# Supplementary Information

## Stereochemical Control and Its Consequences in $VO(acac)_2$ Complexes: An Integrated Study of *Trans*/*Cis* Isomerism with Quinoline and Isoquinoline

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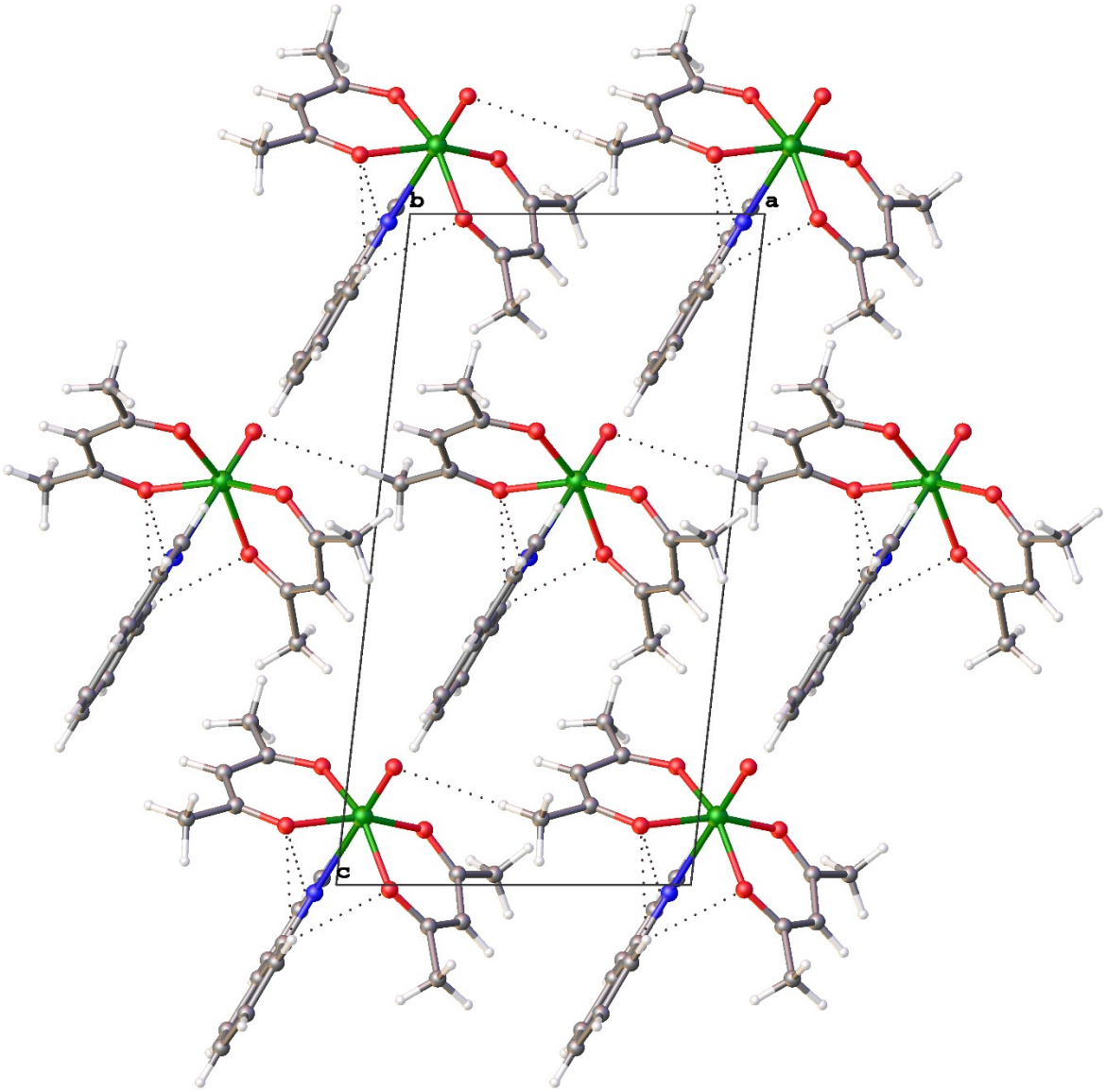


**Figure S1.** Crystal packing of compound (**1**) viewed along the *b*-axis, highlighting intermolecular hydrogen bonds (dashed lines).

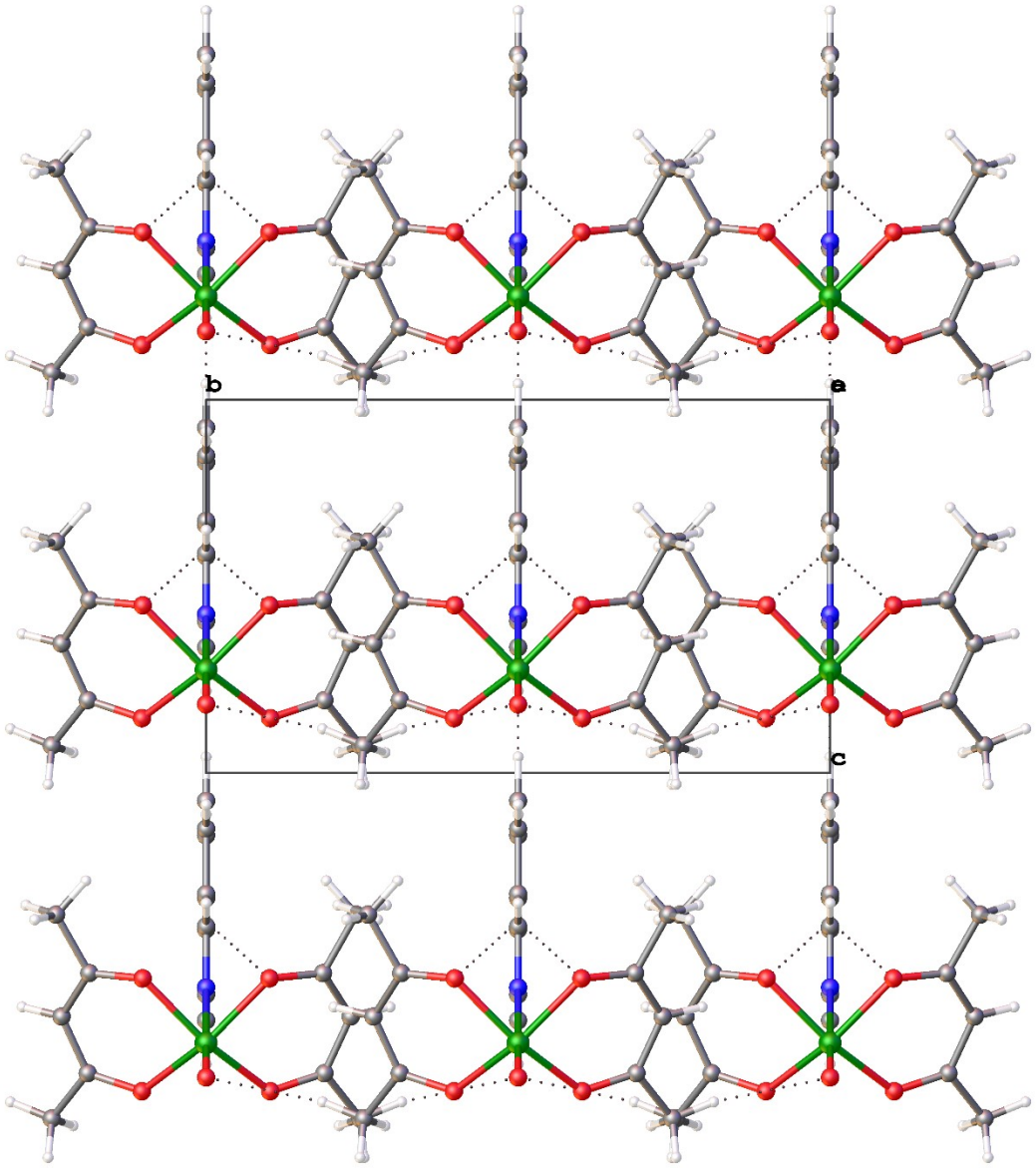


**Figure S2.** Crystal packing of compound (**2**) viewed along the *a*-axis, highlighting intermolecular hydrogen bonds (dashed lines).

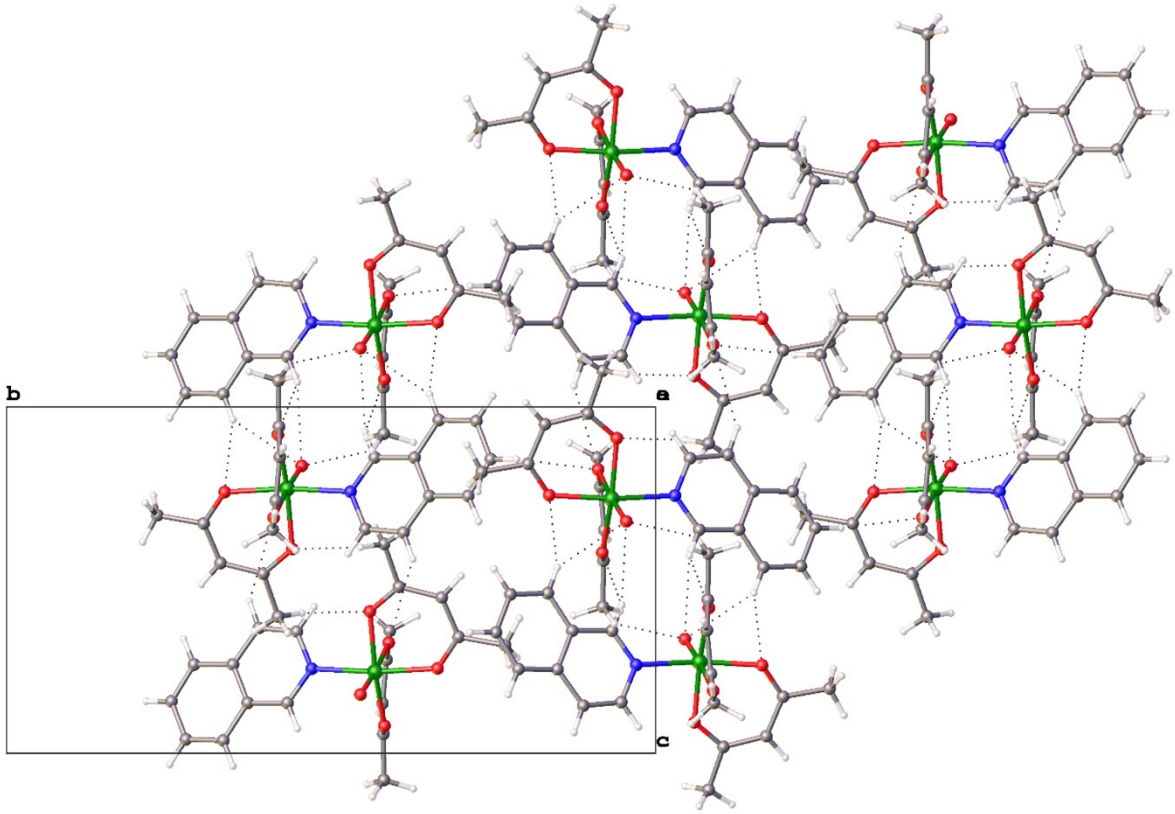


**Figure S3.** Crystal packing of compound (**3**) viewed along the *a*-axis, highlighting intermolecular hydrogen bonds (dashed lines).

