

# Electronic supporting information

## Dual magnetic behavior of Fe(III)-dioxolene complex with tri-substituted catechol

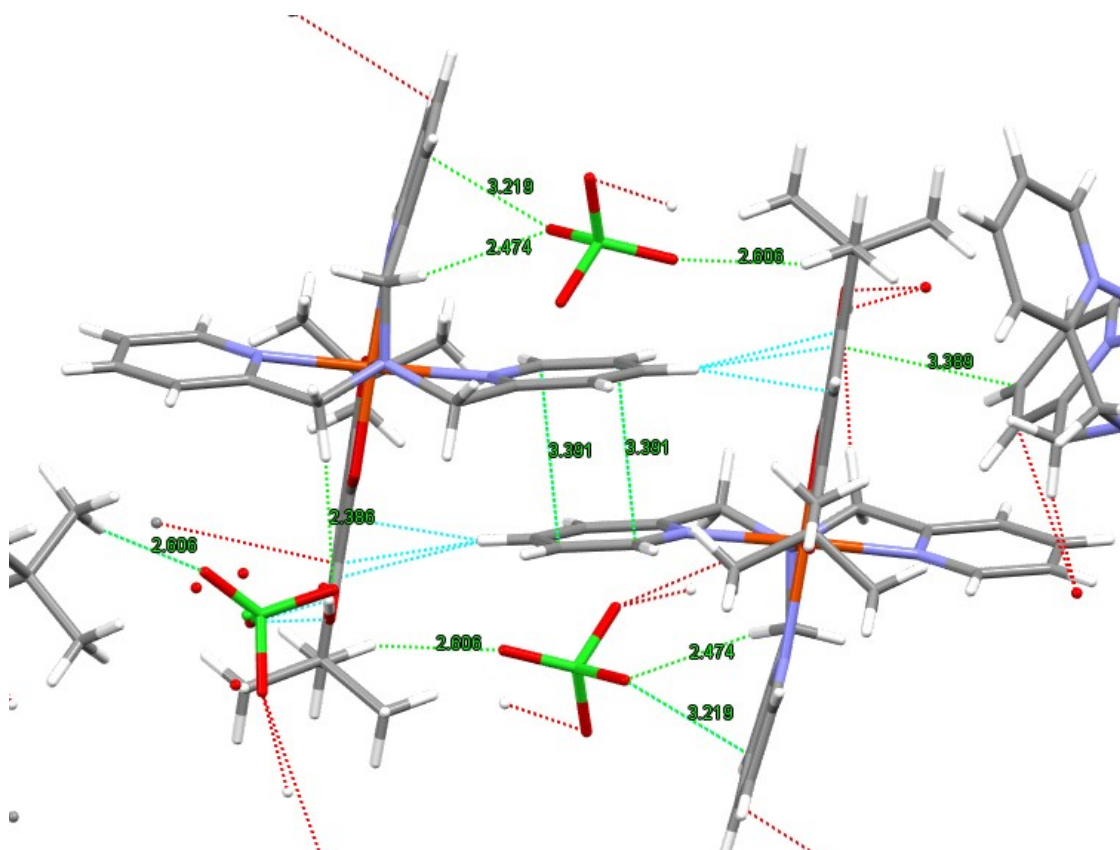
Maxim G. Chegerev,\* Oleg P. Demidov, Stanislav P. Kubrin, Pavel N. Vasiliev, Nikolay N. Efimov,  
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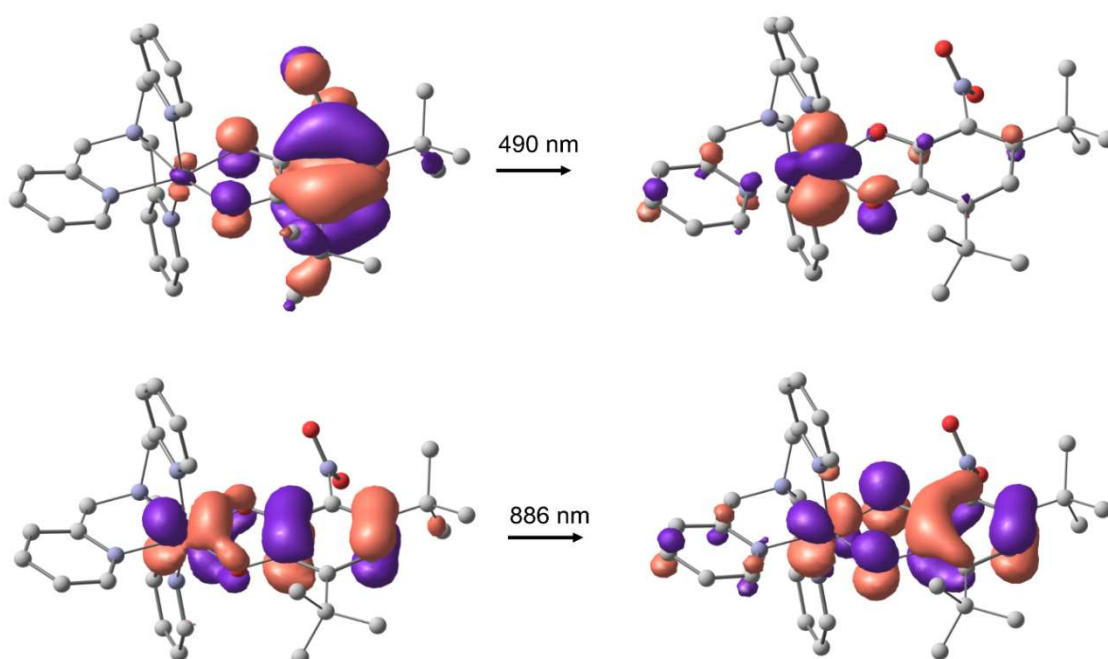
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**Table S1.** Crystallographic data for **1-3**.

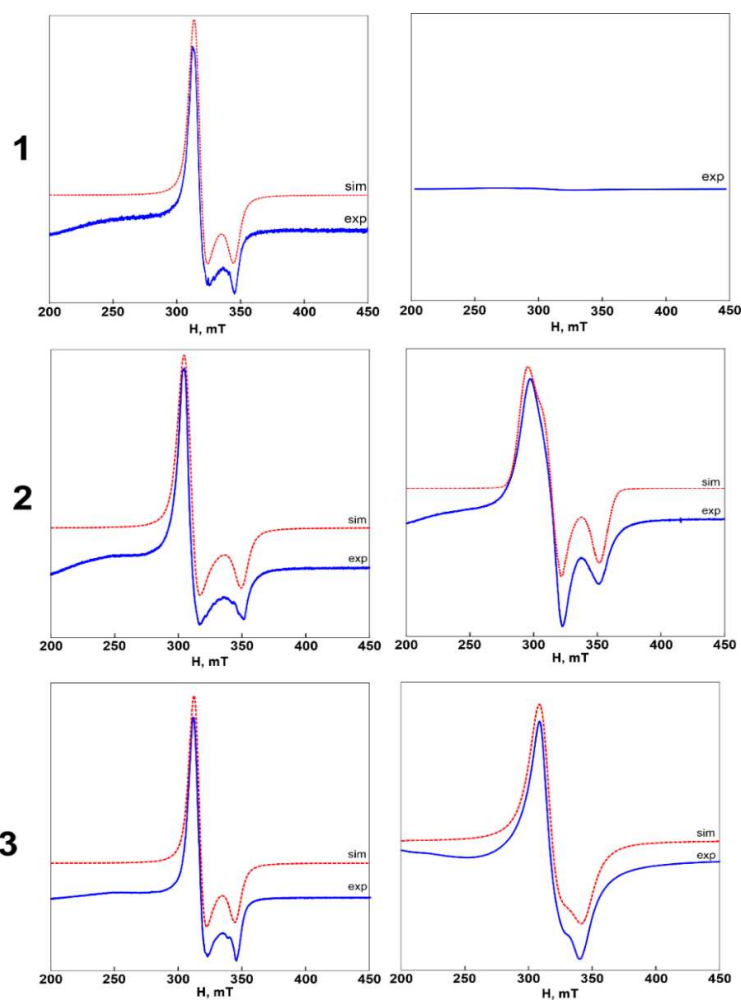
| Parameter                                   | <b>1</b>                                                          |                                                                   | <b>2</b>                                                          |                                                                   | <b>3</b>                                                          |                                                                   |
|---------------------------------------------|-------------------------------------------------------------------|-------------------------------------------------------------------|-------------------------------------------------------------------|-------------------------------------------------------------------|-------------------------------------------------------------------|-------------------------------------------------------------------|
| Temperature/K                               | 100                                                               | 300                                                               | 100                                                               | 295                                                               | 100                                                               | 293                                                               |
| CCDC Number                                 | 2418484                                                           | 2418478                                                           | 2418490                                                           | 2418488                                                           | 2418506                                                           | 2418502                                                           |
