 2.82313600 2.79624800 -1.13326000  C 4.15585900 3.09082300 -1.38436800  C 5.05969900 3.18309200 -0.32963300  C 3.27974500 2.69671100 1.22168200  C 4.61676900 2.98969600 0.97271800  H 2.12059700 2.72425700 -1.95942100  H 4.49198300 3.25295300 -2.40304700  H 6.10085300 3.41655400 -0.52404100  H 2.90107100 2.56854000 2.22951400  H 5.31348300 3.07780600 1.79995200  H -5.66736400 -1.23162200 0.55347800  H -3.97708000 -1.72682300 0.57078700  H -4.60766700 -0.65135500 1.83267700  H 1.12888000 -5.26038600 1.10129600  H 1.35130300 -3.91912700 2.21912700  H -0.04167700 -3.94547000 1.11746200  O 0.56513700 2.20630400 1.74170300  H 0.30661600 2.97470300 -0.15243300  N -0.52494500 -0.43561900 -2.17301500  N -1.53053200 -2.10110000 -0.36955500  Ta -0.57812000 -0.51450500 -0.28977100 |
| **2Ta +PhCHO -TS-HN transfer**  N -1.55053200 -2.05756000 -0.35320000  O -2.17479100 -3.07654200 -0.39016600  P 1.67746100 -1.70680200 0.26823000  P -2.56341900 1.05333400 0.24955800  C 1.87766000 -1.23671600 2.06043700  C -2.41835000 1.20648600 2.10084700  H 2.41814500 -0.28496700 2.05773900  H -1.86660500 2.13254200 2.27116500  H 2.48931100 -1.95802500 2.60730600  H -3.39684200 1.28980800 2.57808900  C 0.53061000 -1.05222700 2.74847700  C -1.63746500 0.04048200 2.69495900  H 0.69670100 -0.63636500 3.75218300  H -1.43882100 0.25180200 3.75512200  H 0.03515900 -2.01788400 2.88304100  H -2.22215400 -0.88362500 2.65515700  N -0.36241900 -0.17286700 1.98406900  C -2.54237300 2.84649400 -0.29243500  C 3.29101500 -1.09968400 -0.47080500  H -1.57512100 3.14899100 0.12593000  H 3.25286800 -0.03057500 -0.23410500  C -4.28950500 0.39709500 -0.08220400  C 1.73001200 -3.58060200 0.19332800  C -4.65226100 -0.76169200 0.84455000  C 0.88810700 -4.22704200 1.29101200  O -0.51426800 -0.43478900 -3.36544700  H 2.77855400 -3.85317800 0.35443500  H -4.97016500 1.23113300 0.12117600  C 1.28602700 -4.07774200 -1.18262100  C -4.43556300 -0.02500200 -1.54394200  H 1.87155000 -3.64986100 -1.99609200  H -4.22102600 0.78528800 -2.24091100  H 0.23718300 -3.83780600 -1.36157100  H -3.76190500 -0.85177700 -1.77623100  H 1.39595000 -5.16521600 -1.22985900  H -5.45987500 -0.36155700 -1.72978300  C -2.49995700 3.01329000 -1.80989700  C 3.32843000 -1.23275900 -1.99176000  H -3.47689000 2.83419000 -2.26549500  H 3.50693200 -2.26493600 -2.30105000  H -1.78104500 2.33979500 -2.28004400  H 2.40147600 -0.89360100 -2.45764400  H -2.21264300 4.03904400 -2.05817400  H 4.14814000 -0.62913300 -2.39038000  C -3.64289500 3.69930000 0.33258300  C 4.54287500 -1.68577100 0.17664600  H -3.66981700 3.61756500 1.42111400  H 4.55389900 -1.55900900 1.26098800  H -4.63173200 3.43885700 -0.05446700  H 4.65512100 -2.75011300 -0.04504300  H -3.47067300 4.75236900 0.09072500  H 5.42793500 -1.17904800 -0.21831100  H 1.08837000 0.99805500 -0.52622600  H 0.07405400 0.80480000 1.81131700  C 0.97228400 2.07637700 -0.10006800  C 2.41365000 2.57114800 -0.05495800  C 3.18150700 2.67540200 -1.21490900  C 4.48889800 3.13833600 -1.15790400  C 5.04525600 3.50699300 0.06375800  C 2.97239400 2.94827200 1.16058700  C 4.28199100 3.41410300 1.22059400  H 2.74789900 2.39754500 -2.17218200  H 5.07477200 3.21995600 -2.06748500  H 6.06498500 3.87366400 0.10915900  H 2.34459600 2.88886600 2.04274400  H 4.70595800 3.71325500 2.17374500  H -5.66948200 -1.09717200 0.62161100  H -3.98838700 -1.61475000 0.69390400  H -4.62901000 -0.48056400 1.89914900  H 0.94569100 -5.31506100 1.19404000  H 1.23766900 -3.97244000 2.29334200  H -0.16379200 -3.94916000 1.20072800  O 0.29044200 2.13288000 1.05915400  H 0.47616700 2.60163300 -0.94034200  N -0.54018400 -0.46974800 -2.18225000  Ta -0.55680700 -0.50301000 -0.29974800 | **2Ta + Ph-COCH3-TS**  O 2.06144200 3.07248000 -0.56507700  P -1.66674000 1.66306700 0.27217500  P 2.72552600 -0.85405000 0.17085400  C -1.70034100 1.42193400 2.12042400  C 2.59333900 -1.06622300 2.02179300  H -2.22465600 0.47710300 2.29199600  H 2.07228200 -2.01269300 2.19166300  H -2.25482800 2.21267800 2.63058400  H 3.57344400 -1.14624300 2.49787500  C -0.29352500 1.31002100 2.69297800  C 1.79597800 0.06695800 2.65708100  H -0.35770500 1.09435700 3.76829600  H 1.66481400 -0.14037600 3.72794100  H 0.25354600 2.24854000 2.57879600  H 2.33858900 1.01119900 2.57280400  N 0.47800400 0.24590400 2.01687000  C 3.00870600 -2.61382300 -0.41992500  C -3.34935800 1.02783700 -0.25045100  H 2.08825100 -3.09952800 -0.08934400  H -3.27621900 -0.03191700 0.00761500  C 4.36326400 0.02081600 -0.12692700  C -1.74192500 3.52016900 -0.01847200  C 4.62785800 1.14277800 0.87468100  C -0.89548500 4.31470200 0.97340300  O 0.33817100 0.17812500 -3.38138500  H -2.79231800 3.79341200 0.13061700  H 5.13331500 -0.74650400 0.00740300  C -1.33769900 3.86366300 -1.45287400  C 4.43832700 0.55792300 -1.55679000  H -1.91656800 3.31840800 -2.19780100  H 4.27315000 -0.21359800 -2.30852400  H -0.28375900 3.64192700 -1.62112800  H 3.69833000 1.34274600 -1.71472400  H -1.49018900 4.93310800 -1.62836100  H 5.42928800 0.98741300 -1.73277600  C 3.05073100 -2.71230500 -1.94389200  C -3.55400400 1.12357500 -1.76093000  H 4.00048200 -2.35162400 -2.34458100  H -3.74534600 2.15189600 -2.07699300  H 2.24475400 -2.14359900 -2.41130900  H -2.69091200 0.74830300 -2.31402300  H 2.95043500 -3.75812500 -2.24865100  H -4.42342200 0.52730600 -2.04932200  C 4.19103000 -3.33107700 0.22585500  C -4.52489300 1.63058500 0.51373800  H 4.15435300 -3.30428700 1.31703200  H -4.42477900 1.51665500 1.59485900  H 5.14698300 -2.90770000 -0.09182400  H -4.65553200 2.69342100 0.29355600  H 4.19254300 -4.38319300 -0.07501500  H -5.44861800 1.12498500 0.21760700  H -0.44979100 -1.31460700 -0.01816200  H -0.06185800 -0.63035300 2.15408900  C -1.25801200 -2.45447000 1.03440500  C -2.57889600 -2.48643900 0.29989400  C -2.67780100 -2.65533400 -1.08094000  C -3.91835500 -2.79183600 -1.68544500  C -5.07843200 -2.76986000 -0.91637800  C -3.74450800 -2.46197800 1.06389800  C -4.98831600 -2.60351300 0.45936700  H -1.77853500 -2.64015800 -1.68644600  H -3.98286100 -2.90929300 -2.76165700  H -6.04746900 -2.88147500 -1.39048000  H -3.65512000 -2.33930200 2.13715100  H -5.88778900 -2.58929100 1.06557500  H 5.59900700 1.59633600 0.65520400  H 3.87826400 1.93158800 0.79516400  H 4.66502600 0.78736400 1.90641200  H -1.00153600 5.38278100 0.76092100  H -1.20262000 4.16024000 2.00971500  H 0.16365200 4.07064300 0.87524900  O -1.20973400 -1.96397100 2.18275200  N 0.42003700 0.28813700 -2.20311600  C -0.36041400 -3.63415500 0.70698700  H -0.86809900 -4.53395600 1.07309700  H -0.18089200 -3.75611800 -0.36000300  H 0.58171400 -3.54181500 1.24417900  Ta 0.52985400 0.41989900 -0.32814100  N 1.46130300 2.04063200 -0.46441900 |

**Table S6.** Computed Energetic Data For All Optimized Structures

|  |  |
| --- | --- |
| **H2**  HF= -1.178636  ZPE= 0.010066  NImag= 0  Htot = -1.165265  Gtot = -1.180063 | **Ph-C≡N**  HF=-324.462850  ZPE= 0.099090  NImag=0  Htot = -324.356685  Gtot = -324.394045 |
| **Ph-CH=NH**  HF= -325.672096  ZPE= 0.122298  NImag=0  Htot = -325.542367  Gtot = -325.580493 | **Ph-CH2NH2**  HF= -326.893009  ZPE= 0.145861  NImag=0  Htot = -326.738985  Gtot = -326.778961 |
| **Ph-CH=NCH2-Ph**  HF= -596.010269  ZPE= 0.230904  NImag=0  Htot = -595.765983  Gtot = -595.821242 | **Ph-CH2NHCH2-Ph**  HF= -597.227352  ZPE= 0.255195  NImag=0  Htot = -596.958369  Gtot = -597.014546 |
| **Ph-CH=N-Ph**  HF= -556.704384  ZPE= 0.202432  NImag=0  Htot = -556.489963  Gtot = -556.540191 | **Ph-CH2NH-Ph**  HF= -557.923968  ZPE= 0.226160  NImag=0  Htot = -557.685119  Gtot = -557.737696 |
| **Ph-C≡CH**  HF= -308.368341  ZPE= 0.109270  NImag=0  Htot = -308.251652  Gtot = -308.289517 | **Ph-CH=CH2**  HF= -309.625103  ZPE= 0.132940  NImag=0  Htot = -309.484357  Gtot = -309.523956 |
| **Ph-CH2CH3**  HF= -310.859083  ZPE= 0.156438  NImag=0  Htot = -310.694324  Gtot = -310.735616 | **Ph-CH=O**  HF=-345.550677  ZPE= 0.109586  NImag=0  Htot = -345.433783  Gtot = -345.471689 |
| **Ph-CH2OH**  HF= -346.757584  ZPE= 0.132478  NImag=0  Htot = -346.617721  Gtot = -346.655623 | **Ph-CO-CH3**  HF= -384.871415  ZPE= 0.137519  NImag=0  Htot = -384.725019  Gtot = -384.766910 |