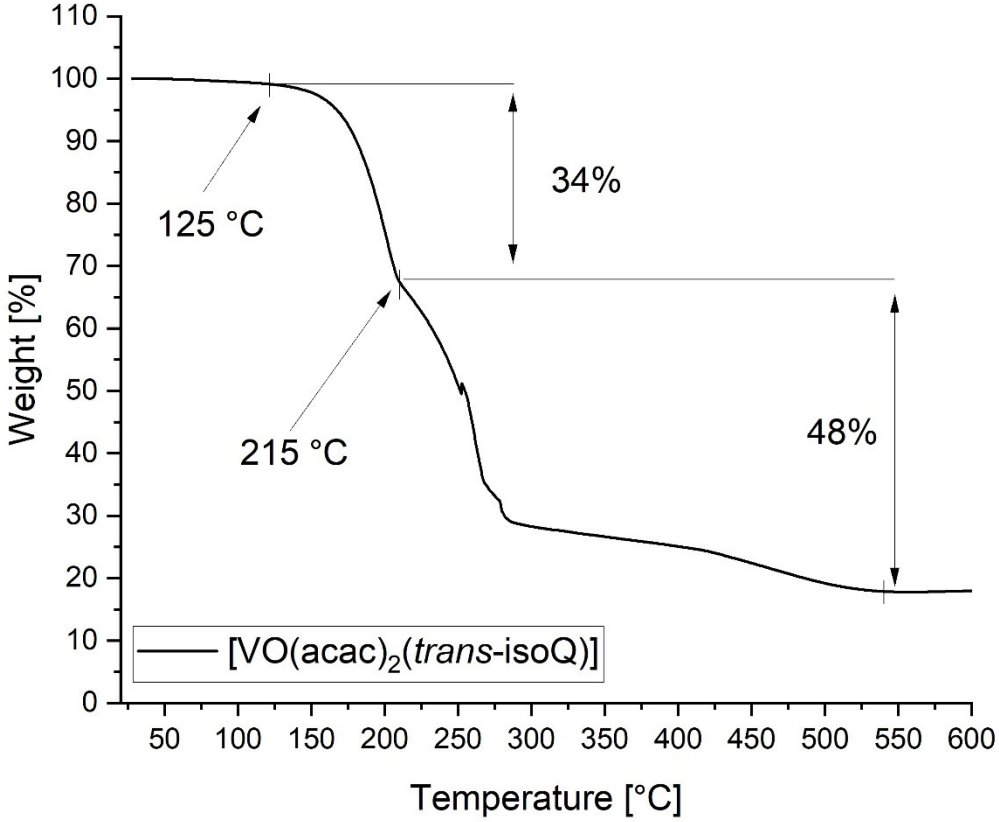


**Figure S4.** TGA curve of thermal decomposition of compound (**2**).

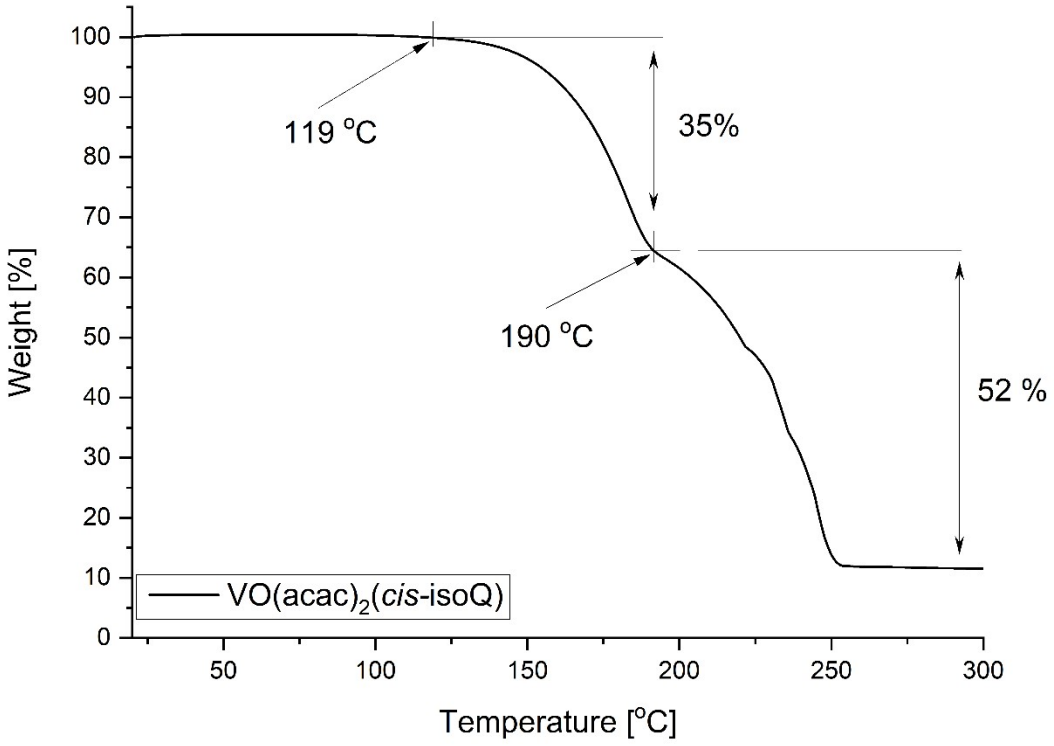


**Figure S5.** TGA curve of thermal decomposition of compound (**3**).

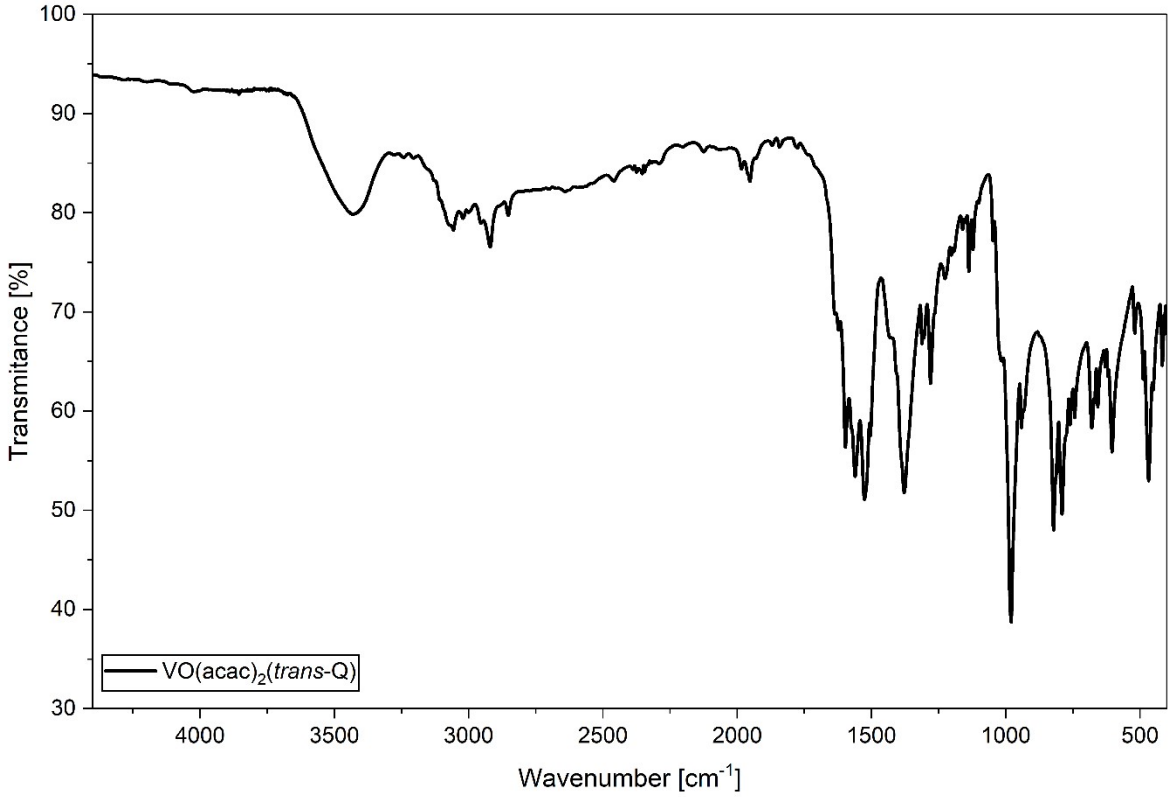


**Figure S6.** Infrared spectrum of compound (**1**).

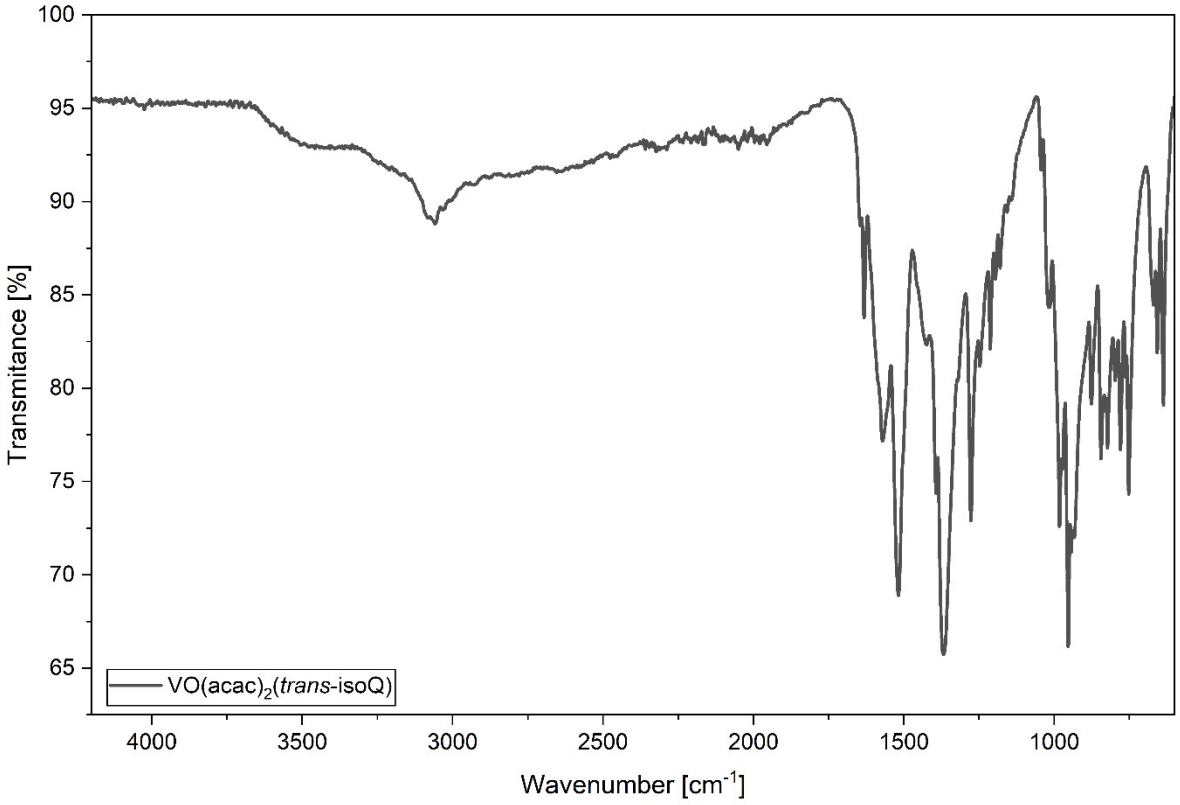


**Figure S7**. Infrared spectrum of compound (**2**).

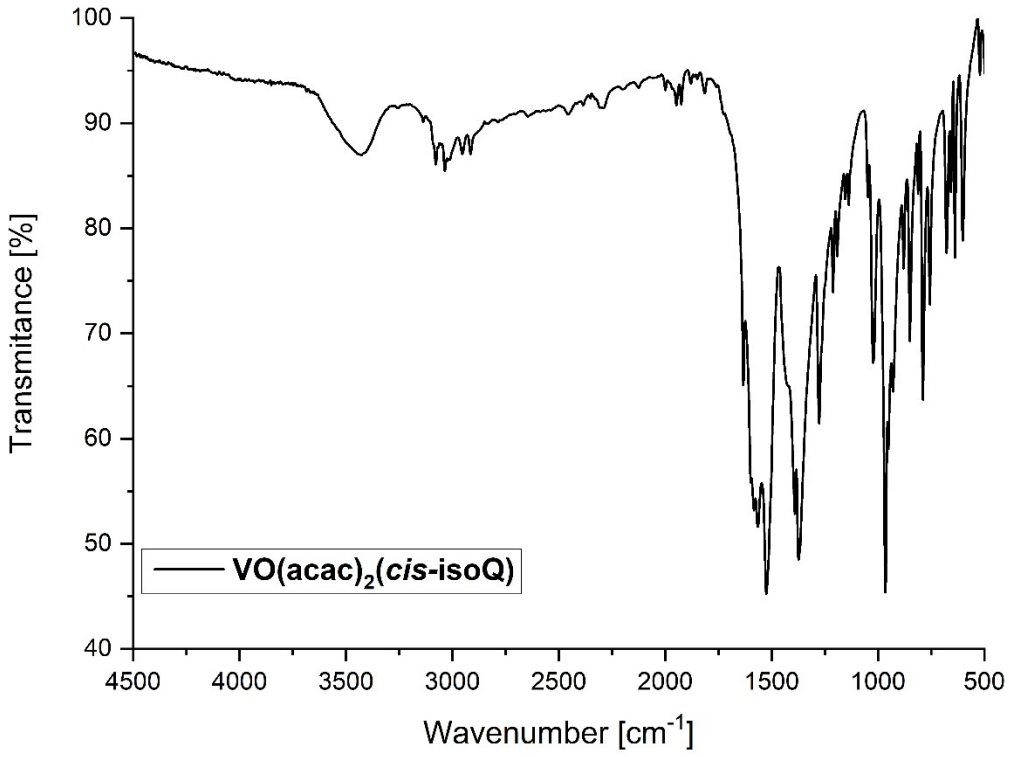


**Figure S8.** Infrared spectrum of compound (**3**).

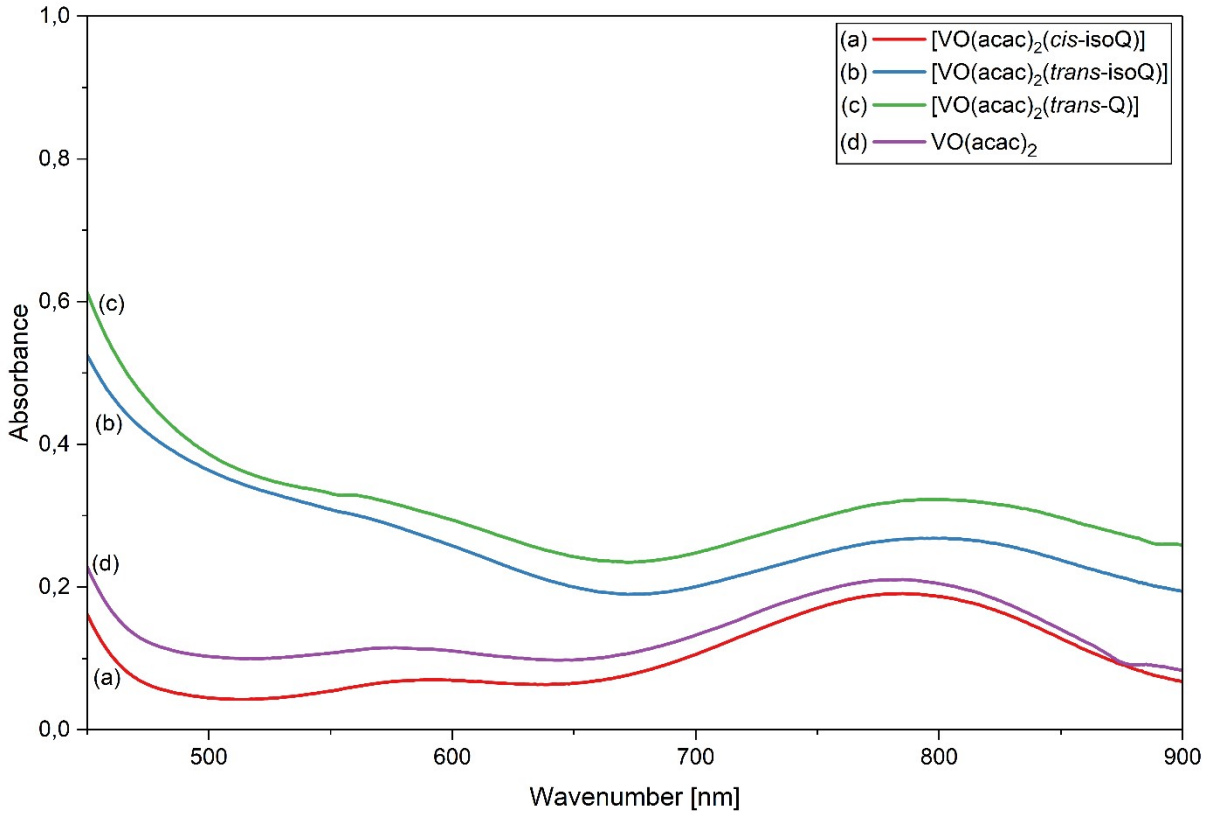


**Figure S9.** UV-Vis absorption spectra of: $VO(acac)_2$ (d) and its adducts with isoquinoline: $VO(acac)_2$(*cis*-isoQ) (a), $VO(acac)_2$(*trans*-*iso*Q) (b) and quinoline: $VO(acac)_2$(*trans*-Q) (c), acquired in DMSO (c = 7 mM).

**Tabels**

**Table S1.** Crystal and structure refinement data for compounds **1**-**3**.

| | (**1**) | (**2**) | (**3**) |
|---|---|---|---|
| Empirical formula | $C_{19}H_{21}NO_5V$ | $C_{19}H_{21}NO_5V$ | $C_{19}H_{21}NO_5V$ |
| Formula weight | 394.31 | 394.31 | 394.31 |
| Temperature /K | 120(2) | 120(2) | 120(2) |
| Wavelength /Å | 0.71073 (Mo $K_\alpha$) | 0.71073 (Mo $K_\alpha$) | 0.71073 (Mo $K_\alpha$) |
| Crystal system | monoclinic | monoclinic | monoclinic |
| Space group | *Pn* | *Cm* | *P* $2_1/c$ |
| *a* /Å | 8.0583(3) | 8.7229(6) | 8.222(2) |
| *b* /Å | 7.7264(4) | 13.5442(8) | 20.454(8) |
| *c* /Å | 15.3312(6) | 8.0885(5) | 11.506(4) |
| $\alpha$ /deg | 90 | 90 | 90 |
| $\beta$ /deg | 96.296(3) | 90.419(5) | 108.51(2) |
| γ /deg | 90 | 90 | 90 |
| *V* /Å$^3$ | 948.79(7) | 955.59(10) | 1834.8(11) |
| *Z* | 2 | 2 | 4 |
| $D_c$ /Mg m$^{-3}$ | 1.380 | 1.370 | 1.427 |
| $\mu$ /mm$^{-1}$ | 0.551 | 0.547 | 0.570 |
| *F*(000) | 410 | 410 | 820 |
| Crystal size /mm | 0.17 x 0.14 x 0.13 | 0.20 x 0.15 x 0.11 | 0.21 x 0.08 x 0.05 |
| $\Theta$ range/deg | 2.636 to 29.212 | 2.518 to 29.151 | 2.613 to 29.295 |
| Index ranges | -11<=h<=11<br>-10<=k<=10<br>-20<=l<=21 | -11<=h<=11<br>-18<=k<=18<br>-11<=l<=11 | -11<=h<=11<br>-28<=k<=27<br>-15<=l<=15 |
| Reflections collected / unique | 14705 / 4882<br>[*R*(int) = 0.0276] | 7425 / 2530<br>[*R*(int) = 0.0281] | 27562 / 4955<br>[*R*(int) = 0.0597] |
| Completeness to $\theta_{max}$ /% | 99.8 | 99.9 | 99.9 |
| Data / restraints / parameters | 4882 / 2 / 240 | 2530 / 2 / 139 | 4955 / 0 / 239 |
| Goodness of fit on $F^2$ | 1.052 | 1.083 | 1.029 |
| Final *R* indices [$I>2\sigma(I)$] | $R_1$ = 0.0362<br>*w* $R_2$ = 0.0967 | $R_1$ = 0.0445<br>*w* $R_2$ = 0.1161 | $R_1$ = 0.0445<br>*w* $R_2$ = 0.1080 |
| *R* indices (all data) | $R_1$ = 0.0387 | $R_1$ = 0.0473 | $R_1$ = 0.0685 |

| | | | |
|---|---|---|---|
| | $w\,R_2 = 0.1012$ | $w\,R_2 = 0.1243$ | $w\,R_2 = 0.1175$ |
| Largest diff. peaks[e Å $^{-3}$] | 0.681, -0.596 | 0.321, -0.709 | 0.484, -0.389 |

**Table S2**. Selected geometric parameters (Å, º) for compounds **1-3.**

| | Bond lengths (Å) | | Bond angles (°) |
|---|---|---|---|
| **(1)** | | | |
| N(1)-V(1) | 2.615(2) | O(1)-V(1)-O(5) | 101.63(12) |
| O(1)-V(1) | 1.596(2) | O(1)-V(1)-O(4) | 100.09(12) |
| O(2)-V(1) | 1.991(2) | O(5)-V(1)-O(4) | 88.63(9) |
| O(3)-V(1) | 1.994(2) | O(1)-V(1)-O(2) | 99.84(12) |
| O(4)-V(1) | 1.989(2) | O(5)-V(1)-O(2) | 158.52(9) |
| O(5)-V(1) | 1.988(2) | O(4)-V(1)-O(2) | 86.83(9) |
| | | O(1)-V(1)-O(3) | 101.08(12) |
| | | O(5)-V(1)-O(3) | 88.07(9) |
| | | O(4)-V(1)-O(3) | 158.81(9) |
| | | O(2)-V(1)-O(3) | 88.63(9) |
| | | O(1)-V(1)-N(1) | 174.80(12) |
| | | O(5)-V(1)-N(1) | 82.22(8) |
| | | O(4)-V(1)-N(1) | 76.37(8) |
| | | O(2)-V(1)-N(1) | 76.30(8) |
| | | O(3)-V(1)-N(1) | 82.45(8) |
| **(2)** | | | |
| N(1)-V(1) | 2.405(5) | O(1)-V(1)-O(3)#1 | 99.16(15) |
| O(1)-V(1) | 1.606(4) | O(1)-V(1)-O(3) | 99.16(15) |
| O(2)-V(1) | 1.999(3) | O(3)#1-V(1)-O(3) | 87.15(17) |
| O(3)-V(1) | 1.997(3) | O(1)-V(1)-O(2) | 100.81(14) |
| | | O(3)#1-V(1)-O(2) | 160.01(11) |
| | | O(3)-V(1)-O(2) | 88.83(11) |
| | | O(1)-V(1)-O(2)#1 | 100.81(14) |
| | | O(3)#1-V(1)-O(2)#1 | 88.83(11) |
| | | O(3)-V(1)-O(2)#1 | 160.01(11) |
| | | O(2)-V(1)-O(2)#1 | 88.29(17) |
| | | O(1)-V(1)-N(1) | 177.9(2) |
| | | O(3)#1-V(1)-N(1) | 79.31(12) |
| | | O(3)-V(1)-N(1) | 79.31(12) |
| | | O(2)-V(1)-N(1) | 80.70(12) |
| | | O(2)#1-V(1)-N(1) | 80.70(12) |
| **(3)** | | | |
| N(1)-V(1) | 2.1558(18) | O(1)-V(1)-O(5) | 94.92(7) |

| | | | |
|---|---|---|---|
| O(1)-V(1) | 1.6001(15) | O(1)-V(1)-O(3) | 98.85(7) |
| O(2)-V(1) | 2.0007(16) | O(5)-V(1)-O(3) | 166.23(6) |
| O(3)-V(1) | 1.9998(15) | O(1)-V(1)-O(2) | 99.45(7) |
| O(4)-V(1) | 2.1350(15) | O(5)-V(1)-O(2) | 89.20(6) |
| O(5)-V(1) | 1.9916(15) | O(3)-V(1)-O(2) | 88.78(6) |
| | | O(1)-V(1)-O(4) | 174.52(7) |
| | | O(5)-V(1)-O(4) | 84.08(6) |
| | | O(3)-V(1)-O(4) | 82.19(6) |
| | | O(2)-V(1)-O(4) | 85.94(6) |
| | | O(1)-V(1)-N(1) | 93.92(7) |
| | | O(5)-V(1)-N(1) | 89.35(6) |
| | | O(3)-V(1)-N(1) | 89.48(6) |
| | | O(2)-V(1)-N(1) | 166.63(6) |
| | | O(4)-V(1)-N(1) | 80.69(6) |

Symmetry transformations used to generate equivalent atoms:
#1 x,-y+1,z

**Table S3**. Hydrogen-bonding geometry (Å and º) for compounds **1**-**3**.

| D-H...A | d(D-H) | d(H...A) | d(D...A) | <(DHA) |
|---|---|---|---|---|
| **(1)** | | | | |
| C(11)-H(11)...O(2)#1 | 0.95 | 2.52 | 2.989(4) | 111 |
| C(11)-H(11)...O(4) #1 | 0.95 | 2.51 | 2.973(4) | 110 |
| C(12)-H(12)...O(5)#2 | 0.95 | 2.54 | 3.400(4) | 150 |
| C(17)-H(17)...O(1)#3 | 0.95 | 2.46 | 3.177(4) | 132 |
| C(18)-H(18)...O(3) #1 | 0.95 | 2.51 | 3.216(4) | 131 |
| C(3)-H(3)...Cg(4) #8 | 0.95 | 2.87 | 3.730(3) | 151 |
| C(6)-H(6C)...Cg(4) #4 | 0.98 | 2.72 | 3.554(4) | 143 |
| C(6)-H(6C)...Cg(5) #4 | 0.98 | 2.82 | 3.463(4) | 124 |
| Cg(4) and Cg(5) are the centers of gravity of the C14–C19 and N1-C11–C17 rings, respectively | | | | |
| **(2)** | | | | |
| C(7)-H(7)...O(1)#4 | 0.95 | 2.41 | 3.354(7) | 176 |
| C(9)-H(9)...O(3) #4 | 0.95 | 2.51 | 3.347(6) | 147 |
| C(9)-H(9)...O(3)#5 | 0.95 | 2.51 | 3.347(6) | 147 |
| C(10)-H(10)...O(1)#6 | 0.95 | 2.45 | 3.151(8) | 131 |
| C(5)-H(5C)...Cg(5) #9 | 0.98 | 3.0 | 3.520(5) | 115 |
| C(5)-H(5C)...Cg(5) #10 | 0.98 | 3.0 | 3.520(5) | 115 |
| Cg(5) is the center of gravity of the N1-C6–C12 | | | | |
| **(3)** | | | | |
| C(6)-H(6C)...O(1)#7 | 0.98 | 2.52 | 3.323(3) | 139 |
| C(10)-H(10B)...O(1)#5 | 0.98 | 2.50 | 3.447(3) | 163 |
| C(11)-H(11)...O(3) | 0.95 | 2.55 | 3.064(3) | 114 |
| C(6)-H(6A)...Cg(4) #9 | 0.98 | 2.95 | 3.632(3) | 128 |
| C(10)-H(10B)...Cg(1) #4 | 0.98 | 2.74 | 3.448(3) | 130 |
| Cg(1) and Cg(4) are the centers of gravity of the V1-O2-C2-C3-C4–O3 and C13–C18 rings, respectively | | | | |

Symmetry transformations used to generate equivalent atoms:

#1 1/2+x,1-y,-1/2+z; #2 1/2+x,-y,-1/2+z; #3 x,1+y,z; #4 -1+x,y,z; #5-1+x,1-y,z: #6 -1+x,y,-1+z: #7 2-x,-y,1-z; #8 1/2+x,1-y,1/2+z; #9 1/2+x,-1/2+y,z; #10 1/2+x,1/2-y,z; #11 1-x,-y,1-z

**Table S4**. The cartesian coordinates (in Å) of all structures obtained at MN15/aug-cc-pVDZ level of theory within the SMD solvation model.