| Empirical formula                           | C <sub>32</sub> H <sub>38</sub> ClFeN <sub>4</sub> O <sub>7</sub> | C <sub>32</sub> H <sub>38</sub> ClFeN <sub>4</sub> O <sub>7</sub> | C <sub>32</sub> H <sub>37</sub> ClFeN <sub>5</sub> O <sub>8</sub> | C <sub>32</sub> H <sub>37</sub> ClFeN <sub>5</sub> O <sub>8</sub> | C <sub>34</sub> H <sub>42</sub> ClFeN <sub>4</sub> O <sub>7</sub> | C <sub>34</sub> H <sub>42</sub> ClFeN <sub>4</sub> O <sub>7</sub> |
| Formula weight                              | 681.96                                                            | 681.96                                                            | 710.96                                                            | 710.96                                                            | 710.01                                                            | 710.01                                                            |
| Crystal system                              | monoclinic                                                        | monoclinic                                                        | orthorhombic                                                      | orthorhombic                                                      | monoclinic                                                        | monoclinic                                                        |
| Space group                                 | P2 <sub>1</sub> /n                                                | P2 <sub>1</sub> /n                                                | Pbca                                                              | Pbca                                                              | I2/a                                                              | I2/a                                                              |
| a/Å                                         | 9.17500(10)                                                       | 9.29920(10)                                                       | 17.3716(2)                                                        | 17.5634(4)                                                        | 23.3854(5)                                                        | 19.7345(6)                                                        |
| b/Å                                         | 17.13730(10)                                                      | 17.2625(2)                                                        | 14.5066(1)                                                        | 14.6900(3)                                                        | 16.8312(3)                                                        | 17.2149(6)                                                        |