| **Ph-CH(OH)-CH3**  HF= -386.077179  ZPE= 0.161141  NImag=0  Htot = -385.906715  Gtot = -385.949373 |  |
| **1V-cs**  HF = -1700.085762  ZPE = 0.516447  NImag = 0  Htot = -1699.535961  Gtot = -1699.632776 | **1V-C1**  HF = -1700.089278  ZPE = 0.516666  NImag = 0  Htot = -1699.539447  Gtot = -1699.635307 |
| **2V-cs**  HF = -1701.279264  ZPE = 0.536996  NImag= 0  Htot = -1700.708847  Gtot = -1700.804507 | **2V-C1**  HF= -1701.276739  ZPE= 0.537201  NImag= 0  Htot = -1700.706168  Gtot = -1700.801743 |
| **1Nb-cs**  HF = -1685.090677  ZPE = 0.514782  NImag = 0  Htot = -1684.541982  Gtot = -1684.641074 | **1Nb-C1**  HF = -1685.093923  ZPE = 0.514853  NImag = 0  Htot = -1684.545277  Gtot = -1684.643202 |
| **2Nb-cs**  HF = -1686.282799  ZPE = 0.534755  NImag = 0  Htot = -1685.713896  Gtot = -1685.811691 | **2Nb-C1**  HF = -1686.279956  ZPE = 0.535017  NImag = 0  Htot = -1685.710806  Gtot = -1685.809118 |
| **1Ta-cs**  HF = -1686.603194  ZPE = 0.514967  NImag = 0  Htot = -1686.054331  Gtot = -1686.153510 | **1Ta-C1**  HF = -1686.606382  ZPE = 0.515034  NImag = 0  Htot = -1686.057576  Gtot = -1686.155578 |
| **2Ta-cs**  HF = -1687.796001  ZPE = 0.535141  NImag = 0  Htot = -1687.226790  Gtot = -1687.324692 | **2Ta-C1**  HF = -1687.792963  ZPE = 0.535413  NImag = 0  Htot = -1687.223511  Gtot = -1687.321737 |
| **1V + H2-TS**  HF = -1701.244566  ZPE = 0.531233  NImag = -855.8573  Htot = -1700.679877  Gtot = -1700.776326 | **2V + PhCN-TS-HM transfer**  HF = -2025.73496  ZPE = 0.636632  NImag = -280.4584  Htot = -2025.057798  Gtot = -2025.170066 |
| **2V + PhCN-interm**  HF = -2025.740568  ZPE = 0.638106  NImag = 0  Htot = -2025.061776  Gtot = -2025.174014 | **2V + PhCN-TS-HN transfer**  HF = -2025.739722  ZPE = 0.635141  NImag = -777.0578  Htot = -2025.064161  Gtot =-2025.17589 |
| **2V + Ph-CHNH-TS**  HF = -2026.935107  ZPE = 0.659645  NImag = -513.1119  Htot = -2026.234698  Gtot = -2026.347099 | **2V + Ph-CHNCH2Ph-TS**  HF = -2297.257658  ZPE = 0.768303  NImag = -614.7925  Htot = -2296.442386  Gtot = -2296.571881 |
| **2V + Ph-CHNPh-TS**  HF = -2257.957104  ZPE =0.740458  NImag = -534.5861  Htot = -2257.17115  Gtot = -2257.29451 | **2V + Ph-CCH-TS-HM transfer to C-H**  HF = -2009.63236  ZPE = 0.645696  NImag = -527.4138  Htot = -2008.94523  Gtot = -2009.061794 |
| **2V + PhCCH-TS-HM transfer to Ph-C**  HF = -2009.622934  ZPE = 0.645469  NImag = -581.5385  Htot = -2008.936397  Gtot = -2009.049229 | **2V + PhCCH-interm to Ph-C**  HF = -2009.630268  ZPE =0.6495  NImag = 0  Htot = -2008.93961  Gtot = -2009.053103 |