| Adducts from $VO(acac)_2$ and two ligand molecules | | | |
|---|---|---|---|
| **isoquinoline: RC (ΔG=0.0)** | | | |
| 1 | -2.506592000 | -0.263723000 | -2.491002000 |
| 1 | 2.855832000 | -3.761209000 | -2.858310000 |
| 1 | 4.137310000 | 0.209628000 | -0.608574000 |
| 23 | 0.886477000 | -1.242803000 | 0.268483000 |
| 8 | -0.265116000 | -0.454095000 | -1.124475000 |
| 8 | 1.982901000 | -1.905992000 | -1.224001000 |
| 8 | 0.371478000 | 0.275925000 | 1.408372000 |
| 8 | 2.498570000 | -1.333298000 | 1.398993000 |
| 8 | 0.069801000 | -2.487866000 | 0.749244000 |
| 7 | -0.142794000 | 3.887283000 | -1.996500000 |
| 6 | 1.655060000 | 2.483119000 | -1.193159000 |
| 6 | 2.654501000 | 2.815725000 | 1.021044000 |
| 6 | -1.146137000 | 0.473149000 | -1.038036000 |
| 6 | -0.554964000 | 1.150798000 | 1.253990000 |
| 6 | 3.131667000 | -2.475493000 | -1.185729000 |
| 6 | 3.605655000 | -1.936382000 | 1.178195000 |
| 6 | 0.779631000 | 4.265447000 | 0.202322000 |
| 1 | 0.771112000 | 4.839849000 | 1.131533000 |
| 6 | 3.507573000 | 1.761085000 | 0.781775000 |
| 6 | 3.938114000 | -2.552226000 | -0.039897000 |
| 1 | 4.904104000 | -3.049801000 | -0.120809000 |
| 6 | 0.700288000 | 2.892305000 | -2.164732000 |
| 6 | -1.334196000 | 1.276265000 | 0.096194000 |
| 1 | -2.099701000 | 2.052133000 | 0.064652000 |
| 6 | -0.104344000 | 4.556348000 | -0.810428000 |
| 1 | -0.824471000 | 5.371007000 | -0.692385000 |
| 6 | 1.707871000 | 3.203068000 | 0.032405000 |
| 6 | -0.770446000 | 2.075155000 | 2.412059000 |
| 1 | -1.042932000 | 1.479709000 | 3.297240000 |
| 1 | -1.550249000 | 2.820223000 | 2.211705000 |
| 6 | 4.587643000 | -1.922612000 | 2.307306000 |
| 1 | 4.887623000 | -0.878549000 | 2.493422000 |
| 1 | 5.478731000 | -2.523963000 | 2.094611000 |
| 6 | 3.450414000 | 1.042656000 | -0.442422000 |
| 6 | -1.990079000 | 0.679796000 | -2.256586000 |
| 1 | -1.335966000 | 0.904471000 | -3.113135000 |
| 1 | -2.724079000 | 1.484426000 | -2.127302000 |
| 6 | 3.609970000 | -3.055243000 | -2.479819000 |
| 1 | 4.576841000 | -3.560902000 | -2.377962000 |
| 1 | 3.694058000 | -2.245903000 | -3.221481000 |
| 6 | 2.534335000 | 1.388851000 | -1.410422000 |
| 1 | 2.469184000 | 0.835079000 | -2.350963000 |
| 1 | 0.179612000 | 2.580922000 | 2.646028000 |
| 1 | 4.096190000 | -2.283678000 | 3.222533000 |
| 1 | 2.689971000 | 3.367150000 | 1.964095000 |

| | | | |
|---|---|---|---|
| 1 | 4.234717000 | 1.462829000 | 1.541310000 |
| 1 | -4.482760000 | 1.369504000 | 2.938885000 |
| 7 | -4.736911000 | -1.694232000 | -1.995098000 |
| 6 | -4.435333000 | -0.574594000 | 0.127504000 |
| 6 | -2.892547000 | -1.440036000 | 1.827535000 |
| 6 | -3.139984000 | -2.559573000 | -0.403157000 |
| 1 | -2.388504000 | -3.309716000 | -0.149164000 |
| 6 | -3.266230000 | -0.416157000 | 2.669673000 |
| 6 | -5.028284000 | -0.723289000 | -1.157151000 |
| 6 | -3.786788000 | -2.595239000 | -1.616383000 |
| 1 | -3.553265000 | -3.382608000 | -2.338546000 |
| 6 | -3.467574000 | -1.538521000 | 0.529657000 |
| 6 | -4.211602000 | 0.561185000 | 2.256383000 |
| 6 | -4.789179000 | 0.483115000 | 1.008752000 |
| 1 | -5.526877000 | 1.219630000 | 0.679780000 |
| 1 | -2.158201000 | -2.185276000 | 2.139263000 |
| 1 | -2.830010000 | -0.347087000 | 3.668957000 |
| 1 | -5.782408000 | 0.010272000 | -1.467231000 |
| 1 | 0.668417000 | 2.349083000 | -3.117394000 |
| **isoquinoline: TS1 (ΔG=2.0) $\nu_1$= -70cm$^{-1}$** | | | |
| 1 | -2.074888000 | 0.627052000 | -2.500034000 |
| 1 | 2.335100000 | -3.790874000 | -3.384922000 |
| 1 | 1.063043000 | 5.638116000 | -2.581658000 |
| 23 | 0.520858000 | -1.802797000 | 0.248285000 |
| 8 | -0.434755000 | -0.555585000 | -0.944117000 |
| 8 | 1.485196000 | -2.300870000 | -1.398737000 |
| 8 | 0.150264000 | -0.539208000 | 1.717322000 |
| 8 | 2.162291000 | -2.224311000 | 1.249698000 |
| 8 | -0.423699000 | -3.022516000 | 0.507080000 |
| 7 | 2.533847000 | 0.588375000 | -0.116408000 |
| 6 | 1.976871000 | 2.795614000 | -0.920186000 |
| 6 | 2.026479000 | 4.742723000 | 0.567826000 |
| 6 | -0.915052000 | 0.609591000 | -0.711093000 |
| 6 | -0.405722000 | 0.614874000 | 1.701604000 |
| 6 | 2.669143000 | -2.765410000 | -1.550569000 |
| 6 | 3.290291000 | -2.666606000 | 0.835807000 |
| 6 | 2.616886000 | 2.454986000 | 1.401868000 |
| 1 | 2.804497000 | 2.833505000 | 2.409185000 |
| 6 | 1.619652000 | 5.538985000 | -0.480291000 |
| 6 | 3.581265000 | -2.964203000 | -0.503493000 |
| 1 | 4.571826000 | -3.348086000 | -0.745380000 |
| 6 | 2.152464000 | 1.392812000 | -1.082652000 |
| 1 | 1.950818000 | 0.947791000 | -2.065950000 |
| 6 | -0.909561000 | 1.231251000 | 0.546539000 |
| 1 | -1.355071000 | 2.222075000 | 0.637841000 |
| 6 | 2.757276000 | 1.117354000 | 1.117869000 |
| 1 | 3.046854000 | 0.406965000 | 1.899478000 |
| 6 | 2.213375000 | 3.347347000 | 0.370874000 |
| 6 | -0.494172000 | 1.311690000 | 3.024298000 |
| 1 | -1.055240000 | 2.252129000 | 2.964135000 |
| 1 | 0.526261000 | 1.513302000 | 3.387197000 |

| | | | |
|---|---|---|---|
| 6 | 4.340959000 | -2.836044000 | 1.888675000 |
| 1 | 4.609452000 | -1.839293000 | 2.274675000 |
| 1 | 5.242184000 | -3.328019000 | 1.505329000 |
| 6 | 1.383662000 | 4.985792000 | -1.766931000 |
| 6 | -1.477485000 | 1.326779000 | -1.898183000 |
| 1 | -0.635315000 | 1.659960000 | -2.528624000 |
| 1 | -2.077853000 | 2.199872000 | -1.614139000 |
| 6 | 3.062677000 | -3.083584000 | -2.959525000 |
| 1 | 4.072595000 | -3.503738000 | -3.026808000 |
| 1 | 3.005671000 | -2.163183000 | -3.560665000 |
| 6 | 1.559376000 | 3.637590000 | -1.985432000 |
| 1 | 1.384590000 | 3.196234000 | -2.970370000 |
| 1 | -0.967799000 | 0.637875000 | 3.754027000 |
| 1 | 3.926041000 | -3.407687000 | 2.731376000 |
| 1 | 2.207963000 | 5.166252000 | 1.558480000 |
| 1 | 1.475144000 | 6.610423000 | -0.325023000 |
| 1 | -4.313948000 | 1.420823000 | 3.067360000 |
| 7 | -4.626939000 | -0.453781000 | -2.426707000 |
| 6 | -4.354469000 | 0.116381000 | -0.092094000 |
| 6 | -3.229322000 | -1.398230000 | 1.475385000 |
| 6 | -3.455596000 | -1.968928000 | -0.955532000 |
| 1 | -2.911143000 | -2.905986000 | -0.820010000 |
| 6 | -3.472438000 | -0.503473000 | 2.494557000 |
| 6 | -4.807298000 | 0.369167000 | -1.417444000 |
| 6 | -3.941929000 | -1.608791000 | -2.189840000 |
| 1 | -3.793300000 | -2.266524000 | -3.050852000 |
| 6 | -3.665668000 | -1.105068000 | 0.153638000 |
| 6 | -4.141777000 | 0.724474000 | 2.243840000 |
| 6 | -4.577273000 | 1.030150000 | 0.973433000 |
| 1 | -5.101891000 | 1.966290000 | 0.765312000 |
| 1 | -2.703495000 | -2.336649000 | 1.663350000 |
| 1 | -3.143356000 | -0.734388000 | 3.510474000 |
| 1 | -5.346900000 | 1.304522000 | -1.610218000 |
| **isoquinoline: trans bound product (ΔG=0.1)** | | | |
| 1 | -1.934250000 | 1.902840000 | -2.244070000 |
| 1 | 2.285686000 | -2.486346000 | -3.896253000 |
| 1 | 4.864952000 | 4.292618000 | -2.056262000 |
| 23 | -0.043088000 | -1.574664000 | -0.099929000 |
| 8 | -0.722165000 | 0.064630000 | -0.974714000 |
| 8 | 1.092235000 | -1.835209000 | -1.703570000 |
| 8 | -0.576072000 | -0.802992000 | 1.641333000 |
| 8 | 1.225873000 | -2.709389000 | 0.912564000 |
| 8 | -1.215917000 | -2.578646000 | -0.399310000 |
| 7 | 1.770962000 | 0.000977000 | 0.319911000 |
| 6 | 3.167194000 | 1.805475000 | -0.444941000 |
| 6 | 4.741487000 | 2.919065000 | 1.066614000 |
| 6 | -1.063110000 | 1.174658000 | -0.437462000 |
| 6 | -0.917410000 | 0.401120000 | 1.909614000 |
| 6 | 2.281598000 | -2.300958000 | -1.770062000 |
| 6 | 2.402700000 | -3.083739000 | 0.576745000 |
| 6 | 3.296522000 | 1.033381000 | 1.860069000 |

| | | | |
|---|---|---|---|
| 1 | 3.716985000 | 1.089016000 | 2.866010000 |
| 6 | 5.125201000 | 3.746483000 | 0.034122000 |
| 6 | 2.964817000 | -2.894610000 | -0.696002000 |
| 1 | 3.977841000 | -3.257237000 | -0.868735000 |
| 6 | 2.174108000 | 0.809576000 | -0.636409000 |
| 1 | 1.702678000 | 0.695632000 | -1.620083000 |
| 6 | -1.134426000 | 1.399961000 | 0.946809000 |
| 1 | -1.437102000 | 2.389022000 | 1.291369000 |
| 6 | 2.327928000 | 0.107553000 | 1.559378000 |
| 1 | 1.950536000 | -0.592690000 | 2.310244000 |
| 6 | 3.749289000 | 1.925164000 | 0.849352000 |
| 6 | -1.052674000 | 0.729347000 | 3.364626000 |
| 1 | -1.592779000 | 1.669170000 | 3.532901000 |
| 1 | -0.037700000 | 0.821767000 | 3.787283000 |
| 6 | 3.206225000 | -3.738454000 | 1.657382000 |
| 1 | 3.438211000 | -2.976436000 | 2.419661000 |
| 1 | 4.142139000 | -4.168577000 | 1.282889000 |
| 6 | 4.542770000 | 3.623976000 | -1.255625000 |
| 6 | -1.359167000 | 2.290293000 | -1.391145000 |
| 1 | -0.398217000 | 2.662502000 | -1.786051000 |
| 1 | -1.892460000 | 3.121046000 | -0.913041000 |
| 6 | 2.960949000 | -2.151273000 | -3.096004000 |
| 1 | 3.910168000 | -2.696754000 | -3.146688000 |
| 1 | 3.152139000 | -1.077896000 | -3.261524000 |
| 6 | 3.579758000 | 2.670155000 | -1.494120000 |
| 1 | 3.120060000 | 2.561419000 | -2.479650000 |
| 1 | -1.550212000 | -0.099487000 | 3.887379000 |
| 1 | 2.600730000 | -4.513443000 | 2.148841000 |
| 1 | 5.188323000 | 3.012845000 | 2.058950000 |
| 1 | 5.887588000 | 4.509807000 | 0.204039000 |
| 1 | -4.734334000 | 1.338070000 | 3.234075000 |
| 7 | -4.669363000 | 1.316954000 | -2.579226000 |
| 6 | -4.595002000 | 1.089497000 | -0.172493000 |
| 6 | -3.878726000 | -0.998489000 | 0.896504000 |
| 6 | -3.902853000 | -0.752108000 | -1.598193000 |
| 1 | -3.514890000 | -1.763682000 | -1.735139000 |
| 6 | -4.107305000 | -0.430499000 | 2.130687000 |
| 6 | -4.848710000 | 1.809424000 | -1.373585000 |
| 6 | -4.187174000 | 0.045643000 | -2.680915000 |
| 1 | -4.034514000 | -0.332624000 | -3.695630000 |
| 6 | -4.116386000 | -0.246467000 | -0.287010000 |
| 6 | -4.568620000 | 0.908544000 | 2.243664000 |
| 6 | -4.810440000 | 1.656603000 | 1.112715000 |
| 1 | -5.172867000 | 2.685505000 | 1.182017000 |
| 1 | -3.510496000 | -2.022620000 | 0.807606000 |
| 1 | -3.925904000 | -1.011114000 | 3.038356000 |
| 1 | -5.225351000 | 2.836315000 | -1.291239000 |
| **isoquinoline: TS2 (ΔG=11.1) $\nu_1$= -72cm$^{-1}$** | | | |
| 1 | -1.946671000 | 0.563950000 | -3.500560000 |
| 1 | 4.238518000 | -1.935099000 | -3.005978000 |
| 1 | 1.606351000 | 3.253878000 | -3.127382000 |

| | | | |
|---|---|---|---|
| 23 | 0.696133000 | -1.489056000 | -0.412776000 |
| 8 | -0.016538000 | -0.286082000 | -1.796271000 |
| 8 | 2.415893000 | -1.237004000 | -1.285441000 |
| 8 | 0.071717000 | -0.015686000 | 0.902882000 |
| 8 | 1.690912000 | -2.057843000 | 1.213470000 |
| 8 | 0.328250000 | -2.901405000 | -0.982101000 |
| 6 | 3.319315000 | 1.066487000 | 1.997458000 |
| 6 | 2.553944000 | 2.101119000 | -0.060605000 |
| 6 | 1.030408000 | 4.002369000 | -0.004612000 |
| 6 | -0.769836000 | 0.752227000 | -1.741887000 |
| 6 | -0.714080000 | 0.966997000 | 0.713600000 |
| 6 | 3.533310000 | -1.802996000 | -0.999148000 |
| 6 | 2.881000000 | -2.513755000 | 1.271996000 |
| 6 | 1.809994000 | 2.960947000 | 2.121011000 |
| 1 | 1.218773000 | 3.682216000 | 2.691312000 |
| 7 | 0.976704000 | 4.085056000 | -1.315861000 |
| 6 | 3.790220000 | -2.482667000 | 0.196219000 |
| 1 | 4.780878000 | -2.911816000 | 0.343691000 |
| 6 | 3.342792000 | 1.134819000 | 0.622525000 |
| 1 | 3.973920000 | 0.460625000 | 0.042292000 |
| 6 | -1.168402000 | 1.376168000 | -0.556859000 |
| 1 | -1.811034000 | 2.255127000 | -0.619266000 |
| 6 | 2.541437000 | 1.982133000 | 2.755589000 |
| 1 | 2.539768000 | 1.913552000 | 3.845374000 |
| 6 | 1.796326000 | 3.033191000 | 0.701727000 |
| 6 | -1.212883000 | 1.705618000 | 1.922822000 |
| 1 | -2.272460000 | 1.442347000 | 2.081315000 |
| 1 | -1.167767000 | 2.793174000 | 1.767781000 |
| 6 | 3.307020000 | -3.068254000 | 2.595798000 |
| 1 | 3.273307000 | -2.257844000 | 3.341064000 |
| 1 | 4.316171000 | -3.494373000 | 2.565397000 |
| 6 | 1.682336000 | 3.170932000 | -2.039206000 |
| 6 | -1.232672000 | 1.282390000 | -3.064883000 |
| 1 | -0.375469000 | 1.345978000 | -3.751108000 |
| 1 | -1.716965000 | 2.262242000 | -2.974369000 |
| 6 | 4.613984000 | -1.627941000 | -2.019030000 |
| 1 | 5.521111000 | -2.189337000 | -1.767917000 |
| 1 | 4.856784000 | -0.554179000 | -2.086616000 |
| 6 | 2.467036000 | 2.191199000 | -1.475936000 |
| 1 | 3.014079000 | 1.481823000 | -2.102117000 |
| 1 | -0.636449000 | 1.421625000 | 2.811602000 |
| 1 | 2.584602000 | -3.832333000 | 2.918440000 |
| 1 | 0.452429000 | 4.730465000 | 0.578479000 |
| 1 | -6.651672000 | 0.816252000 | 2.486840000 |
| 7 | -2.050107000 | -1.762317000 | 0.060100000 |
| 6 | -4.078642000 | -0.719213000 | 0.844706000 |
| 6 | -5.952110000 | -0.273776000 | -0.671194000 |
| 6 | -3.857389000 | -1.383764000 | -1.483596000 |
| 1 | -4.251753000 | -1.464345000 | -2.498864000 |
| 6 | -6.648738000 | 0.288961000 | 0.375290000 |
| 6 | -2.761946000 | -1.223430000 | 1.024346000 |
| 1 | -2.297190000 | -1.142521000 | 2.014609000 |

| | | | |
|---|---|---|---|
| 6 | -2.600157000 | -1.850022000 | -1.181853000 |
| 1 | -1.967579000 | -2.302140000 | -1.950727000 |
| 6 | -4.644863000 | -0.791341000 | -0.459423000 |
| 6 | -6.079473000 | 0.363120000 | 1.674881000 |
| 6 | -4.816580000 | -0.132415000 | 1.908239000 |
| 1 | -4.362871000 | -0.083639000 | 2.901755000 |
| 1 | -6.387811000 | -0.330678000 | -1.671424000 |
| 1 | -7.652547000 | 0.686104000 | 0.209298000 |
| 1 | 3.914312000 | 0.307607000 | 2.513075000 |
| **isoquinoline: cis bound product (ΔG=0.9)** | | | |
| 1 | -0.946854000 | 2.103535000 | -3.603027000 |
| 1 | 3.586540000 | -3.878604000 | -1.509260000 |
| 1 | 3.189864000 | 1.478173000 | -2.974193000 |
| 23 | -0.359608000 | -1.556034000 | -1.124674000 |
| 8 | 0.171731000 | 0.028503000 | -2.201373000 |
| 8 | 1.513978000 | -2.236539000 | -1.150527000 |
| 8 | 0.282889000 | -0.248854000 | 0.473616000 |
| 8 | -0.710335000 | -2.741217000 | 0.417443000 |
| 8 | -0.988708000 | -2.412735000 | -2.282322000 |
| 6 | 3.648766000 | 0.485904000 | 2.750060000 |
| 6 | 3.440512000 | 1.043009000 | 0.398285000 |
| 6 | 3.325892000 | 3.369857000 | -0.319939000 |
| 6 | 0.075442000 | 1.281231000 | -1.936644000 |
| 6 | 0.150395000 | 1.013242000 | 0.509967000 |
| 6 | 2.106818000 | -2.968282000 | -0.287028000 |
| 6 | 0.131043000 | -3.360929000 | 1.156421000 |
| 6 | 3.543850000 | 2.820611000 | 2.099977000 |
| 1 | 3.541474000 | 3.886747000 | 2.341345000 |
| 7 | 3.253609000 | 3.045163000 | -1.592263000 |
| 6 | 1.499317000 | -3.484150000 | 0.871350000 |
| 1 | 2.114016000 | -4.068473000 | 1.555499000 |
| 6 | 3.537641000 | 0.077610000 | 1.439174000 |
| 1 | 3.527898000 | -0.984532000 | 1.183159000 |
| 6 | -0.010823000 | 1.811537000 | -0.643994000 |
| 1 | -0.091082000 | 2.893033000 | -0.528382000 |
| 6 | 3.656788000 | 1.866866000 | 3.086014000 |
| 1 | 3.747376000 | 2.164785000 | 4.132585000 |
| 6 | 3.434487000 | 2.425189000 | 0.738876000 |
| 6 | 0.136541000 | 1.658933000 | 1.864052000 |
| 1 | -0.848830000 | 1.457673000 | 2.320569000 |
| 1 | 0.288665000 | 2.744683000 | 1.819513000 |
| 6 | -0.435070000 | -3.989855000 | 2.391877000 |
| 1 | -0.829313000 | -3.193263000 | 3.042286000 |
| 1 | 0.309774000 | -4.574624000 | 2.943631000 |
| 6 | 3.259669000 | 1.720360000 | -1.909584000 |
| 6 | 0.043826000 | 2.193029000 | -3.126352000 |
| 1 | 0.789453000 | 1.863075000 | -3.863779000 |
| 1 | 0.215211000 | 3.241820000 | -2.855448000 |
| 6 | 3.541182000 | -3.293484000 | -0.577555000 |
| 1 | 4.012425000 | -3.863057000 | 0.231835000 |
| 1 | 4.103219000 | -2.364104000 | -0.755785000 |