| c/Å                                         | 20.1420(2)                                                        | 20.3500(2)                                                        | 25.5452(3)                                                        | 26.3985(4)                                                        | 19.8747(4)                                                        | 23.6446(9)                                                        |
| α/°                                         | 90                                                                | 90                                                                | 90                                                                | 90                                                                | 90                                                                | 90                                                                |
| β/°                                         | 96.1030(10)                                                       | 95.8830(10)                                                       | 90                                                                | 90                                                                | 112.072(2)                                                        | 110.789(4)                                                        |
| γ/°                                         | 90                                                                | 90                                                                | 90                                                                | 90                                                                | 90                                                                | 90                                                                |
| Volume/Å <sup>3</sup>                       | 3149.07(5)                                                        | 3249.53(6)                                                        | 6437.46(11)                                                       | 6811.0(2)                                                         | 7249.5(3)                                                         | 7509.7(5)                                                         |
| Z                                           | 4                                                                 | 4                                                                 | 8                                                                 | 8                                                                 | 8                                                                 | 8                                                                 |
| ρ <sub>calc</sub> /g/cm <sup>3</sup>        | 1.438                                                             | 1.394                                                             | 1.467                                                             | 1.387                                                             | 1.301                                                             | 1.256                                                             |
| μ/mm <sup>-1</sup>                          | 5.076                                                             | 4.919                                                             | 5.025                                                             | 4.662                                                             | 4.430                                                             | 4.276                                                             |
| F(000)                                      | 1428.0                                                            | 1428.0                                                            | 2968                                                              | 2868                                                              | 2984.0                                                            | 2984.0                                                            |
| Crystal size/mm <sup>3</sup>                | 0.428 × 0.264 × 0.16                                              | 0.417 × 0.26 × 0.162                                              | 0.413 × 0.198 × 0.054                                             | 0.475 × 0.198 × 0.065                                             | 0.364 × 0.22 × 0.205                                              | 0.391 × 0.231 × 0.204                                             |
| Radiation                                   | Cu Kα (λ = 1.54184)                                               | Cu Kα (λ = 1.54184)                                               | Cu Kα (λ = 1.54184)                                               | Cu Kα (λ = 1.54184)                                               | Cu Kα (λ = 1.54184)                                               | Cu Kα (λ = 1.54184)                                               |