| **2V + PhCCH-TS-HN transfer to C-H**  HF = -2009.626039  ZPE =0.647494  NImag = -611.5415  Htot = -2008.937755  Gtot = -2009.049824 | **2V + PhCHCH2-TS-HM transfer**  HF = -2010.885728  ZPE = 0.669958  NImag = -624.8225  Htot = -2010.174458  Gtot = -2010.288922 |
| **2V + Ph-CHCH2-interm**  HF = -2010.894244  ZPE = 0.672813  NImag = 0  Htot = -2010.179794  Gtot = -2010.294096 | **2V + Ph-CHCH2-TS-HN transfer**  HF = -2010.89224  ZPE = 0.669334  NImag = -837.653  Htot = -2010.18161  Gtot = -2010.295234 |
| **2V + PhCHO-TS-HM transfer**  HF = -2046.828257  ZPE = 0.647695  NImag = -213.7581  Htot = -2046.139913  Gtot = -2046.252242 | **2V + PhCHO-interm**  HF = -2046.841038  ZPE = 0.648637  NImag = 0  Htot = -2046.151267  Gtot = -2046.265353 |
| **2V +PhCHO-TS-HN transfer**  HF = -2046.840369  ZPE = 0.648637  NImag = -477.8354  Htot = -2046.152846  Gtot = -2046.266838 | **2V + Ph-COCH3-TS**  HF = -2086.134719  ZPE = 0.675815  NImag = -422.1179  Htot = -2085.41696  Gtot = -2085.531519 |
| **1Nb + H2-TS**  HF = -1686.251018  ZPE = 0.528872  NImag = -917.6823  Htot = -1685.6879  Gtot = -1685.787172 | **2Nb+PhCN-TS-HM transfer**  HF = -2010.740698  ZPE = 0.634426  NImag = -251.5601  Htot = -2010.064879  Gtot = -2010.180566 |
| **2Nb + PhCN-interm**  HF = -2010.746267  ZPE = 0.635931  NImag = 0  Htot = -2010.068764  Gtot = -2010.184702 | **2Nb + PhCN-TS-HN transfer**  HF = -2010.745444  ZPE = 0.632959  NImag = -732.7051  Htot = -2010.071207  Gtot = -2010.18661 |
| **2Nb + Ph-CHNH-TS**  HF = -2011.941572  ZPE = 0.657459  NImag = -484.9541  Htot = -2011.242515  Gtot = -2011.358226 | **2Nb + Ph-CHNCH2Ph-TS**  HF = -2282.267928  ZPE = 0.766159  NImag = -464.1694  Htot = -2281.454008  Gtot = -2281.585206 |
| **2Nb + Ph-CHNPh-TS**  HF = -2242.965079  ZPE = 0.738177  NImag = -479.4662  Htot = -2242.180505  Gtot = -2242.308145 | **2Nb + Ph-CCH-TS-HM transfer to C-H**  HF = -1994.635466  ZPE = 0.643611  NImag = -548.6001  Htot = -1993.949652  Gtot = -1994.068914 |
| **2Nb + PhCCH-TS-HM transfer to Ph-C**  HF = -1994.62727  ZPE = 0.643139  NImag = -559.5328  Htot = -1993.942115  Gtot = -1994.058888 | **2Nb + PhCCH-interm to Ph-C**  HF = -1994.63591  ZPE = 0.647674  NImag = 0  Htot = -1993.947219  Gtot = -1994.060283 |
| **2Nb + PhCCH-TS-HN transfer to C-H**  HF = -1994.630144  ZPE = 0.645367  NImag = -648.5162  Htot = -1993.943129  Gtot = -1994.058698 | **2Nb + PhCHCH2-TS-HM transfer**  HF = -1995.889758  ZPE = 0.667893  NImag = -251.5601  Htot = -1995.179818  Gtot = -1995.296686 |
| **2Nb + Ph-CHCH2-interm**  HF = -1995.898672  ZPE = 0.670489  NImag = 0  Htot = -1995.185667  Gtot = -1995.303663 | **2Nb + Ph-CHCH2-TS-HN transfer**  HF = -1995.897536  ZPE = 0.667367  NImag = -646.1459  Htot = -1995.188072  Gtot = -1995.30495 |