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|---|---|---|---|
| 6 | 3.343526000 | 0.711228000 | -0.979664000 |
| 1 | 3.317129000 | -0.334033000 | -1.293376000 |
| 1 | 0.895847000 | 1.189611000 | 2.505978000 |
| 1 | -1.285612000 | -4.630302000 | 2.115569000 |
| 1 | 3.313932000 | 4.436034000 | -0.062833000 |
| 1 | -5.779766000 | 1.376032000 | 3.409288000 |
| 7 | -2.203343000 | -0.555943000 | -0.717902000 |
| 6 | -3.820116000 | 0.346471000 | 0.810056000 |
| 6 | -5.706253000 | 1.687329000 | 0.009566000 |
| 6 | -4.020956000 | 0.744669000 | -1.583794000 |
| 1 | -4.534962000 | 1.181320000 | -2.441833000 |
| 6 | -6.134485000 | 1.831716000 | 1.311281000 |
| 6 | -2.651914000 | -0.395961000 | 0.512276000 |
| 1 | -2.076618000 | -0.858103000 | 1.319799000 |
| 6 | -2.878238000 | 0.009761000 | -1.763777000 |
| 1 | -2.449284000 | -0.160399000 | -2.753777000 |
| 6 | -4.532742000 | 0.938732000 | -0.271344000 |
| 6 | -5.418339000 | 1.243733000 | 2.387777000 |
| 6 | -4.278610000 | 0.512089000 | 2.144923000 |
| 1 | -3.713905000 | 0.050779000 | 2.958749000 |
| 1 | -6.255770000 | 2.141124000 | -0.817972000 |
| 1 | -7.037862000 | 2.407135000 | 1.524529000 |
| 1 | 3.730808000 | -0.257772000 | 3.545768000 |
| **quinoline: RC (ΔG=0.0)** | | | |
| 1 | -2.413370000 | -0.235473000 | -2.576362000 |
| 1 | 2.862102000 | -3.727924000 | -2.887758000 |
| 1 | 4.129352000 | 0.232300000 | -0.568731000 |
| 23 | 0.884937000 | -1.249683000 | 0.270046000 |
| 8 | -0.274343000 | -0.455067000 | -1.115436000 |
| 8 | 1.979277000 | -1.898083000 | -1.230847000 |
| 8 | 0.373879000 | 0.260607000 | 1.420640000 |
| 8 | 2.501916000 | -1.343037000 | 1.394687000 |
| 8 | 0.074309000 | -2.499924000 | 0.748010000 |
| 6 | -0.102653000 | 3.771301000 | -1.992979000 |
| 6 | 1.626924000 | 2.478190000 | -1.200284000 |
| 6 | 2.628515000 | 2.846921000 | 1.016703000 |
| 6 | -1.144657000 | 0.481451000 | -1.026105000 |
| 6 | -0.547199000 | 1.142751000 | 1.269183000 |
| 6 | 3.133043000 | -2.457545000 | -1.202445000 |
| 6 | 3.612077000 | -1.936643000 | 1.164383000 |
| 6 | 0.759397000 | 4.280577000 | 0.190730000 |
| 1 | 0.775004000 | 4.857515000 | 1.119411000 |
| 6 | 3.489798000 | 1.794153000 | 0.805172000 |
| 6 | 3.944592000 | -2.538695000 | -0.060505000 |
| 1 | 4.914320000 | -3.027469000 | -0.149937000 |
| 7 | 0.743610000 | 2.783949000 | -2.194162000 |
| 6 | -1.326790000 | 1.278090000 | 0.114029000 |
| 1 | -2.086771000 | 2.059320000 | 0.086471000 |
| 6 | -0.137942000 | 4.558426000 | -0.813170000 |
| 1 | -0.867188000 | 5.364920000 | -0.722888000 |
| 6 | 1.682761000 | 3.214611000 | 0.019718000 |

| | | | |
|---|---|---|---|
| 6 | -0.754879000 | 2.066659000 | 2.429268000 |
| 1 | -1.014807000 | 1.471606000 | 3.318312000 |
| 1 | -1.540455000 | 2.807721000 | 2.236284000 |
| 6 | 4.598563000 | -1.925261000 | 2.289616000 |
| 1 | 4.892904000 | -0.880628000 | 2.481638000 |
| 1 | 5.492527000 | -2.519461000 | 2.068987000 |
| 6 | 3.437466000 | 1.063119000 | -0.410679000 |
| 6 | -1.972281000 | 0.718348000 | -2.250208000 |
| 1 | -1.304975000 | 1.060238000 | -3.056355000 |
| 1 | -2.759920000 | 1.463593000 | -2.084688000 |
| 6 | 3.611554000 | -3.019669000 | -2.504284000 |
| 1 | 4.583135000 | -3.517992000 | -2.411470000 |
| 1 | 3.685797000 | -2.201531000 | -3.237332000 |
| 6 | 2.523789000 | 1.390551000 | -1.387145000 |
| 1 | 2.462096000 | 0.829008000 | -2.322011000 |
| 1 | 0.194711000 | 2.578386000 | 2.652482000 |
| 1 | 4.113228000 | -2.295700000 | 3.204338000 |
| 1 | 2.653325000 | 3.417938000 | 1.948794000 |
| 1 | 4.215079000 | 1.512075000 | 1.572191000 |
| 1 | -4.488676000 | 1.357034000 | 2.926130000 |
| 6 | -4.716917000 | -1.630353000 | -1.922833000 |
| 6 | -4.438120000 | -0.584318000 | 0.106803000 |
| 6 | -2.893268000 | -1.443513000 | 1.820301000 |
| 6 | -3.120105000 | -2.572783000 | -0.394419000 |
| 1 | -2.366240000 | -3.310356000 | -0.108879000 |
| 6 | -3.263604000 | -0.423367000 | 2.667469000 |
| 7 | -5.054515000 | -0.652404000 | -1.109907000 |
| 6 | -3.746373000 | -2.619210000 | -1.617175000 |
| 1 | -3.516068000 | -3.395096000 | -2.348831000 |
| 6 | -3.466462000 | -1.543517000 | 0.522061000 |
| 6 | -4.211042000 | 0.547271000 | 2.247501000 |
| 6 | -4.786752000 | 0.467731000 | 0.998825000 |
| 1 | -5.526159000 | 1.197787000 | 0.662769000 |
| 1 | -2.157895000 | -2.190705000 | 2.126189000 |
| 1 | -2.827401000 | -0.353320000 | 3.666401000 |
| 1 | -0.813416000 | 3.989235000 | -2.798307000 |
| 1 | -5.224351000 | -1.668757000 | -2.893035000 |
| **quinoline: TS1 (ΔG=2.1) $\nu_1$= -81cm$^{-1}$** | | | |
| 1 | -1.450103000 | 1.865245000 | -2.099560000 |
| 1 | 3.062486000 | -1.783639000 | -3.964439000 |
| 1 | 2.145388000 | 3.340588000 | -3.077652000 |
| 23 | 0.577297000 | -1.608975000 | -0.209354000 |
| 8 | -0.275809000 | 0.038805000 | -0.868211000 |
| 8 | 1.818896000 | -1.386348000 | -1.730340000 |
| 8 | -0.178928000 | -1.184133000 | 1.566614000 |
| 8 | 2.080597000 | -2.347321000 | 0.818344000 |
| 8 | -0.297030000 | -2.815826000 | -0.684098000 |
| 6 | 2.240354000 | 0.765437000 | 2.009571000 |
| 6 | 2.148940000 | 2.023437000 | 0.078846000 |
| 6 | 1.710852000 | 4.443121000 | 0.116370000 |
| 6 | -0.911025000 | 0.954912000 | -0.235835000 |

| | | | |
|---|---|---|---|
| 6 | -0.810672000 | -0.145202000 | 1.969566000 |
| 6 | 3.055149000 | -1.699232000 | -1.834277000 |
| 6 | 3.299664000 | -2.542707000 | 0.472754000 |
| 6 | 1.805274000 | 3.116897000 | 2.230307000 |
| 1 | 1.602532000 | 4.016507000 | 2.817180000 |
| 6 | 1.810385000 | 4.482904000 | -1.256694000 |
| 6 | 3.816948000 | -2.266202000 | -0.800190000 |
| 1 | 4.867874000 | -2.482228000 | -0.990043000 |
| 7 | 2.320588000 | 0.819118000 | 0.698095000 |
| 6 | -1.174757000 | 0.926663000 | 1.142295000 |
| 1 | -1.722856000 | 1.760871000 | 1.581457000 |
| 6 | 1.991236000 | 1.895082000 | 2.831588000 |
| 1 | 1.943569000 | 1.775277000 | 3.915170000 |
| 6 | 1.881263000 | 3.215521000 | 0.814386000 |
| 6 | -1.133775000 | -0.105844000 | 3.431388000 |
| 1 | -1.528697000 | -1.081789000 | 3.747963000 |
| 1 | -1.844715000 | 0.691881000 | 3.679292000 |
| 6 | 4.191852000 | -3.082102000 | 1.546569000 |
| 1 | 4.283045000 | -2.319736000 | 2.337112000 |
| 1 | 5.190409000 | -3.335849000 | 1.172944000 |
| 6 | 2.074822000 | 3.295417000 | -1.988734000 |
| 6 | -1.349627000 | 2.139583000 | -1.041147000 |
| 1 | -0.572620000 | 2.919501000 | -0.958360000 |
| 1 | -2.288800000 | 2.560758000 | -0.659806000 |
| 6 | 3.691922000 | -1.390173000 | -3.153285000 |
| 1 | 4.707635000 | -1.794254000 | -3.232410000 |
| 1 | 3.728514000 | -0.295184000 | -3.273933000 |
| 6 | 2.236406000 | 2.091991000 | -1.339236000 |
| 1 | 2.421391000 | 1.166078000 | -1.888030000 |
| 1 | -0.196169000 | 0.062075000 | 3.987621000 |
| 1 | 3.722203000 | -3.965592000 | 2.002778000 |
| 1 | 1.507254000 | 5.348828000 | 0.693146000 |
| 1 | 1.684123000 | 5.427753000 | -1.789227000 |
| 1 | -4.879728000 | -0.223875000 | 3.030262000 |
| 6 | -4.243400000 | 0.781107000 | -2.543884000 |
| 6 | -4.369979000 | 0.159451000 | -0.332875000 |
| 6 | -3.346431000 | -1.917077000 | 0.501946000 |
| 6 | -3.163302000 | -1.266118000 | -1.900189000 |
| 1 | -2.570353000 | -2.160327000 | -2.108616000 |
| 6 | -3.799496000 | -1.631532000 | 1.770668000 |
| 7 | -4.680022000 | 1.039793000 | -1.330236000 |
| 6 | -3.474388000 | -0.361203000 | -2.886425000 |
| 1 | -3.146099000 | -0.502209000 | -3.917328000 |
| 6 | -3.617347000 | -1.028453000 | -0.574697000 |
| 6 | -4.533214000 | -0.441657000 | 2.017392000 |
| 6 | -4.815301000 | 0.431709000 | 0.990155000 |
| 1 | -5.385490000 | 1.347598000 | 1.159424000 |
| 1 | -2.769877000 | -2.822720000 | 0.300183000 |
| 1 | -3.591366000 | -2.317175000 | 2.595104000 |
| 1 | 2.361693000 | -0.221497000 | 2.472386000 |
| 1 | -4.498969000 | 1.501371000 | -3.328954000 |

**quinoline: trans bound product (ΔG=1.2)**

| | | | |
|---|---|---|---|
| 1 | -1.971021000 | 2.605737000 | -1.233597000 |
| 1 | 2.812588000 | -0.369222000 | -4.294093000 |
| 1 | 2.390074000 | 3.826088000 | -1.924441000 |
| 23 | 0.227867000 | -1.259017000 | -0.650353000 |
| 8 | -0.607343000 | 0.523755000 | -0.756776000 |
| 8 | 1.467249000 | -0.697363000 | -2.086360000 |
| 8 | -0.471643000 | -1.390170000 | 1.190917000 |
| 8 | 1.579421000 | -2.603744000 | -0.117168000 |
| 8 | -0.785654000 | -2.138119000 | -1.459914000 |
| 6 | 2.326627000 | -0.466117000 | 1.845304000 |
| 6 | 2.514690000 | 1.372148000 | 0.455262000 |
| 6 | 4.010640000 | 3.250068000 | 1.010737000 |
| 6 | -1.120180000 | 1.242145000 | 0.169683000 |
| 6 | -0.977556000 | -0.478386000 | 1.934775000 |
| 6 | 2.697637000 | -0.999002000 | -2.262277000 |
| 6 | 2.803489000 | -2.706292000 | -0.477556000 |
| 6 | 3.825778000 | 1.280807000 | 2.515560000 |
| 1 | 4.550335000 | 1.730767000 | 3.198993000 |
| 6 | 3.631351000 | 3.900788000 | -0.140566000 |
| 6 | 3.397995000 | -1.943833000 | -1.494764000 |
| 1 | 4.448022000 | -2.121089000 | -1.725676000 |
| 7 | 1.967121000 | 0.148139000 | 0.734273000 |
| 6 | -1.287901000 | 0.818187000 | 1.497701000 |
| 1 | -1.733840000 | 1.512732000 | 2.209830000 |
| 6 | 3.256501000 | 0.057672000 | 2.774817000 |
| 1 | 3.501710000 | -0.514337000 | 3.670450000 |
| 6 | 3.463137000 | 1.978507000 | 1.334127000 |
| 6 | -1.203594000 | -0.859510000 | 3.364956000 |
| 1 | -1.610304000 | -1.879090000 | 3.417805000 |
| 1 | -1.863231000 | -0.155061000 | 3.886499000 |
| 6 | 3.620968000 | -3.698800000 | 0.288935000 |
| 1 | 3.740911000 | -3.318120000 | 1.317126000 |
| 1 | 4.611419000 | -3.858515000 | -0.152453000 |
| 6 | 2.687317000 | 3.301838000 | -1.013409000 |
| 6 | -1.522308000 | 2.627647000 | -0.230398000 |
| 1 | -0.608465000 | 3.242811000 | -0.295363000 |
| 1 | -2.209010000 | 3.088435000 | 0.489961000 |
| 6 | 3.393224000 | -0.263677000 | -3.365807000 |
| 1 | 4.419242000 | -0.615372000 | -3.523352000 |
| 1 | 3.407821000 | 0.809511000 | -3.115162000 |
| 6 | 2.140737000 | 2.069424000 | -0.727734000 |
| 1 | 1.414551000 | 1.604600000 | -1.393283000 |
| 1 | -0.223005000 | -0.871278000 | 3.871116000 |
| 1 | 3.076021000 | -4.651057000 | 0.358587000 |
| 1 | 4.734918000 | 3.693745000 | 1.698259000 |
| 1 | 4.052466000 | 4.877695000 | -0.386296000 |
| 1 | -4.947546000 | -0.634592000 | 3.184873000 |
| 6 | -4.640104000 | 1.893378000 | -1.914378000 |
| 6 | -4.637900000 | 0.678147000 | 0.038467000 |
| 6 | -3.683591000 | -1.586717000 | 0.167359000 |
| 6 | -3.626881000 | -0.284674000 | -1.960824000 |
| 1 | -3.098868000 | -1.101683000 | -2.459010000 |

| | | | |
|---|---|---|---|
| 6 | -4.036003000 | -1.660889000 | 1.496532000 |
| 7 | -4.968615000 | 1.814835000 | -0.643083000 |
| 6 | -3.960571000 | 0.870552000 | -2.625877000 |
| 1 | -3.716985000 | 1.015342000 | -3.679507000 |
| 6 | -3.973071000 | -0.417728000 | -0.588768000 |
| 6 | -4.680862000 | -0.565142000 | 2.127761000 |
| 6 | -4.976991000 | 0.576540000 | 1.416060000 |
| 1 | -5.480796000 | 1.425824000 | 1.882326000 |
| 1 | -3.173976000 | -2.416606000 | -0.327566000 |
| 1 | -3.814263000 | -2.561515000 | 2.073535000 |
| 1 | 1.863023000 | -1.439491000 | 2.033935000 |
| 1 | -4.913985000 | 2.812942000 | -2.443384000 |
| **quinoline: TS2 (ΔG=10.2) $\nu_1$= -101cm$^{-1}$** | | | |
| 1 | 5.453918000 | -2.660823000 | -0.873373000 |
| 6 | 4.746389000 | -1.892152000 | -1.204489000 |
| 1 | 4.759020000 | -1.807036000 | -2.300463000 |
| 1 | 5.059996000 | -0.914965000 | -0.799881000 |
| 1 | -2.532048000 | 1.117052000 | 1.826037000 |
| 1 | -1.052419000 | 0.691012000 | 2.733306000 |
| 23 | 0.533541000 | -1.388099000 | -0.948435000 |
| 8 | 0.449885000 | 0.336704000 | -1.930388000 |
| 8 | 0.802384000 | -2.696878000 | 0.514515000 |
| 8 | -0.197706000 | -0.273329000 | 0.605581000 |
| 8 | 2.452913000 | -1.381954000 | -1.220747000 |
| 7 | -2.417959000 | -1.311059000 | -1.036603000 |
| 8 | 0.074280000 | -2.358157000 | -2.089329000 |
| 6 | -0.267996000 | 1.382257000 | -1.730932000 |
| 6 | 3.350985000 | -2.161953000 | -0.736751000 |
| 6 | 1.847111000 | -3.372222000 | 0.802406000 |
| 6 | -3.231221000 | -1.082427000 | 0.033179000 |
| 6 | -2.959075000 | -1.751390000 | 1.257982000 |
| 1 | -2.092689000 | -2.416692000 | 1.293293000 |
| 6 | -0.803385000 | 0.849463000 | 0.608922000 |
| 6 | -4.571891000 | 0.469118000 | -1.282512000 |
| 1 | -5.411807000 | 1.163578000 | -1.366683000 |
| 6 | -4.334290000 | -0.183473000 | -0.041783000 |
| 6 | -2.663140000 | -0.688217000 | -2.167382000 |
| 1 | -1.973411000 | -0.884999000 | -2.996708000 |
| 6 | -3.742065000 | 0.215380000 | -2.348655000 |
| 1 | -3.888695000 | 0.696621000 | -3.316982000 |
| 6 | -3.756592000 | -1.533314000 | 2.358509000 |
| 1 | -3.543172000 | -2.046764000 | 3.298550000 |
| 6 | -4.856812000 | -0.638044000 | 2.286147000 |
| 1 | -5.477821000 | -0.476901000 | 3.169746000 |
| 6 | -0.397956000 | 2.314053000 | -2.897202000 |
| 1 | -0.860768000 | 3.268764000 | -2.618350000 |
| 1 | -1.019856000 | 1.821405000 | -3.663712000 |
| 6 | 3.102502000 | -3.172379000 | 0.199646000 |
| 1 | 3.939064000 | -3.786901000 | 0.530861000 |
| 6 | -5.139902000 | 0.024436000 | 1.111949000 |
| 1 | -5.984467000 | 0.714758000 | 1.044537000 |