| 2θ range for data collection/°              | 6.788 to 152.706                                                  | 6.73 to 152.318                                                   | 8.592 to 152.322                                                  | 8.38 to 152.428                                                   | 7.114 to 152.428                                                  | 7.024 to 153.072                                                  |
| Index ranges                                | -11 ≤ h ≤ 10, -21 ≤ k ≤ 21, -21 ≤ l ≤ 25                          | -11 ≤ h ≤ 11, -21 ≤ k ≤ 21, -25 ≤ l ≤ 25                          | -21 ≤ h ≤ 21, -18 ≤ k ≤ 15, -32 ≤ l ≤ 31                          | -21 ≤ h ≤ 22, -17 ≤ k ≤ 18, -32 ≤ l ≤ 33                          | -29 ≤ h ≤ 29, -21 ≤ k ≤ 20, -25 ≤ l ≤ 24                          | -23 ≤ h ≤ 24, -20 ≤ k ≤ 21, -29 ≤ l ≤ 29                          |
| Reflections collected                       | 30800                                                             | 34602                                                             | 35742                                                             | 37885                                                             | 38895                                                             | 39992                                                             |
| Independent reflections                     | 6566 [R <sub>int</sub> = 0.0280, R <sub>sigma</sub> = 0.0217]     | 6788 [R <sub>int</sub> = 0.0300, R <sub>sigma</sub> = 0.0209]     | 6693 [R <sub>int</sub> = 0.0337, R <sub>sigma</sub> = 0.0226]     | 7094 [R <sub>int</sub> = 0.0448, R <sub>sigma</sub> = 0.0283]     | 7538 [R <sub>int</sub> = 0.0365, R <sub>sigma</sub> = 0.0244]     | 7790 [R <sub>int</sub> = 0.0360, R <sub>sigma</sub> = 0.0231]     |
| Data/restraints/parameters                  | 6566/502/447                                                      | 6788/428/460                                                      | 6693/44/458                                                       | 7094/92/489                                                       | 7538/695/696                                                      | 7790/793/653                                                      |