| **2Nb + PhCHO-TS-HM transfer**  HF = -2031.83521  ZPE = 0.645468  NImag = -155.7126  Htot = -2031.148264  Gtot = -2031.264044 | **2Nb + PhCHO-interm**  HF = -2031.849215  ZPE = 0.647415  NImag = 0  Htot = -2031.160072  Gtot = -2031.276216 |
| **2Nb +PhCHO -TS-HN transfer**  HF = -2031.849155  ZPE = 0.645372  NImag = -216.4131  Htot = -2031.162474  Gtot = -2031.277769 | **2Nb + Ph-COCH3-TS**  HF = -2071.1447  ZPE = 0.673659  NImag = -330.7437  Htot = -2070.42829  Gtot = -2070.545838 |
| **1Ta + H2-TS**  HF = -1687.762099  ZPE = 0.529135  NImag = -921.8268  Htot = -1687.198784  Gtot = -1687.297772 | **2Ta +PhCN-TS-HM transfer**  HF = -2012.253054  ZPE = 0.63464  NImag = -247.9951  Htot = -2011.57713  Gtot = -2011.692483 |
| **2Ta + PhCN-interm**  HF = -2012.256048  ZPE = 0.635796  NImag = 0  Htot = -2011.578743  Gtot = -2011.694475 | **2Ta + PhCN-TS-HN transfer**  HF = -2012.255333  ZPE = 0.633062  NImag = -655.3483  Htot = -2011.58111  Gtot = -2011.696041 |
| **2Ta + Ph-CHNH-TS**  HF = -2244.4768  ZPE = 0.738547  NImag = -489.6871  Htot = -2243.692011  Gtot = -2243.819019 | **2Ta + Ph-CHNCH2Ph-TS**  HF = -2283.779619  ZPE = 0.766445  NImag = -465.5506  Htot = -2282.965566  Gtot = -2283.096098 |
| **2Ta + Ph-CHNPh-TS**  HF = -2013.453218  ZPE = 0.657579  NImag = -456.7003  Htot = -2012.754133  Gtot = -2012.869618 | **2Ta + Ph-CCH-TS-HM transfer to C-H**  HF = -1996.146975  ZPE = 0.644006  NImag = -557.6819  Htot = -1995.460948  Gtot = -1995.579166 |
| **2Ta + PhCCH-TS-HM transfer to Ph-C**  HF = -1996.139738  ZPE = 0.643413  NImag = -563.4816  Htot = -1995.454448  Gtot = -1995.570789 | **2Ta + PhCCH-interm to Ph-C**  HF = -1996.143979  ZPE = 0.647473  NImag = 0  Htot = -1995.45462  Gtot = -1995.571706 |
| **2Ta + PhCCH-TS-HN transfer to C-H**  HF = -1996.139609  ZPE = 0.645114  NImag = -596.2289  Htot = -1995.452935  Gtot = -1995.568147 | **2Ta + PhCHCH2-TS-HM transfer**  HF = -1997.400863  ZPE = 0.667959  NImag = -646.6309  Htot = -1996.690859  Gtot = -1996.808322 |
| **2Ta + Ph-CHCH2-interm**  HF = -1997.406595  ZPE = 0.670216  NImag = 0  Htot = -1996.693967  Gtot = -1996.811583 | **2Ta + Ph-CHCH2-TS-HN transfer**  HF = -1997.406148  ZPE = 0.667954  NImag = -417.2688  Htot = -1996.696337  Gtot = -1996.812405 |
| **2Ta + PhCHO-TS-HM transfer**  HF = -2033.347547  ZPE = 0.645932  NImag = -181.2908  Htot = -2032.660308  Gtot = -2032.775425 | **2Ta + PhCHO-interm**  HF = -2033.357754  ZPE = 0.646845  NImag = 0  Htot = -2032.669196  Gtot = -2032.785648 |
| **2Ta +PhCHO -TS-HN transfer**  HF = -2033.355682  ZPE = 0.64877  NImag = -119.8161  Htot = -2032.666014  Gtot = -2032.779741 | **2Ta + Ph-COCH3-TS**  HF = -2072.656717  ZPE = 0.673932  NImag = -338.5074  Htot = -2071.940136  Gtot = -2072.057428 |