| | | | |
|---|---|---|---|
| 6 | -0.919629000 | 1.672571000 | -0.526270000 |
| 1 | -1.471333000 | 2.609774000 | -0.440605000 |
| 6 | -1.443782000 | 1.283372000 | 1.896356000 |
| 1 | -1.288905000 | 2.356234000 | 2.077995000 |
| 6 | 1.684982000 | -4.408606000 | 1.869796000 |
| 1 | 1.344941000 | -3.916927000 | 2.793840000 |
| 1 | 2.613884000 | -4.956651000 | 2.063751000 |
| 1 | 0.893284000 | -5.110856000 | 1.568499000 |
| 1 | 0.592243000 | 2.488428000 | -3.341904000 |
| 6 | 3.026698000 | 1.244323000 | 0.362101000 |
| 6 | 2.311404000 | 2.471246000 | 0.353156000 |
| 7 | 2.265069000 | 3.200189000 | -0.800838000 |
| 6 | 1.726854000 | 2.079534000 | 2.709398000 |
| 1 | 1.210886000 | 2.413467000 | 3.613469000 |
| 6 | 1.654927000 | 2.893621000 | 1.546419000 |
| 6 | 3.072018000 | 0.466721000 | 1.498855000 |
| 1 | 3.619028000 | -0.480161000 | 1.493353000 |
| 6 | 2.416233000 | 0.887235000 | 2.684693000 |
| 1 | 2.461408000 | 0.260354000 | 3.577676000 |
| 6 | 1.554516000 | 4.306868000 | -0.807485000 |
| 1 | 1.515576000 | 4.868435000 | -1.747780000 |
| 6 | 0.855208000 | 4.809725000 | 0.321150000 |
| 1 | 0.291201000 | 5.739885000 | 0.236907000 |
| 6 | 0.916056000 | 4.106520000 | 1.500377000 |
| 1 | 0.399625000 | 4.452956000 | 2.399895000 |
| 1 | 3.519182000 | 0.934633000 | -0.561704000 |
| **quinoline: cis bound product (ΔG=6.1)** | | | |
| 1 | 3.198984000 | -4.809337000 | -0.787573000 |
| 6 | 2.990266000 | -3.779379000 | -1.099609000 |
| 1 | 3.079745000 | -3.689250000 | -2.191798000 |
| 1 | 3.746785000 | -3.111379000 | -0.656953000 |
| 1 | -1.410856000 | 2.068676000 | 2.089343000 |
| 1 | -0.156776000 | 1.052581000 | 2.856365000 |
| 23 | -0.533091000 | -1.340643000 | -1.074458000 |
| 8 | 0.318372000 | 0.214844000 | -1.987900000 |
| 8 | -1.010213000 | -2.673774000 | 0.318332000 |
| 8 | -0.084713000 | -0.127702000 | 0.645276000 |
| 8 | 1.241517000 | -2.200428000 | -1.150596000 |
| 7 | -2.390174000 | -0.055478000 | -0.942995000 |
| 8 | -1.176845000 | -2.031518000 | -2.328286000 |
| 6 | 0.330078000 | 1.465471000 | -1.690672000 |
| 6 | 1.626532000 | -3.323831000 | -0.676893000 |
| 6 | -0.392839000 | -3.732326000 | 0.683184000 |
| 6 | -3.048049000 | 0.367777000 | 0.186633000 |
| 6 | -2.958131000 | -0.382349000 | 1.388506000 |
| 1 | -2.375153000 | -1.302625000 | 1.377587000 |
| 6 | -0.097443000 | 1.139140000 | 0.711388000 |
| 6 | -3.972551000 | 2.259390000 | -1.053407000 |
| 1 | -4.568876000 | 3.174853000 | -1.077092000 |
| 6 | -3.833480000 | 1.556898000 | 0.171648000 |
| 6 | -2.578031000 | 0.602605000 | -2.074787000 |

| | | | |
|---|---|---|---|
| 1 | -2.047120000 | 0.222148000 | -2.951565000 |
| 6 | -3.370304000 | 1.765676000 | -2.185658000 |
| 1 | -3.466397000 | 2.257509000 | -3.154010000 |
| 6 | -3.598017000 | 0.054275000 | 2.527005000 |
| 1 | -3.527708000 | -0.533659000 | 3.444619000 |
| 6 | -4.347251000 | 1.258715000 | 2.526370000 |
| 1 | -4.838476000 | 1.591735000 | 3.442694000 |
| 6 | 0.627117000 | 2.395379000 | -2.828758000 |
| 1 | 0.765722000 | 3.431800000 | -2.496738000 |
| 1 | -0.211685000 | 2.350424000 | -3.543530000 |
| 6 | 0.869444000 | -4.112731000 | 0.203512000 |
| 1 | 1.299039000 | -5.047993000 | 0.561144000 |
| 6 | -4.465117000 | 1.993415000 | 1.368979000 |
| 1 | -5.053930000 | 2.913228000 | 1.339491000 |
| 6 | 0.061843000 | 1.976036000 | -0.417891000 |
| 1 | 0.081633000 | 3.057037000 | -0.271387000 |
| 6 | -0.346990000 | 1.773283000 | 2.050587000 |
| 1 | 0.254540000 | 2.682037000 | 2.192970000 |
| 6 | -1.102458000 | -4.580557000 | 1.692751000 |
| 1 | -1.263000000 | -3.986512000 | 2.605650000 |
| 1 | -0.544072000 | -5.490278000 | 1.941333000 |
| 1 | -2.096149000 | -4.847073000 | 1.302764000 |
| 1 | 1.525962000 | 2.047991000 | -3.358800000 |
| 6 | 3.378501000 | -0.284825000 | 0.235374000 |
| 6 | 3.352599000 | 1.134852000 | 0.211424000 |
| 7 | 3.558913000 | 1.779879000 | -0.974396000 |
| 6 | 2.888564000 | 1.107621000 | 2.626413000 |
| 1 | 2.690209000 | 1.662025000 | 3.547517000 |
| 6 | 3.101961000 | 1.838430000 | 1.426204000 |
| 6 | 3.156821000 | -0.970664000 | 1.409277000 |
| 1 | 3.165642000 | -2.063974000 | 1.415867000 |
| 6 | 2.911675000 | -0.269333000 | 2.617835000 |
| 1 | 2.738386000 | -0.827701000 | 3.540173000 |
| 6 | 3.482622000 | 3.092747000 | -0.987882000 |
| 1 | 3.638732000 | 3.591088000 | -1.951312000 |
| 6 | 3.221453000 | 3.886287000 | 0.160043000 |
| 1 | 3.175855000 | 4.972418000 | 0.067193000 |
| 6 | 3.040096000 | 3.256633000 | 1.368258000 |
| 1 | 2.841483000 | 3.820991000 | 2.283611000 |
| 1 | 3.558981000 | -0.805945000 | -0.706909000 |
| **pyridine: RC (ΔG=0.0)** | | | |
| 1 | 3.708044000 | -2.836349000 | 2.739749000 |
| 1 | -2.132303000 | 0.013450000 | 3.160129000 |
| 23 | 0.668485000 | -1.175855000 | -0.155117000 |
| 8 | 2.043416000 | -1.440877000 | 1.234421000 |
| 8 | -0.393834000 | -0.379300000 | 1.287944000 |
| 8 | 2.135704000 | -0.844035000 | -1.419451000 |
| 8 | -0.383837000 | -0.057463000 | -1.406623000 |
| 8 | 0.149338000 | -2.627251000 | -0.416103000 |
| 7 | 1.210327000 | 2.558817000 | 1.578889000 |
| 6 | 0.255158000 | 4.286304000 | 0.199689000 |

| | | | |
|---|---|---|---|
| 6 | 3.318368000 | -1.497748000 | 1.136227000 |
| 6 | 3.406064000 | -0.907189000 | -1.257163000 |
| 6 | -1.304605000 | 0.524201000 | 1.263715000 |
| 6 | -1.299878000 | 0.807446000 | -1.181288000 |
| 6 | 1.503946000 | 2.505073000 | -0.811010000 |
| 1 | 1.913283000 | 1.979468000 | -1.676837000 |
| 6 | -1.770515000 | 1.142782000 | 0.097625000 |
| 1 | -2.555768000 | 1.893796000 | 0.183549000 |
| 6 | 0.499480000 | 3.683350000 | 1.435017000 |
| 1 | 0.104816000 | 4.138274000 | 2.349549000 |
| 6 | 4.029672000 | -1.237873000 | -0.046235000 |
| 1 | 5.117865000 | -1.282792000 | -0.018208000 |
| 6 | 1.686686000 | 1.981737000 | 0.470065000 |
| 1 | 2.249041000 | 1.048931000 | 0.597589000 |
| 6 | 0.772944000 | 3.685809000 | -0.948794000 |
| 6 | 4.227155000 | -0.579679000 | -2.464773000 |
| 1 | 5.298899000 | -0.734692000 | -2.296291000 |
| 1 | 4.049160000 | 0.474012000 | -2.733326000 |
| 6 | -1.861759000 | 1.495052000 | -2.386503000 |
| 1 | -1.088712000 | 2.164466000 | -2.798749000 |
| 1 | -2.757047000 | 2.082220000 | -2.148483000 |
| 6 | 4.052409000 | -1.850531000 | 2.392035000 |
| 1 | 3.791612000 | -1.124029000 | 3.176096000 |
| 1 | 5.138768000 | -1.868481000 | 2.249241000 |
| 6 | -1.860507000 | 0.918091000 | 2.596445000 |
| 1 | -2.727815000 | 1.583266000 | 2.506818000 |
| 1 | -1.064860000 | 1.427288000 | 3.164018000 |
| 1 | 3.885670000 | -1.190403000 | -3.313304000 |
| 1 | -2.093083000 | 0.748101000 | -3.158745000 |
| 1 | 0.606064000 | 4.127660000 | -1.933930000 |
| 1 | -0.328872000 | 5.206569000 | 0.145838000 |
| 7 | -3.956037000 | -1.128138000 | -1.519043000 |
| 6 | -3.096095000 | -2.206522000 | 0.455351000 |
| 6 | -4.898757000 | -0.633981000 | 0.641134000 |
| 1 | -5.634492000 | -0.074056000 | 1.221194000 |
| 6 | -3.104140000 | -1.968978000 | -0.920347000 |
| 1 | -2.387740000 | -2.489112000 | -1.564376000 |
| 6 | -4.823683000 | -0.468050000 | -0.743021000 |
| 1 | -5.506159000 | 0.225851000 | -1.244897000 |
| 6 | -4.019321000 | -1.528824000 | 1.252534000 |
| 1 | -4.049624000 | -1.691103000 | 2.332542000 |
| 1 | -2.373958000 | -2.903813000 | 0.883865000 |
| **pyridine: TS1 (ΔG=0.4) $\nu_1$= -153cm$^{-1}$** | | | |
| 1 | 3.659979000 | -2.555512000 | 2.942881000 |
| 1 | -2.080938000 | 0.132273000 | 3.201243000 |
| 23 | 0.632297000 | -1.176408000 | -0.119332000 |
| 8 | 2.011772000 | -1.383693000 | 1.277733000 |
| 8 | -0.438857000 | -0.345794000 | 1.308123000 |
| 8 | 2.094879000 | -0.972635000 | -1.421080000 |
| 8 | -0.410632000 | -0.088018000 | -1.401454000 |
| 8 | 0.091827000 | -2.629849000 | -0.309683000 |

| | | | |
|---|---|---|---|
| 7 | 1.744295000 | 1.770520000 | 0.282482000 |
| 6 | 0.718432000 | 3.640403000 | 1.390036000 |
| 6 | 3.286903000 | -1.427338000 | 1.176540000 |
| 6 | 3.364170000 | -1.035379000 | -1.258205000 |
| 6 | -1.323944000 | 0.579183000 | 1.256125000 |
| 6 | -1.289702000 | 0.820479000 | -1.195550000 |
| 6 | 0.908485000 | 3.620209000 | -1.004358000 |
| 1 | 0.752760000 | 4.067214000 | -1.987895000 |
| 6 | -1.751422000 | 1.198594000 | 0.073427000 |
| 1 | -2.509771000 | 1.978697000 | 0.140406000 |
| 6 | 1.339407000 | 2.390305000 | 1.395712000 |
| 1 | 1.511006000 | 1.863628000 | 2.341099000 |
| 6 | 3.991625000 | -1.271053000 | -0.027124000 |
| 1 | 5.080036000 | -1.311888000 | 0.000362000 |
| 6 | 1.523430000 | 2.371937000 | -0.890955000 |
| 1 | 1.839736000 | 1.828014000 | -1.788628000 |
| 6 | 0.499237000 | 4.267516000 | 0.162450000 |
| 6 | 4.183339000 | -0.814109000 | -2.491360000 |
| 1 | 5.253855000 | -0.971030000 | -2.316851000 |
| 1 | 4.018776000 | 0.218207000 | -2.839436000 |
| 6 | -1.825992000 | 1.495436000 | -2.419595000 |
| 1 | -0.997259000 | 2.009291000 | -2.932503000 |
| 1 | -2.617185000 | 2.217260000 | -2.184234000 |
| 6 | 4.031381000 | -1.640569000 | 2.457895000 |
| 1 | 3.811333000 | -0.803552000 | 3.138335000 |
| 1 | 5.114162000 | -1.712899000 | 2.304910000 |
| 6 | -1.890699000 | 1.013487000 | 2.572487000 |
| 1 | -2.807482000 | 1.604018000 | 2.453616000 |
| 1 | -1.134849000 | 1.628591000 | 3.089440000 |
| 1 | 3.828629000 | -1.483248000 | -3.288883000 |
| 1 | -2.212218000 | 0.730765000 | -3.109317000 |
| 1 | 0.012944000 | 5.244315000 | 0.115274000 |
| 1 | 0.410174000 | 4.104039000 | 2.328801000 |
| 7 | -3.956700000 | -1.136458000 | -1.498266000 |
| 6 | -3.179886000 | -2.104145000 | 0.565704000 |
| 6 | -4.938806000 | -0.472583000 | 0.597867000 |
| 1 | -5.671640000 | 0.145715000 | 1.119374000 |
| 6 | -3.146571000 | -1.959883000 | -0.822577000 |
| 1 | -2.431792000 | -2.543515000 | -1.411284000 |
| 6 | -4.822981000 | -0.401031000 | -0.791483000 |
| 1 | -5.470512000 | 0.277569000 | -1.356529000 |
| 6 | -4.102258000 | -1.348636000 | 1.291016000 |
| 1 | -4.163553000 | -1.435720000 | 2.378376000 |
| 1 | -2.488995000 | -2.790317000 | 1.059143000 |
| **pyridine: trans bound product (ΔG=-2.0)** | | | |
| 1 | 3.362320000 | -2.269619000 | 3.166242000 |
| 1 | -2.224394000 | 0.702641000 | 3.212341000 |
| 23 | 0.355015000 | -1.075992000 | -0.024347000 |
| 8 | 1.726430000 | -1.412371000 | 1.361950000 |
| 8 | -0.656744000 | -0.109602000 | 1.376123000 |
| 8 | 1.743783000 | -1.363089000 | -1.404253000 |

| | | | |
|---|---|---|---|
| 8 | -0.642400000 | -0.041638000 | -1.388706000 |
| 8 | -0.402524000 | -2.452826000 | -0.062342000 |
| 7 | 1.524647000 | 1.064802000 | 0.021541000 |
| 6 | 2.466940000 | 2.886366000 | 1.259688000 |
| 6 | 2.997597000 | -1.462728000 | 1.224468000 |
| 6 | 3.012883000 | -1.421327000 | -1.253431000 |
| 6 | -1.409567000 | 0.917406000 | 1.251996000 |
| 6 | -1.387531000 | 0.985487000 | -1.223155000 |
| 6 | 2.483205000 | 2.925442000 | -1.144042000 |
| 1 | 2.724030000 | 3.396721000 | -2.097862000 |
| 6 | -1.755057000 | 1.509275000 | 0.026585000 |
| 1 | -2.408539000 | 2.381617000 | 0.044701000 |
| 6 | 1.828877000 | 1.649414000 | 1.186547000 |
| 1 | 1.546073000 | 1.100982000 | 2.091051000 |
| 6 | 3.666154000 | -1.451940000 | -0.010533000 |
| 1 | 4.754767000 | -1.500729000 | -0.004662000 |
| 6 | 1.844420000 | 1.687085000 | -1.119683000 |
| 1 | 1.573596000 | 1.168579000 | -2.045213000 |
| 6 | 2.799424000 | 3.536349000 | 0.070280000 |
| 6 | 3.814474000 | -1.425330000 | -2.518104000 |
| 1 | 4.878605000 | -1.619663000 | -2.341688000 |
| 1 | 3.701581000 | -0.438629000 | -2.996967000 |
| 6 | -1.859528000 | 1.654217000 | -2.477163000 |
| 1 | -1.002213000 | 2.180263000 | -2.929681000 |
| 1 | -2.662442000 | 2.376859000 | -2.287379000 |
| 6 | 3.784148000 | -1.505347000 | 2.497907000 |
| 1 | 3.667058000 | -0.532620000 | 3.003704000 |
| 1 | 4.850086000 | -1.695812000 | 2.328272000 |
| 6 | -1.915085000 | 1.508621000 | 2.531966000 |
| 1 | -2.741744000 | 2.211035000 | 2.369888000 |
| 1 | -1.080748000 | 2.043502000 | 3.016163000 |
| 1 | 3.401612000 | -2.170461000 | -3.213177000 |
| 1 | -2.194318000 | 0.893189000 | -3.195298000 |
| 1 | 3.298668000 | 4.507322000 | 0.089376000 |
| 1 | 2.694833000 | 3.326492000 | 2.231395000 |
| 7 | -4.241748000 | -0.648924000 | -1.436310000 |
| 6 | -3.576131000 | -1.576633000 | 0.684149000 |
| 6 | -5.135309000 | 0.245605000 | 0.613219000 |
| 1 | -5.790821000 | 0.973564000 | 1.094475000 |
| 6 | -3.530216000 | -1.518941000 | -0.709972000 |
| 1 | -2.886912000 | -2.213233000 | -1.259835000 |
| 6 | -5.016046000 | 0.221422000 | -0.777489000 |
| 1 | -5.583085000 | 0.935187000 | -1.384237000 |
| 6 | -4.402848000 | -0.678450000 | 1.360051000 |
| 1 | -4.470496000 | -0.693584000 | 2.450416000 |
| 1 | -2.966341000 | -2.306688000 | 1.219459000 |
| **pyridine: TS2 (ΔG=9.2) $\nu_1$= -82cm$^{-1}$** | | | |
| 1 | -4.172104000 | -0.318463000 | -2.776234000 |
| 1 | 2.605388000 | 1.358979000 | -2.743286000 |
| 23 | -0.384443000 | -1.305734000 | -0.525775000 |
| 8 | -2.025608000 | -0.568905000 | -1.237395000 |

| | | | |
|---|---|---|---|
| 8 | 0.502422000 | 0.181095000 | -1.483829000 |
| 8 | -1.491098000 | -2.267219000 | 0.821547000 |
| 8 | 0.244666000 | -0.340015000 | 1.154389000 |
| 8 | -0.056425000 | -2.500977000 | -1.484916000 |
| 6 | -1.886623000 | 2.267859000 | 0.558147000 |
| 6 | -0.565793000 | 4.032538000 | 1.507875000 |
| 6 | -3.252695000 | -0.785987000 | -0.916625000 |
| 6 | -2.758488000 | -2.343553000 | 0.930307000 |
| 6 | 1.288186000 | 1.113494000 | -1.095980000 |
| 6 | 1.032942000 | 0.652143000 | 1.307872000 |
| 6 | -0.905306000 | 3.781901000 | -0.853240000 |
| 1 | -0.741462000 | 4.120775000 | -1.881613000 |
| 6 | 1.609848000 | 1.367058000 | 0.244107000 |
| 1 | 2.265172000 | 2.207896000 | 0.473061000 |
| 6 | -1.362980000 | 2.901344000 | 1.687042000 |
| 1 | -1.575171000 | 2.507911000 | 2.682964000 |
| 6 | -3.662397000 | -1.643534000 | 0.107426000 |
| 1 | -4.729801000 | -1.758577000 | 0.292939000 |
| 7 | -1.677946000 | 2.701151000 | -0.690232000 |
| 6 | -0.326818000 | 4.480545000 | 0.208098000 |
| 6 | -3.271209000 | -3.231392000 | 2.021432000 |
| 1 | -4.366006000 | -3.250862000 | 2.064948000 |
| 1 | -2.867036000 | -2.884248000 | 2.984248000 |
| 6 | 1.354766000 | 1.042996000 | 2.720026000 |
| 1 | 0.491173000 | 0.843757000 | 3.368699000 |
| 1 | 1.658976000 | 2.095006000 | 2.795967000 |
| 6 | -4.257288000 | -0.021914000 | -1.719560000 |
| 1 | -4.002098000 | 1.047784000 | -1.666741000 |
| 1 | -5.283867000 | -0.183908000 | -1.371961000 |
| 6 | 1.872925000 | 1.963529000 | -2.182863000 |
| 1 | 2.370911000 | 2.858340000 | -1.789979000 |
| 1 | 1.079180000 | 2.249186000 | -2.888459000 |
| 1 | -2.887750000 | -4.250303000 | 1.860766000 |
| 1 | 2.190863000 | 0.415854000 | 3.073385000 |
| 1 | 0.291669000 | 5.358264000 | 0.012979000 |
| 1 | -0.136443000 | 4.553990000 | 2.366449000 |
| 7 | 2.379935000 | -1.925490000 | 0.019398000 |
| 6 | 4.247216000 | -1.038446000 | -1.205737000 |
| 6 | 4.315897000 | -1.119504000 | 1.193033000 |
| 1 | 4.809682000 | -0.942157000 | 2.149985000 |
| 6 | 2.977602000 | -1.614308000 | -1.134922000 |
| 1 | 2.406960000 | -1.815676000 | -2.047318000 |
| 6 | 3.039921000 | -1.681369000 | 1.156906000 |
| 1 | 2.520977000 | -1.930550000 | 2.088198000 |
| 6 | 4.928963000 | -0.783909000 | -0.015478000 |
| 1 | 5.922500000 | -0.330555000 | -0.028887000 |
| 1 | 4.684273000 | -0.794451000 | -2.175633000 |
| 1 | -2.511401000 | 1.375473000 | 0.678626000 |
| **pyridine: cis bound product (ΔG=-0.1)** | | | |
| 1 | -2.068491000 | -4.101876000 | -1.907788000 |
| 1 | -0.157247000 | 3.481386000 | -2.280042000 |

| | | | |
|---|---|---|---|
| 23 | 0.966365000 | -0.675895000 | -0.975532000 |
| 8 | -0.604311000 | -1.858871000 | -1.206637000 |
| 8 | -0.147784000 | 0.863382000 | -1.552083000 |
| 8 | 1.795873000 | -2.074488000 | 0.146434000 |
| 8 | 0.087417000 | -0.198036000 | 0.929936000 |
| 8 | 1.741917000 | -0.901937000 | -2.324755000 |
| 6 | -3.262860000 | -0.397588000 | 0.697126000 |
| 6 | -4.120110000 | 1.720099000 | 1.431384000 |
| 6 | -0.889842000 | -2.936219000 | -0.584243000 |
| 6 | 1.245421000 | -3.109918000 | 0.660543000 |
| 6 | -0.558448000 | 1.899874000 | -0.917731000 |
| 6 | -0.303770000 | 0.936347000 | 1.338211000 |
| 6 | -3.882055000 | 1.139400000 | -0.883694000 |
| 1 | -3.988656000 | 1.387162000 | -1.945062000 |
| 6 | -0.581167000 | 2.021344000 | 0.476292000 |
| 1 | -0.949102000 | 2.951936000 | 0.909699000 |
| 6 | -3.616394000 | 0.456973000 | 1.743620000 |
| 1 | -3.491935000 | 0.134705000 | 2.778952000 |
| 6 | -0.054256000 | -3.549275000 | 0.367346000 |
| 1 | -0.411611000 | -4.456837000 | 0.853640000 |
| 7 | -3.402060000 | -0.075594000 | -0.593262000 |
| 6 | -4.251367000 | 2.072142000 | 0.087345000 |
| 6 | 2.092463000 | -3.873155000 | 1.631819000 |
| 1 | 1.601182000 | -4.784259000 | 1.991889000 |
| 1 | 2.325286000 | -3.219635000 | 2.487040000 |
| 6 | -0.448896000 | 1.114345000 | 2.821452000 |
| 1 | -0.836447000 | 0.189435000 | 3.270355000 |
| 1 | -1.087340000 | 1.967363000 | 3.084268000 |
| 6 | -2.196295000 | -3.572893000 | -0.949352000 |
| 1 | -2.950376000 | -2.789439000 | -1.107220000 |
| 1 | -2.532771000 | -4.294613000 | -0.195450000 |
| 6 | -1.030744000 | 3.035971000 | -1.775934000 |
| 1 | -1.545402000 | 3.812434000 | -1.196429000 |
| 1 | -1.695242000 | 2.648836000 | -2.562074000 |
| 1 | 3.049201000 | -4.128733000 | 1.152628000 |
| 1 | 0.558304000 | 1.287026000 | 3.238658000 |
| 1 | -4.637757000 | 3.048494000 | -0.210468000 |
| 1 | -4.405351000 | 2.417681000 | 2.222020000 |
| 7 | 2.395266000 | 0.740354000 | -0.235724000 |
| 6 | 3.541028000 | 2.811840000 | -0.576162000 |
| 6 | 3.731310000 | 1.653741000 | 1.523107000 |
| 1 | 4.115269000 | 1.559571000 | 2.539395000 |
| 6 | 2.709464000 | 1.787039000 | -1.015220000 |
| 1 | 2.272636000 | 1.794126000 | -2.017295000 |
| 6 | 2.891817000 | 0.670782000 | 1.008841000 |
| 1 | 2.596388000 | -0.198326000 | 1.600575000 |
| 6 | 4.059415000 | 2.744966000 | 0.717626000 |
| 1 | 4.712069000 | 3.535070000 | 1.094313000 |
| 1 | 3.770574000 | 3.645641000 | -1.240304000 |
| 1 | -2.855196000 | -1.390164000 | 0.921396000 |

for trans ⇌ cis isomerization

| **$VO(acac)_2$(trans-isoQ) (ΔG=0.0)** | | | |
|---|---|---|---|
| 1 | -13.275072000 | 10.281348000 | 2.772287000 |
| 1 | -7.932284000 | 6.721841000 | 2.872261000 |
| 1 | -7.653357000 | 13.476362000 | -0.473852000 |
| 23 | -10.057304000 | 9.414659000 | 5.859066000 |
| 8 | -11.344175000 | 9.921365000 | 4.439577000 |
| 8 | -9.063726000 | 8.406169000 | 4.471287000 |
| 8 | -10.649154000 | 11.002851000 | 6.884828000 |
| 8 | -8.391441000 | 9.488651000 | 6.929207000 |
| 8 | -10.836444000 | 8.257865000 | 6.574609000 |
| 7 | -8.847070000 | 11.205849000 | 4.727674000 |
| 6 | -8.229992000 | 12.327010000 | 2.690239000 |
| 6 | -6.968072000 | 14.426749000 | 2.732525000 |
| 6 | -11.974677000 | 11.024391000 | 4.293003000 |
| 6 | -11.353530000 | 11.993447000 | 6.486794000 |
| 6 | -7.799990000 | 8.247579000 | 4.357754000 |
| 6 | -7.197585000 | 9.216054000 | 6.558583000 |
| 6 | -7.601830000 | 13.254344000 | 4.852186000 |
| 1 | -7.118480000 | 14.021310000 | 5.460421000 |
| 6 | -6.998693000 | 14.456455000 | 1.355575000 |
| 6 | -6.858182000 | 8.637062000 | 5.324605000 |
| 1 | -5.804615000 | 8.450197000 | 5.118155000 |
| 6 | -8.843563000 | 11.271015000 | 3.413650000 |
| 1 | -9.349832000 | 10.463550000 | 2.870843000 |
| 6 | -11.996832000 | 12.061663000 | 5.240182000 |
| 1 | -12.570433000 | 12.958249000 | 5.006699000 |
| 6 | -8.230103000 | 12.186933000 | 5.444966000 |
| 1 | -8.268475000 | 12.074170000 | 6.532411000 |
| 6 | -7.586370000 | 13.356866000 | 3.434198000 |
| 6 | -11.444436000 | 13.145738000 | 7.438855000 |
| 1 | -12.153438000 | 13.912537000 | 7.106454000 |
| 1 | -10.441590000 | 13.594183000 | 7.531516000 |
| 6 | -6.119538000 | 9.580637000 | 7.531913000 |
| 1 | -6.086507000 | 10.679574000 | 7.612521000 |
| 1 | -5.133946000 | 9.211789000 | 7.225752000 |
| 6 | -7.642720000 | 13.428317000 | 0.616817000 |
| 6 | -12.695120000 | 11.189391000 | 2.990730000 |
| 1 | -11.939227000 | 11.290611000 | 2.193890000 |
| 1 | -13.347663000 | 12.069937000 | 2.978910000 |
| 6 | -7.339982000 | 7.625639000 | 3.075602000 |
| 1 | -6.270919000 | 7.384411000 | 3.083587000 |
| 1 | -7.544704000 | 8.336708000 | 2.258083000 |
| 6 | -8.248676000 | 12.379657000 | 1.270610000 |
| 1 | -8.749413000 | 11.579865000 | 0.719304000 |
| 1 | -11.725221000 | 12.776320000 | 8.435861000 |
| 1 | -6.377382000 | 9.191876000 | 8.527679000 |
| 1 | -6.473603000 | 15.217038000 | 3.301866000 |
| 1 | -6.522999000 | 15.280286000 | 0.819111000 |
| **$VO(acac)_2$(trans-isoQ) TS1 (ΔG=19.9) $\nu_1$= -74$cm^{-1}$** | | | |
| 1 | 0.465212000 | 4.154501000 | 1.806543000 |
| 1 | 5.384504000 | 1.500830000 | 1.329569000 |

| | | | |
|---|---|---|---|
| 1 | -5.381423000 | -0.678761000 | 2.900752000 |
| 23 | 1.486740000 | 0.378438000 | -0.445866000 |
| 8 | 0.764935000 | 2.003534000 | 0.374955000 |
| 8 | 2.957433000 | 0.624504000 | 0.821500000 |
| 8 | -0.500581000 | 1.305636000 | -2.107567000 |
| 8 | 1.986937000 | -1.551123000 | -0.431808000 |
| 8 | 2.189191000 | 0.754076000 | -1.788535000 |
| 7 | -0.446218000 | -0.554786000 | -0.130800000 |
| 6 | -2.575637000 | -0.765492000 | 0.957469000 |
| 6 | -4.369309000 | -2.107361000 | -0.030116000 |
| 6 | -0.337835000 | 2.678787000 | 0.486609000 |
| 6 | -1.455005000 | 1.950468000 | -1.638674000 |
| 6 | 4.015772000 | -0.087348000 | 0.973519000 |
| 6 | 3.123422000 | -2.070697000 | -0.169498000 |
| 6 | -2.139886000 | -1.909821000 | -1.150260000 |
| 1 | -2.455284000 | -2.559742000 | -1.968310000 |
| 6 | -5.183774000 | -1.771414000 | 1.030151000 |
| 6 | 4.173256000 | -1.378362000 | 0.457723000 |
| 1 | 5.107485000 | -1.906121000 | 0.647062000 |
| 6 | -1.250842000 | -0.262758000 | 0.869891000 |
| 1 | -0.862812000 | 0.383180000 | 1.663960000 |
| 6 | -1.405022000 | 2.673291000 | -0.395386000 |
| 1 | -2.276863000 | 3.272093000 | -0.125970000 |
| 6 | -0.879677000 | -1.376992000 | -1.135731000 |
| 1 | -0.157058000 | -1.579221000 | -1.928781000 |
| 6 | -3.041657000 | -1.609061000 | -0.090047000 |
| 6 | -2.770183000 | 1.944455000 | -2.377602000 |
| 1 | -2.604874000 | 1.729130000 | -3.441315000 |
| 1 | -3.326732000 | 2.883148000 | -2.254283000 |
| 6 | 3.286604000 | -3.511635000 | -0.540810000 |
| 1 | 2.524908000 | -4.104095000 | -0.011582000 |
| 1 | 4.284515000 | -3.894277000 | -0.298696000 |
| 6 | -4.715667000 | -0.930129000 | 2.072996000 |
| 6 | -0.419768000 | 3.503671000 | 1.740375000 |
| 1 | -0.386561000 | 2.830854000 | 2.612864000 |
| 1 | -1.330134000 | 4.113383000 | 1.786804000 |
| 6 | 5.101890000 | 0.541597000 | 1.788586000 |
| 1 | 5.983551000 | -0.103346000 | 1.876130000 |
| 1 | 4.709177000 | 0.768495000 | 2.791480000 |
| 6 | -3.431691000 | -0.433782000 | 2.040306000 |
| 1 | -3.054305000 | 0.217264000 | 2.832535000 |
| 1 | -3.388057000 | 1.132647000 | -1.955238000 |
| 1 | 3.093547000 | -3.627741000 | -1.617806000 |
| 1 | -4.728306000 | -2.754924000 | -0.833111000 |
| 1 | -6.205267000 | -2.155382000 | 1.072548000 |
| **$VO(acac)_2$(trans-isoQ) INT (ΔG=13.9)** | | | |
| 1 | 0.133971000 | 1.195208000 | 3.638969000 |
| 1 | 5.754191000 | 1.413683000 | 0.482337000 |
| 1 | -4.627933000 | -3.447604000 | 1.926635000 |
| 23 | 1.440659000 | 0.361154000 | -0.422835000 |
| 8 | 0.750943000 | 1.358172000 | 1.073520000 |

| | | | |
|---|---|---|---|
| 8 | 3.227708000 | 0.683013000 | 0.393699000 |
| 8 | -0.302272000 | 3.259621000 | -0.816451000 |
| 8 | 1.976638000 | -1.491913000 | -0.672285000 |
| 8 | 1.586784000 | 1.125350000 | -1.778354000 |
| 7 | -0.537146000 | -0.319744000 | -0.727985000 |
| 6 | -2.387371000 | -1.531587000 | 0.205369000 |
| 6 | -4.660329000 | -1.208204000 | -0.650056000 |
| 6 | -0.425090000 | 1.560506000 | 1.612585000 |
| 6 | -1.335394000 | 3.115173000 | -0.148174000 |
| 6 | 4.244852000 | -0.083974000 | 0.453997000 |
| 6 | 3.118488000 | -2.062560000 | -0.496557000 |
| 6 | -2.723216000 | 0.027010000 | -1.637968000 |
| 1 | -3.368730000 | 0.528123000 | -2.361808000 |
| 6 | -5.122049000 | -2.109534000 | 0.283566000 |
| 6 | 4.249338000 | -1.422823000 | 0.015851000 |
| 1 | 5.167814000 | -1.999440000 | 0.121011000 |
| 6 | -1.013809000 | -1.198541000 | 0.134734000 |
| 1 | -0.300887000 | -1.667862000 | 0.821683000 |
| 6 | -1.422582000 | 2.344309000 | 1.077620000 |
| 1 | -2.363587000 | 2.398124000 | 1.629647000 |
| 6 | -1.378171000 | 0.291453000 | -1.615012000 |
| 1 | -0.916382000 | 1.009829000 | -2.293473000 |
| 6 | -3.276257000 | -0.895250000 | -0.708837000 |
| 6 | -2.622024000 | 3.755600000 | -0.611685000 |
| 1 | -3.109877000 | 4.303794000 | 0.207347000 |
| 1 | -3.319784000 | 2.964392000 | -0.932601000 |
| 6 | 3.172071000 | -3.509493000 | -0.872755000 |
| 1 | 2.420159000 | -4.058323000 | -0.285438000 |
| 1 | 4.162589000 | -3.947491000 | -0.705667000 |
| 6 | -4.233385000 | -2.738894000 | 1.196135000 |
| 6 | -0.635268000 | 0.860623000 | 2.925356000 |
| 1 | -0.493020000 | -0.224027000 | 2.793112000 |
| 1 | -1.629193000 | 1.050791000 | 3.348805000 |
| 6 | 5.481721000 | 0.511855000 | 1.050794000 |
| 1 | 6.322728000 | -0.190648000 | 1.058791000 |
| 1 | 5.260113000 | 0.835431000 | 2.079145000 |
| 6 | -2.887054000 | -2.458412000 | 1.159978000 |
| 1 | -2.188229000 | -2.932194000 | 1.853358000 |
| 1 | -2.426329000 | 4.428672000 | -1.455933000 |
| 1 | 2.891526000 | -3.615565000 | -1.931551000 |
| 1 | -5.342497000 | -0.723554000 | -1.351832000 |
| 1 | -6.187017000 | -2.347168000 | 0.327880000 |
| **$VO(acac)_2$(trans-isoQ) TS2 (ΔG=14.9) $\nu_1$= -66$cm^{-1}$** | | | |
| 1 | 0.226901000 | 0.941135000 | 3.742487000 |
| 1 | 5.391481000 | 0.671874000 | 1.798807000 |
| 1 | -4.917521000 | -3.321187000 | 1.698319000 |
| 23 | 1.407899000 | 0.295293000 | -0.489885000 |
| 8 | 0.867013000 | 1.093836000 | 1.202370000 |
| 8 | 3.262397000 | 0.576702000 | 0.187811000 |
| 8 | 0.239405000 | 3.093216000 | -0.681331000 |
| 8 | 1.774943000 | -1.600372000 | -0.495101000 |

| | | | |
|---|---|---|---|
| 8 | 1.561363000 | 0.829719000 | -1.953526000 |
| 7 | -0.644357000 | -0.234834000 | -0.705277000 |
| 6 | -2.567485000 | -1.390881000 | 0.146710000 |
| 6 | -4.810655000 | -0.906665000 | -0.712416000 |
| 6 | -0.249327000 | 1.504858000 | 1.736949000 |
| 6 | -0.808165000 | 3.194115000 | -0.022627000 |
| 6 | 4.218024000 | -0.258108000 | 0.294795000 |
| 6 | 2.888202000 | -2.235984000 | -0.341265000 |
| 6 | -2.803532000 | 0.294455000 | -1.596797000 |
| 1 | -3.414142000 | 0.876558000 | -2.289700000 |
| 6 | -5.326627000 | -1.849530000 | 0.149085000 |
| 6 | 4.095107000 | -1.635176000 | 0.014225000 |
| 1 | 4.974462000 | -2.268025000 | 0.128910000 |
| 6 | -1.177065000 | -1.125890000 | 0.109694000 |
| 1 | -0.498091000 | -1.670105000 | 0.774517000 |
| 6 | -1.076892000 | 2.466306000 | 1.197169000 |
| 1 | -1.997181000 | 2.702836000 | 1.734949000 |
| 6 | -1.445446000 | 0.474317000 | -1.556565000 |
| 1 | -0.937398000 | 1.197864000 | -2.195790000 |
| 6 | -3.413092000 | -0.655538000 | -0.733259000 |
| 6 | -1.909966000 | 4.100840000 | -0.514918000 |
| 1 | -2.383166000 | 4.653227000 | 0.308890000 |
| 1 | -2.689960000 | 3.474044000 | -0.980035000 |
| 6 | 2.808898000 | -3.713038000 | -0.561462000 |
| 1 | 2.062880000 | -4.139087000 | 0.126401000 |
| 1 | 3.774924000 | -4.208653000 | -0.413341000 |
| 6 | -4.481103000 | -2.579698000 | 1.026567000 |
| 6 | -0.606808000 | 0.832341000 | 3.031926000 |
| 1 | -0.737232000 | -0.248390000 | 2.857788000 |
| 1 | -1.522492000 | 1.240501000 | 3.476988000 |
| 6 | 5.525098000 | 0.292203000 | 0.773937000 |
| 1 | 5.808184000 | 1.150481000 | 0.147307000 |
| 1 | 6.323016000 | -0.458936000 | 0.766103000 |
| 6 | -3.123515000 | -2.356313000 | 1.029047000 |
| 1 | -2.457403000 | -2.909002000 | 1.695706000 |
| 1 | -1.520003000 | 4.795421000 | -1.269843000 |
| 1 | 2.447132000 | -3.901414000 | -1.583717000 |
| 1 | -5.459072000 | -0.344616000 | -1.388081000 |
| 1 | -6.401360000 | -2.042925000 | 0.161086000 |
| **$VO(acac)_2$(cis-isoQ) (ΔG=1.4)** | | | |
| 1 | 0.591617000 | -0.590910000 | 3.708490000 |
| 1 | 5.803515000 | 0.562171000 | -0.235282000 |
| 1 | -5.339400000 | -2.795149000 | 1.347241000 |
| 23 | 1.269895000 | 0.336009000 | -0.895019000 |
| 8 | 0.956327000 | -0.014324000 | 1.233874000 |
| 8 | 3.172382000 | 0.503828000 | -0.348337000 |
| 8 | 0.968935000 | 2.206042000 | -0.320148000 |
| 8 | 1.471329000 | -1.630850000 | -0.830024000 |
| 8 | 1.346386000 | 0.580432000 | -2.445424000 |
| 7 | -0.852707000 | 0.111741000 | -0.884307000 |
| 6 | -2.858127000 | -0.930196000 | -0.075012000 |

| | | | |
|---|---|---|---|
| 6 | -5.061712000 | 0.019270000 | -0.565772000 |
| 6 | 0.229004000 | 0.666586000 | 2.015739000 |
| 6 | 0.244337000 | 2.700665000 | 0.617384000 |
| 6 | 3.940930000 | -0.403689000 | 0.118583000 |
| 6 | 2.412804000 | -2.312553000 | -0.292210000 |
| 6 | -2.970786000 | 1.098653000 | -1.417668000 |
| 1 | -3.537870000 | 1.890315000 | -1.910395000 |
| 6 | -5.643446000 | -0.999649000 | 0.156624000 |
| 6 | 3.608401000 | -1.767750000 | 0.199393000 |
| 1 | 4.343352000 | -2.449085000 | 0.627281000 |
| 6 | -1.450902000 | -0.853101000 | -0.212035000 |
| 1 | -0.812693000 | -1.606437000 | 0.259398000 |
| 6 | -0.188096000 | 1.990713000 | 1.741754000 |
| 1 | -0.802317000 | 2.508965000 | 2.478305000 |
| 6 | -1.602304000 | 1.084678000 | -1.485788000 |
| 1 | -1.041044000 | 1.853090000 | -2.021793000 |
| 6 | -3.649085000 | 0.077928000 | -0.696620000 |
| 6 | -0.140737000 | 4.138355000 | 0.437970000 |
| 1 | -0.661819000 | 4.546882000 | 1.311699000 |
| 1 | -0.795842000 | 4.215004000 | -0.445150000 |
| 6 | 2.171460000 | -3.787950000 | -0.204676000 |
| 1 | 1.313296000 | -3.964096000 | 0.463003000 |
| 1 | 3.043277000 | -4.333654000 | 0.173900000 |
| 6 | -4.851470000 | -2.000753000 | 0.779443000 |
| 6 | -0.231473000 | -0.004749000 | 3.276725000 |
| 1 | -1.030860000 | -0.715518000 | 3.003461000 |
| 1 | -0.629022000 | 0.702043000 | 4.014963000 |
| 6 | 5.282007000 | 0.063747000 | 0.595786000 |
| 1 | 5.899833000 | -0.755711000 | 0.980346000 |
| 1 | 5.136805000 | 0.819452000 | 1.382548000 |
| 6 | -3.480416000 | -1.970242000 | 0.667138000 |
| 1 | -2.853533000 | -2.731306000 | 1.138048000 |
| 1 | 0.758647000 | 4.734312000 | 0.224045000 |
| 1 | 1.890576000 | -4.169641000 | -1.197195000 |
| 1 | -5.670190000 | 0.790265000 | -1.043385000 |
| 1 | -6.730163000 | -1.042197000 | 0.256000000 |
| **$VO(acac)_2$(trans-Q) (ΔG=0.0)** | | | |
| 1 | 0.900194000 | -4.276519000 | -1.834093000 |
| 6 | 0.674577000 | -3.263838000 | -2.187231000 |
| 1 | 0.233563000 | -3.305447000 | -3.194058000 |
| 1 | 1.610119000 | -2.686787000 | -2.268740000 |
| 1 | 0.231419000 | 3.305124000 | -3.194160000 |
| 1 | 0.896431000 | 4.277411000 | -1.834250000 |
| 23 | -1.696258000 | -0.000586000 | -0.733599000 |
| 8 | -2.100028000 | 1.362812000 | 0.641261000 |
| 8 | -2.098837000 | -1.364255000 | 0.641379000 |
| 8 | -0.637323000 | 1.378329000 | -1.676112000 |
| 8 | -0.636335000 | -1.378894000 | -1.676049000 |
| 7 | 0.471561000 | 0.000229000 | 0.709471000 |
| 8 | -3.014229000 | -0.000758000 | -1.575000000 |
| 6 | -1.557991000 | 2.506957000 | 0.830624000 |

| | | | |
|---|---|---|---|
| 6 | -0.256083000 | -2.530832000 | -1.271444000 |
| 6 | -1.556062000 | -2.508079000 | 0.830564000 |
| 6 | 1.781245000 | 0.000644000 | 0.307197000 |
| 6 | 2.104378000 | 0.000740000 | -1.079005000 |
| 1 | 1.287456000 | 0.000473000 | -1.799227000 |
| 6 | -0.258078000 | 2.530600000 | -1.271418000 |
| 6 | 2.519286000 | 0.000843000 | 2.636922000 |
| 1 | 3.324504000 | 0.001056000 | 3.376053000 |
| 6 | 2.848419000 | 0.000968000 | 1.256357000 |
| 6 | 0.207482000 | 0.000150000 | 2.002288000 |
| 1 | -0.850878000 | -0.000150000 | 2.281451000 |
| 6 | 1.198020000 | 0.000445000 | 3.012981000 |
| 1 | 0.896819000 | 0.000320000 | 4.061119000 |
| 6 | 3.419995000 | 0.001168000 | -1.488796000 |
| 1 | 3.652192000 | 0.001231000 | -2.556191000 |
| 6 | 4.478129000 | 0.001512000 | -0.544465000 |
| 1 | 5.513389000 | 0.001876000 | -0.891180000 |
| 6 | -1.925753000 | 3.192411000 | 2.109513000 |
| 1 | -1.564061000 | 4.226156000 | 2.151916000 |
| 1 | -1.480631000 | 2.620337000 | 2.940843000 |
| 6 | -0.648243000 | -3.110921000 | -0.053834000 |
| 1 | -0.257150000 | -4.096139000 | 0.198892000 |
| 6 | 4.195732000 | 0.001407000 | 0.801961000 |
| 1 | 4.995211000 | 0.001644000 | 1.546955000 |
| 6 | -0.650594000 | 3.110394000 | -0.053804000 |
| 1 | -0.260096000 | 4.095857000 | 0.198887000 |
| 6 | 0.672081000 | 3.264368000 | -2.187154000 |
| 1 | 1.608310000 | 2.688330000 | -2.268088000 |
| 6 | -1.923294000 | -3.193878000 | 2.109432000 |
| 1 | -1.476616000 | -2.622765000 | 2.940616000 |
| 1 | -1.562599000 | -4.228003000 | 2.150953000 |
| 1 | -3.013689000 | -3.163538000 | 2.245978000 |
| 1 | -3.016330000 | 3.163194000 | 2.244859000 |
| **$VO(acac)_2$(trans-Q) TS1 ($\Delta G$=19.2) $\nu_1$= -27$cm^{-1}$** | | | |
| 1 | -3.698018000 | -4.031314000 | 0.183998000 |
| 6 | -2.687487000 | -3.630411000 | 0.046160000 |
| 1 | -2.249974000 | -4.027627000 | -0.881740000 |
| 1 | -2.043251000 | -3.963257000 | 0.874285000 |
| 1 | 3.851750000 | 1.421685000 | -2.459639000 |
| 1 | 4.188440000 | 2.375343000 | -0.966634000 |
| 23 | -1.118100000 | 0.311158000 | -0.655628000 |
| 8 | -0.688596000 | 2.202510000 | -0.307172000 |
| 8 | -2.849325000 | 0.742027000 | 0.125261000 |
| 8 | 1.344885000 | 1.075420000 | -1.959238000 |
| 8 | -1.534902000 | -1.593101000 | -0.212492000 |
| 7 | 0.564379000 | -0.181294000 | 0.631060000 |
| 8 | -1.384832000 | 0.214819000 | -2.191072000 |
| 6 | 0.326598000 | 2.916111000 | 0.077495000 |
| 6 | -2.670952000 | -2.134599000 | -0.007195000 |
| 6 | -3.878489000 | -0.012564000 | 0.297785000 |
| 6 | 1.601870000 | -1.016838000 | 0.320084000 |

| | | | |
|---|---|---|---|
| 6 | 1.626852000 | -1.682216000 | -0.933089000 |
| 1 | 0.797102000 | -1.519095000 | -1.624426000 |
| 6 | 2.104488000 | 1.766964000 | -1.259184000 |
| 6 | 2.592156000 | -0.565329000 | 2.504487000 |
| 1 | 3.400278000 | -0.712869000 | 3.225071000 |
| 6 | 2.664833000 | -1.216288000 | 1.245412000 |
| 6 | 0.514320000 | 0.401481000 | 1.816561000 |
| 1 | -0.352630000 | 1.043995000 | 2.007551000 |
| 6 | 1.509826000 | 0.230461000 | 2.800736000 |
| 1 | 1.410194000 | 0.737945000 | 3.760212000 |
| 6 | 2.690468000 | -2.493939000 | -1.254253000 |
| 1 | 2.710752000 | -3.003242000 | -2.219843000 |
| 6 | 3.767710000 | -2.677211000 | -0.346855000 |
| 1 | 4.603556000 | -3.320918000 | -0.627424000 |
| 6 | -0.026158000 | 4.005634000 | 1.050931000 |
| 1 | 0.834136000 | 4.632076000 | 1.316562000 |
| 1 | -0.440945000 | 3.548546000 | 1.964432000 |
| 6 | -3.858589000 | -1.405687000 | 0.193385000 |
| 1 | -4.783938000 | -1.954478000 | 0.365847000 |
| 6 | 3.754025000 | -2.054996000 | 0.879842000 |
| 1 | 4.568203000 | -2.193645000 | 1.594866000 |
| 6 | 1.647502000 | 2.733809000 | -0.294931000 |
| 1 | 2.393107000 | 3.382718000 | 0.167753000 |
| 6 | 3.594098000 | 1.560995000 | -1.400245000 |
| 1 | 3.852560000 | 0.622551000 | -0.876763000 |
| 6 | -5.141862000 | 0.704343000 | 0.655808000 |
| 1 | -4.977772000 | 1.277194000 | 1.581118000 |
| 1 | -5.985754000 | 0.018483000 | 0.791102000 |
| 1 | -5.376203000 | 1.432435000 | -0.135360000 |
| 1 | -0.821016000 | 4.634166000 | 0.621168000 |
| **$VO(acac)_2$(trans-Q) INT (ΔG=14.5)** | | | |
| 1 | -4.798991000 | -3.357923000 | -0.024065000 |
| 6 | -3.723260000 | -3.176908000 | 0.080759000 |
| 1 | -3.173075000 | -3.759903000 | -0.673407000 |
| 1 | -3.381722000 | -3.525498000 | 1.067157000 |
| 1 | 4.106075000 | 1.287974000 | -0.403402000 |
| 1 | 3.831544000 | 2.184384000 | -1.938757000 |
| 23 | -1.168613000 | 0.200779000 | -0.370508000 |
| 8 | -0.530666000 | 1.740268000 | 0.594634000 |
| 8 | -2.932190000 | 1.108239000 | -0.271678000 |
| 8 | 1.357204000 | 2.170736000 | -1.515433000 |
| 8 | -2.119469000 | -1.453460000 | 0.048338000 |
| 7 | 0.568789000 | -0.853809000 | 0.380638000 |
| 8 | -0.940689000 | 0.221068000 | -1.914808000 |
| 6 | 0.521970000 | 2.030075000 | 1.318082000 |
| 6 | -3.370805000 | -1.731466000 | -0.073974000 |
| 6 | -4.101400000 | 0.601687000 | -0.355431000 |
| 6 | 1.793213000 | -1.064913000 | -0.209500000 |
| 6 | 1.967423000 | -0.905184000 | -1.608608000 |
| 1 | 1.113920000 | -0.591645000 | -2.207544000 |
| 6 | 2.165002000 | 2.186156000 | -0.576855000 |

| | | | |
|---|---|---|---|
| 6 | 2.722804000 | -1.663769000 | 1.974220000 |
| 1 | 3.576204000 | -1.965908000 | 2.586190000 |
| 6 | 2.908908000 | -1.473329000 | 0.581034000 |
| 6 | 0.425718000 | -1.075387000 | 1.678852000 |
| 1 | -0.573872000 | -0.901739000 | 2.092871000 |
| 6 | 1.476500000 | -1.481198000 | 2.525082000 |
| 1 | 1.282908000 | -1.632102000 | 3.587047000 |
| 6 | 3.198555000 | -1.131788000 | -2.183870000 |
| 1 | 3.318351000 | -1.006770000 | -3.262081000 |
| 6 | 4.311977000 | -1.525092000 | -1.399548000 |
| 1 | 5.278138000 | -1.696735000 | -1.877814000 |
| 6 | 0.247473000 | 2.169159000 | 2.788572000 |
| 1 | 1.155731000 | 2.376472000 | 3.367817000 |
| 1 | -0.232144000 | 1.253060000 | 3.167414000 |
| 6 | -4.364813000 | -0.779859000 | -0.315781000 |
| 1 | -5.398226000 | -1.115320000 | -0.395999000 |
| 6 | 4.168370000 | -1.691368000 | -0.041588000 |
| 1 | 5.008636000 | -2.000805000 | 0.584166000 |
| 6 | 1.793760000 | 2.210086000 | 0.826100000 |
| 1 | 2.590901000 | 2.398557000 | 1.548946000 |
| 6 | 3.648710000 | 2.182901000 | -0.856541000 |
| 1 | 4.128244000 | 3.058773000 | -0.393133000 |
| 6 | -5.230812000 | 1.576827000 | -0.474192000 |
| 1 | -5.241933000 | 2.218292000 | 0.420233000 |
| 1 | -6.201622000 | 1.079842000 | -0.581014000 |
| 1 | -5.048441000 | 2.233073000 | -1.338138000 |
| 1 | -0.473335000 | 2.988071000 | 2.941419000 |
| **$VO(acac)_2$(trans-Q) TS2 (ΔG=16.2) $\nu_1$= -84$cm^{-1}$** | | | |
| 1 | -4.801210000 | -3.276617000 | 0.068927000 |
| 6 | -3.719888000 | -3.114426000 | 0.141710000 |
| 1 | -3.199485000 | -3.738473000 | -0.600654000 |
| 1 | -3.362404000 | -3.430402000 | 1.133465000 |
| 1 | 3.909409000 | 1.624697000 | -0.303289000 |
| 1 | 3.402622000 | 2.676399000 | -1.669702000 |
| 23 | -1.106948000 | 0.170092000 | -0.463323000 |
| 8 | -0.672024000 | 1.392466000 | 1.000629000 |
| 8 | -2.851862000 | 1.134527000 | -0.431122000 |
| 8 | 1.000759000 | 2.210975000 | -1.110619000 |
| 8 | -2.079378000 | -1.432350000 | 0.003175000 |
| 7 | 0.646705000 | -0.928138000 | 0.188606000 |
| 8 | -0.911682000 | 0.158259000 | -2.016262000 |
| 6 | 0.373816000 | 1.713317000 | 1.708054000 |
| 6 | -3.343631000 | -1.684229000 | -0.079511000 |
| 6 | -4.030280000 | 0.653002000 | -0.453741000 |
| 6 | 1.893460000 | -0.977813000 | -0.392667000 |
| 6 | 2.082700000 | -0.613966000 | -1.751719000 |
| 1 | 1.220641000 | -0.282337000 | -2.327244000 |
| 6 | 1.865650000 | 2.258267000 | -0.221379000 |
| 6 | 2.825767000 | -1.814171000 | 1.710049000 |
| 1 | 3.687318000 | -2.142187000 | 2.296798000 |
| 6 | 3.022262000 | -1.413961000 | 0.363756000 |

| | | | |
|---|---|---|---|
| 6 | 0.498754000 | -1.336748000 | 1.440074000 |
| 1 | -0.512521000 | -1.277164000 | 1.852709000 |
| 6 | 1.560229000 | -1.794172000 | 2.245966000 |
| 1 | 1.359150000 | -2.105975000 | 3.270955000 |
| 6 | 3.337793000 | -0.668673000 | -2.316825000 |
| 1 | 3.467093000 | -0.387221000 | -3.364061000 |
| 6 | 4.463844000 | -1.083237000 | -1.562106000 |
| 1 | 5.449356000 | -1.114512000 | -2.030507000 |
| 6 | 0.168132000 | 1.639335000 | 3.194642000 |
| 1 | 1.069886000 | 1.912326000 | 3.756474000 |
| 1 | -0.144293000 | 0.620256000 | 3.473734000 |
| 6 | -4.320009000 | -0.722819000 | -0.336143000 |
| 1 | -5.361977000 | -1.038723000 | -0.373930000 |
| 6 | 4.306719000 | -1.449088000 | -0.245522000 |
| 1 | 5.155600000 | -1.782424000 | 0.356002000 |
| 6 | 1.595569000 | 2.082815000 | 1.187971000 |
| 1 | 2.410861000 | 2.277663000 | 1.887848000 |
| 6 | 3.308882000 | 2.504370000 | -0.589770000 |
| 1 | 3.711114000 | 3.364470000 | -0.033443000 |
| 6 | -5.145487000 | 1.642707000 | -0.586241000 |
| 1 | -5.134582000 | 2.307020000 | 0.291539000 |
| 1 | -6.125475000 | 1.158793000 | -0.665187000 |
| 1 | -4.964540000 | 2.272997000 | -1.469290000 |
| 1 | -0.655884000 | 2.312192000 | 3.479044000 |
| **$VO(acac)_2$(cis-Q) (ΔG=2.0)** | | | |
| 1 | -4.648093000 | -3.066503000 | -0.489391000 |
| 6 | -3.564904000 | -2.978167000 | -0.630642000 |
| 1 | -3.270875000 | -3.455192000 | -1.577307000 |
| 1 | -3.044916000 | -3.517306000 | 0.176616000 |
| 1 | 2.429303000 | 3.129453000 | 0.313218000 |
| 1 | 1.082531000 | 4.171028000 | 0.798382000 |
| 23 | -0.803090000 | 0.294639000 | -0.781792000 |
| 8 | -1.124607000 | -0.084333000 | 1.327126000 |
| 8 | -2.505273000 | 1.299109000 | -0.630537000 |
| 8 | 0.115187000 | 1.885575000 | -0.047895000 |
| 8 | -1.857213000 | -1.380040000 | -0.873254000 |
| 7 | 0.986506000 | -0.866034000 | -0.339956000 |
| 8 | -0.500379000 | 0.463254000 | -2.315259000 |
| 6 | -0.383886000 | 0.265636000 | 2.293647000 |
| 6 | -3.101989000 | -1.553816000 | -0.633344000 |
| 6 | -3.680454000 | 0.846152000 | -0.414789000 |
| 6 | 2.268754000 | -0.445252000 | -0.615269000 |
| 6 | 2.506074000 | 0.697369000 | -1.425403000 |
| 1 | 1.655640000 | 1.232313000 | -1.843834000 |
| 6 | 0.732507000 | 2.085405000 | 1.059492000 |
| 6 | 3.156056000 | -2.322477000 | 0.678798000 |
| 1 | 4.010057000 | -2.873947000 | 1.079634000 |
| 6 | 3.390526000 | -1.159224000 | -0.097554000 |
| 6 | 0.808733000 | -1.966488000 | 0.375597000 |
| 1 | -0.225765000 | -2.260263000 | 0.563197000 |
| 6 | 1.865325000 | -2.735878000 | 0.904252000 |

| | | | |
|---|---|---|---|
| 1 | 1.636049000 | -3.630135000 | 1.483962000 |
| 6 | 3.795133000 | 1.115070000 | -1.677178000 |
| 1 | 3.959902000 | 1.995211000 | -2.302472000 |
| 6 | 4.908925000 | 0.419920000 | -1.144224000 |
| 1 | 5.920408000 | 0.771905000 | -1.355286000 |
| 6 | -0.549600000 | -0.484605000 | 3.582480000 |
| 1 | -0.049671000 | 0.003353000 | 4.427618000 |
| 1 | -0.114107000 | -1.489001000 | 3.443768000 |
| 6 | -4.015418000 | -0.518593000 | -0.382350000 |
| 1 | -5.053693000 | -0.787432000 | -0.189751000 |
| 6 | 4.707518000 | -0.700705000 | -0.372968000 |
| 1 | 5.547795000 | -1.263593000 | 0.040011000 |
| 6 | 0.584742000 | 1.291711000 | 2.202065000 |
| 1 | 1.162926000 | 1.547070000 | 3.090144000 |
| 6 | 1.649828000 | 3.270887000 | 1.079178000 |
| 1 | 2.119724000 | 3.420452000 | 2.058272000 |
| 6 | -4.742026000 | 1.878643000 | -0.188363000 |
| 1 | -4.471435000 | 2.476791000 | 0.695167000 |
| 1 | -5.733602000 | 1.435445000 | -0.042055000 |
| 1 | -4.764540000 | 2.566196000 | -1.047053000 |
| 1 | -1.618911000 | -0.622353000 | 3.796054000 |
| **$VO(acac)_2$(trans-P) (ΔG=0.0)** | | | |
| 1 | -3.198796000 | 0.971427000 | 3.188059000 |
| 1 | 3.198009000 | 0.963513000 | 3.191212000 |
| 23 | 0.001541000 | 1.407821000 | -0.004091000 |
| 8 | -1.359948000 | 1.012823000 | 1.378584000 |
| 8 | 1.360996000 | 1.010044000 | 1.379824000 |
| 8 | -1.358779000 | 1.004763000 | -1.385934000 |
| 8 | 1.362113000 | 1.002457000 | -1.384767000 |
| 8 | 0.002094000 | 2.975318000 | -0.008317000 |
| 7 | -0.001036000 | -1.044437000 | 0.003207000 |
| 6 | -0.006216000 | -3.112860000 | 1.211689000 |
| 6 | -2.504590000 | 0.460203000 | 1.236273000 |
| 6 | -2.502577000 | 0.451015000 | -1.241363000 |
| 6 | 2.504688000 | 0.455310000 | 1.238308000 |
| 6 | 2.505518000 | 0.448031000 | -1.239356000 |
| 6 | -0.002201000 | -3.120217000 | -1.192591000 |
| 1 | -0.001345000 | -3.635783000 | -2.153838000 |
| 6 | 3.093120000 | 0.148061000 | 0.000552000 |
| 1 | 4.074781000 | -0.325150000 | 0.002305000 |
| 6 | -0.003980000 | -1.720141000 | 1.158530000 |
| 1 | -0.004704000 | -1.115559000 | 2.071450000 |
| 6 | -3.091985000 | 0.152707000 | -0.001871000 |
| 1 | -4.074256000 | -0.319242000 | -0.000919000 |
| 6 | -0.000082000 | -1.727180000 | -1.147959000 |
| 1 | 0.002602000 | -1.128180000 | -2.064577000 |
| 6 | -0.005348000 | -3.825540000 | 0.011707000 |
| 6 | -3.208996000 | 0.086707000 | -2.510537000 |
| 1 | -4.241791000 | -0.237994000 | -2.339387000 |
| 1 | -2.648185000 | -0.732544000 | -2.990212000 |
| 6 | 3.213367000 | 0.085120000 | -2.508116000 |

| | | | |
|---|---|---|---|
| 1 | 2.650372000 | -0.730027000 | -2.992127000 |
| 1 | 4.244539000 | -0.244046000 | -2.335765000 |
| 6 | -3.214284000 | 0.108380000 | 2.507129000 |
| 1 | -2.652275000 | -0.702593000 | 2.999182000 |
| 1 | -4.245383000 | -0.221760000 | 2.336220000 |
| 6 | 3.212264000 | 0.100936000 | 2.509651000 |
| 1 | 4.242786000 | -0.231427000 | 2.339613000 |
| 1 | 2.647824000 | -0.709076000 | 3.000495000 |
| 1 | -3.187802000 | 0.941127000 | -3.202034000 |
| 1 | 3.197154000 | 0.942118000 | -3.196593000 |
| 1 | -0.007113000 | -4.917567000 | 0.015071000 |
| 1 | -0.008617000 | -3.622499000 | 2.176089000 |
| **$VO(acac)_2$(trans-P) TS1 ($\Delta G$=20.0) $\nu_1$= -79$cm^{-1}$** | | | |
| 1 | 1.042153000 | -4.151034000 | 1.064047000 |
| 1 | -4.257655000 | -2.863682000 | 0.096182000 |
| 23 | -0.675970000 | -0.305547000 | -0.513223000 |
| 8 | 0.372539000 | -1.844088000 | 0.068967000 |
| 8 | -2.172879000 | -1.273610000 | 0.283711000 |
| 8 | 1.850737000 | -0.189300000 | -1.805679000 |
| 8 | -1.756914000 | 1.342896000 | -0.244463000 |
| 8 | -0.953493000 | -0.468073000 | -2.041153000 |
| 7 | 0.780255000 | 0.949905000 | 0.491498000 |
| 6 | 2.423872000 | 1.393655000 | 2.166901000 |
| 6 | 1.588228000 | -2.219450000 | 0.330156000 |
| 6 | 2.831798000 | -0.671319000 | -1.214823000 |
| 6 | -3.409354000 | -0.931257000 | 0.360826000 |
| 6 | -3.026765000 | 1.444815000 | -0.148885000 |
| 6 | 2.141079000 | 2.906994000 | 0.315981000 |
| 1 | 2.400985000 | 3.811091000 | -0.235435000 |
| 6 | -3.883755000 | 0.358039000 | 0.096264000 |
| 1 | -4.953202000 | 0.548004000 | 0.182309000 |
| 6 | 1.406829000 | 0.610109000 | 1.625010000 |
| 1 | 1.072814000 | -0.307203000 | 2.116863000 |
| 6 | 2.751200000 | -1.705267000 | -0.214059000 |
| 1 | 3.693247000 | -2.111690000 | 0.158799000 |
| 6 | 1.130289000 | 2.077037000 | -0.151232000 |
| 1 | 0.579207000 | 2.306621000 | -1.066614000 |
| 6 | 2.802744000 | 2.554996000 | 1.495841000 |
| 6 | 4.204841000 | -0.118338000 | -1.509186000 |
| 1 | 4.216390000 | 0.360430000 | -2.496978000 |
| 1 | 4.989339000 | -0.884030000 | -1.440722000 |
| 6 | -3.583705000 | 2.827633000 | -0.282309000 |
| 1 | -3.123469000 | 3.473913000 | 0.480169000 |
| 1 | -4.674265000 | 2.850456000 | -0.177893000 |
| 6 | 1.674826000 | -3.303457000 | 1.368204000 |
| 1 | 1.261972000 | -2.922502000 | 2.316623000 |
| 1 | 2.701756000 | -3.651001000 | 1.533631000 |
| 6 | -4.349603000 | -2.013538000 | 0.788552000 |
| 1 | -5.390205000 | -1.671752000 | 0.822890000 |
| 1 | -4.046956000 | -2.374889000 | 1.783238000 |
| 1 | 4.425020000 | 0.651838000 | -0.749445000 |

| | | | |
|---|---|---|---|
| 1 | -3.295826000 | 3.233271000 | -1.263991000 |
| 1 | 3.602339000 | 3.185638000 | 1.889874000 |
| 1 | 2.906805000 | 1.088259000 | 3.095568000 |
| **VO(acac)$_2$(trans-P) INT (ΔG=13.5)** | | | |
| 1 | 0.682390000 | -1.854233000 | 3.335201000 |
| 1 | -4.270741000 | -2.998893000 | -0.523387000 |
| 23 | -0.729450000 | -0.235574000 | -0.435858000 |
| 8 | 0.277354000 | -1.336010000 | 0.778805000 |
| 8 | -2.267173000 | -1.386576000 | 0.073389000 |
| 8 | 2.083828000 | -1.932827000 | -1.392243000 |
| 8 | -1.927443000 | 1.282899000 | -0.215864000 |
| 8 | -0.567515000 | -0.576895000 | -1.952502000 |
| 7 | 0.848892000 | 1.169445000 | -0.278173000 |
| 6 | 2.042639000 | 2.609608000 | 1.210385000 |
| 6 | 1.415651000 | -1.263632000 | 1.421206000 |
| 6 | 2.944407000 | -1.671399000 | -0.540249000 |
| 6 | -3.513188000 | -1.109933000 | 0.086443000 |
| 6 | -3.212694000 | 1.322744000 | -0.142690000 |
| 6 | 3.003938000 | 1.981954000 | -0.905681000 |
| 1 | 3.805098000 | 2.012447000 | -1.645168000 |
| 6 | -4.028636000 | 0.193320000 | -0.046152000 |
| 1 | -5.108214000 | 0.333012000 | -0.001511000 |
| 6 | 0.928993000 | 1.846638000 | 0.879212000 |
| 1 | 0.072344000 | 1.759829000 | 1.554238000 |
| 6 | 2.663891000 | -1.390292000 | 0.854440000 |
| 1 | 3.523543000 | -1.284092000 | 1.519762000 |
| 6 | 1.858590000 | 1.232943000 | -1.159376000 |
| 1 | 1.742946000 | 0.654076000 | -2.077410000 |
| 6 | 3.101063000 | 2.673273000 | 0.302209000 |
| 6 | 4.399922000 | -1.612874000 | -0.938538000 |
| 1 | 4.524841000 | -1.969581000 | -1.968628000 |
| 1 | 5.021696000 | -2.206470000 | -0.252516000 |
| 6 | -3.811020000 | 2.693585000 | -0.149097000 |
| 1 | -3.412146000 | 3.259653000 | 0.706537000 |
| 1 | -4.905400000 | 2.670863000 | -0.097654000 |
| 6 | 1.276125000 | -1.035225000 | 2.899760000 |
| 1 | 0.710990000 | -0.106250000 | 3.075804000 |
| 1 | 2.244794000 | -0.978386000 | 3.411216000 |
| 6 | -4.441094000 | -2.267872000 | 0.281386000 |
| 1 | -5.493757000 | -1.963465000 | 0.288632000 |
| 1 | -4.192760000 | -2.769789000 | 1.228666000 |
| 1 | 4.748959000 | -0.569270000 | -0.870062000 |
| 1 | -3.490735000 | 3.221458000 | -1.059921000 |
| 1 | 3.992456000 | 3.259884000 | 0.533238000 |
| 1 | 2.074880000 | 3.139541000 | 2.162686000 |
| **VO(acac)$_2$(trans-P) TS2 (ΔG=15.1) $\nu_1$= -57cm$^{-1}$** | | | |
| 23 | -0.677349000 | -0.217850000 | -0.486713000 |
| 8 | -0.613294000 | -0.467050000 | -2.029766000 |
| 8 | 1.612363000 | -2.022983000 | -1.173857000 |
| 8 | 0.164912000 | -1.059429000 | 1.059236000 |
| 7 | 0.954795000 | 1.140209000 | -0.389540000 |

| | | | |
|---|---|---|---|
| 6 | 2.596645000 | -1.853106000 | -0.436667000 |
| 6 | 2.513705000 | -1.448675000 | 0.948049000 |
| 1 | 3.441030000 | -1.427052000 | 1.523972000 |
| 6 | 1.346391000 | -1.118392000 | 1.605142000 |
| 6 | 3.985592000 | -2.045099000 | -0.996158000 |
| 1 | 4.440902000 | -1.051599000 | -1.147025000 |
| 1 | 3.935845000 | -2.562752000 | -1.962556000 |
| 1 | 4.631421000 | -2.596578000 | -0.298344000 |
| 6 | 1.369851000 | -0.781052000 | 3.069042000 |
| 1 | 2.374297000 | -0.862468000 | 3.502185000 |
| 1 | 0.684574000 | -1.454661000 | 3.606565000 |
| 1 | 0.989269000 | 0.242697000 | 3.213882000 |
| 6 | 1.069123000 | 1.879887000 | 0.725476000 |
| 1 | 0.213224000 | 1.869317000 | 1.406331000 |
| 6 | 2.217759000 | 2.608314000 | 1.011812000 |
| 1 | 2.275765000 | 3.191572000 | 1.931254000 |
| 6 | 3.278058000 | 2.566878000 | 0.104416000 |
| 6 | 1.965668000 | 1.104215000 | -1.270479000 |
| 1 | 1.820307000 | 0.477049000 | -2.152462000 |
| 6 | 3.146954000 | 1.809454000 | -1.059894000 |
| 1 | 3.948577000 | 1.754255000 | -1.797509000 |
| 8 | -2.229110000 | -1.377247000 | -0.014918000 |
| 8 | -1.823499000 | 1.307938000 | -0.202055000 |
| 6 | -3.461914000 | -1.065808000 | 0.069978000 |
| 6 | -3.943673000 | 0.258188000 | 0.012069000 |
| 1 | -5.016118000 | 0.424450000 | 0.108034000 |
| 6 | -3.106474000 | 1.369964000 | -0.080359000 |
| 6 | -4.417873000 | -2.200835000 | 0.264857000 |
| 1 | -4.147302000 | -2.741521000 | 1.184338000 |
| 1 | -4.304498000 | -2.909228000 | -0.569518000 |
| 1 | -5.458856000 | -1.864207000 | 0.326703000 |
| 6 | -3.670240000 | 2.753989000 | -0.023518000 |
| 1 | -4.761843000 | 2.755415000 | 0.071653000 |
| 1 | -3.373562000 | 3.300189000 | -0.931582000 |
| 1 | -3.223358000 | 3.285335000 | 0.830628000 |
| 1 | 4.197349000 | 3.121509000 | 0.302905000 |
| **$VO(acac)_2$(cis-P) (ΔG=0.6)** | | | |
| 23 | 0.415395000 | 0.138512000 | -0.921970000 |
| 8 | 0.345017000 | 0.018695000 | -2.487122000 |
| 8 | -0.570118000 | 1.847093000 | -0.735511000 |
| 8 | 0.331800000 | 0.220612000 | 1.241206000 |
| 7 | -1.446626000 | -0.852688000 | -0.585357000 |
| 6 | -1.372906000 | 2.274082000 | 0.170120000 |
| 6 | -1.436917000 | 1.771296000 | 1.473723000 |
| 1 | -2.151127000 | 2.216666000 | 2.166405000 |
| 6 | -0.536324000 | 0.796044000 | 1.962043000 |
| 6 | -2.282599000 | 3.388086000 | -0.253280000 |
| 1 | -2.958581000 | 3.008037000 | -1.036354000 |
| 1 | -1.687024000 | 4.194214000 | -0.706540000 |
| 1 | -2.877271000 | 3.784510000 | 0.577987000 |
| 6 | -0.604294000 | 0.383432000 | 3.403409000 |

| | | | |
|---|---|---|---|
| 1 | -1.227033000 | 1.052676000 | 4.008904000 |
| 1 | 0.412191000 | 0.328043000 | 3.818230000 |
| 1 | -1.027750000 | -0.634039000 | 3.445990000 |
| 6 | -1.589511000 | -1.807330000 | 0.347039000 |
| 1 | -0.680854000 | -2.115433000 | 0.868493000 |
| 6 | -2.826946000 | -2.370782000 | 0.640738000 |
| 1 | -2.900919000 | -3.144613000 | 1.405553000 |
| 6 | -3.950565000 | -1.923921000 | -0.055532000 |
| 6 | -2.524727000 | -0.419759000 | -1.258632000 |
| 1 | -2.350353000 | 0.362972000 | -2.001477000 |
| 6 | -3.796338000 | -0.932194000 | -1.025085000 |
| 1 | -4.646024000 | -0.553109000 | -1.593712000 |
| 8 | 2.124736000 | 1.114930000 | -0.662986000 |
| 8 | 1.349742000 | -1.542273000 | -0.475254000 |
| 6 | 3.205847000 | 0.682225000 | -0.136449000 |
| 6 | 3.426493000 | -0.650352000 | 0.255489000 |
| 1 | 4.388081000 | -0.898463000 | 0.704034000 |
| 6 | 2.507756000 | -1.690853000 | 0.051162000 |
| 6 | 4.289992000 | 1.699702000 | 0.047322000 |
| 1 | 3.905529000 | 2.524031000 | 0.666615000 |
| 1 | 4.546472000 | 2.127989000 | -0.933601000 |
| 1 | 5.188703000 | 1.276381000 | 0.510031000 |
| 6 | 2.854733000 | -3.088193000 | 0.462570000 |
| 1 | 3.887403000 | -3.176543000 | 0.818845000 |
| 1 | 2.690004000 | -3.768479000 | -0.385818000 |
| 1 | 2.165288000 | -3.399129000 | 1.263356000 |
| 1 | -4.936028000 | -2.344049000 | 0.155376000 |