| Goodness-of-fit on F <sup>2</sup>           | 1.032                                                             | 1.027                                                             | 1.040                                                             | 1.017                                                             | 1.051                                                             | 1.036                                                             |
| Final R indexes [I ≥ 2σ (I)]                | R1 = 0.0332, wR2 = 0.0883                                         | R1 = 0.0373, wR2 = 0.1038                                         | R1 = 0.0330, wR2 = 0.0884                                         | R1 = 0.0539, wR2 = 0.1459                                         | R1 = 0.0591, wR2 = 0.1551                                         | R1 = 0.0551, wR2 = 0.1528                                         |
| Final R indexes [all data]                  | R1 = 0.0346, wR2 = 0.0894                                         | R1 = 0.0392, wR2 = 0.1060                                         | R1 = 0.0358, wR2 = 0.0905                                         | R1 = 0.0657, wR2 = 0.1570                                         | R1 = 0.0642, wR2 = 0.1592                                         | R1 = 0.0743, wR2 = 0.1693                                         |
| Largest diff. peak/hole / e Å <sup>-3</sup> | 0.83/-0.53                                                        | 0.45/-0.36                                                        | 0.46/-0.41                                                        | 0.41/-0.53                                                        | 0.52/-0.61                                                        | 0.35/-0.39                                                        |



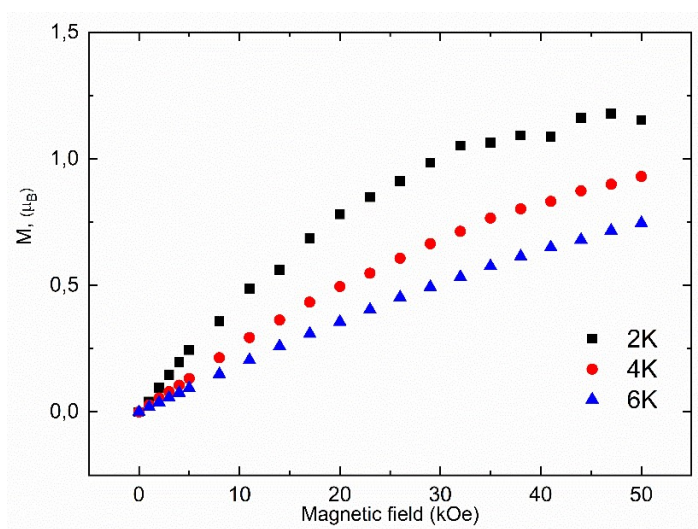
**Figure S1.** Fragment of crystal packing and intermolecular interactions of complex **1**.



**Figure S2.** Characteristic frontier molecular orbitals at transitions of the complex **2** at 490 and 886 nm as calculated by the DFT UTPSSH/6-311++G(d,p) method. Hydrogen atoms are not shown.

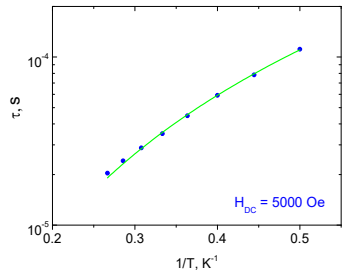
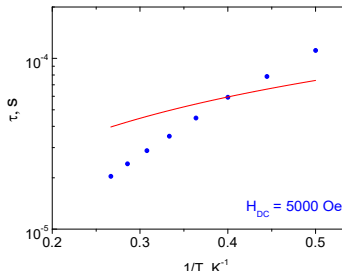
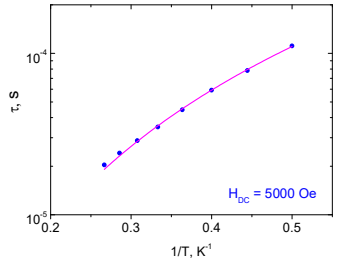
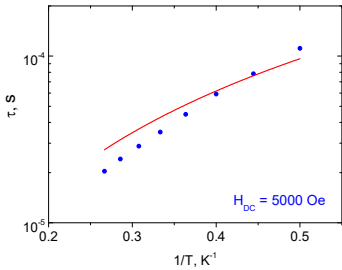
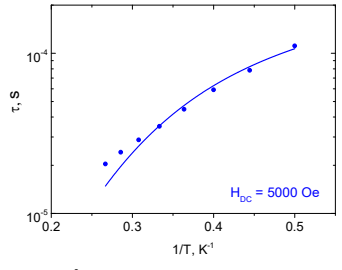
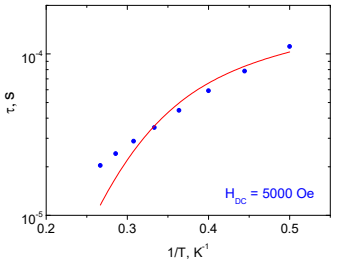
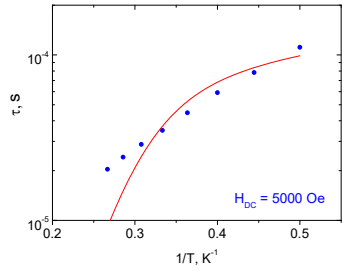


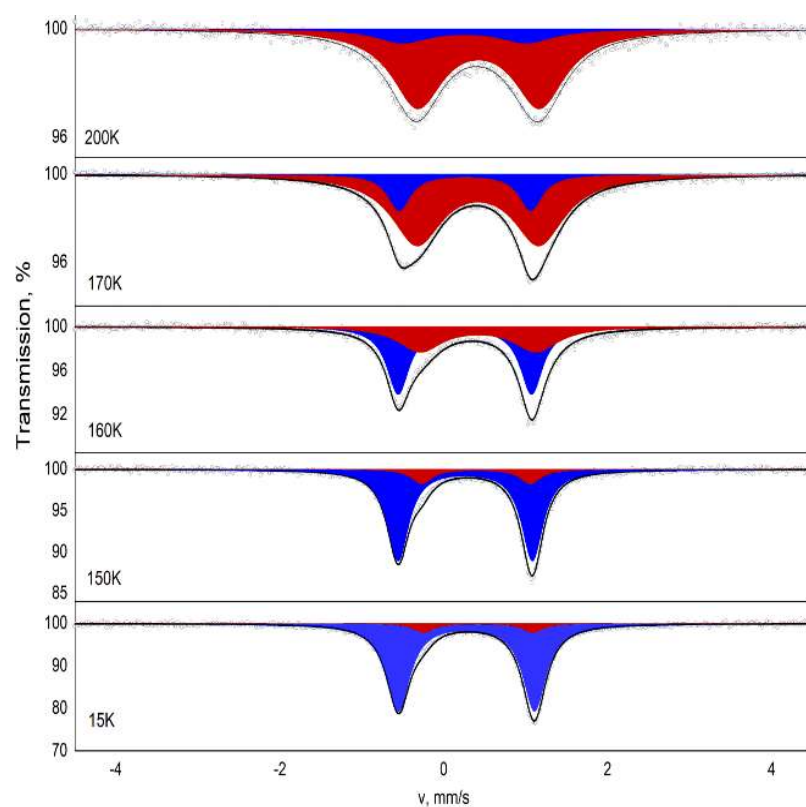
**Figure S3.** Experimental (blue) and theoretical (red) X-band EPR spectra of **1-3** in frozen  $\text{CH}_2\text{Cl}_2$  solutions (left column) and powder (right column) at 100 K.



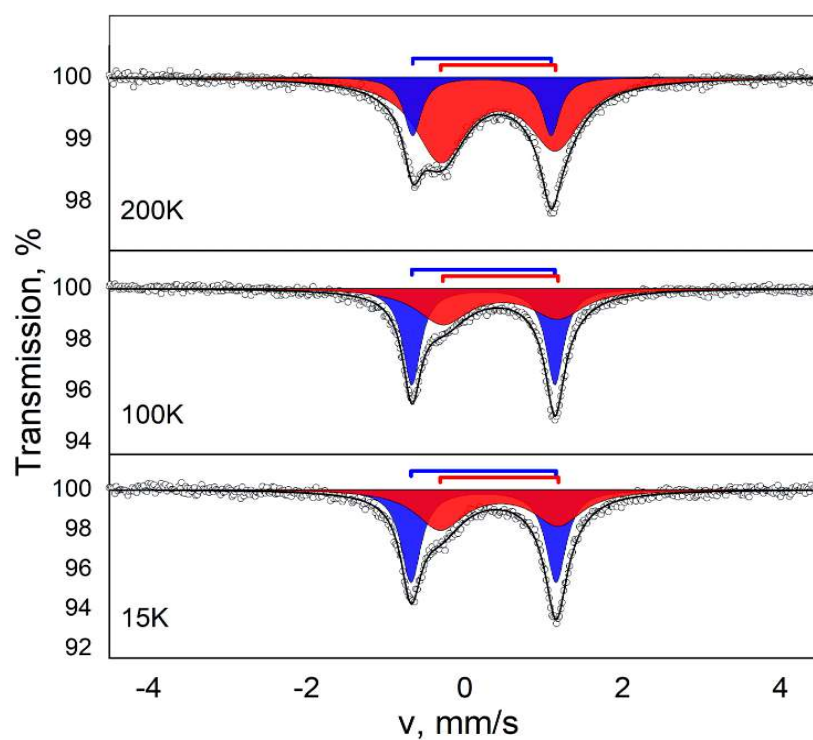
**Figure S4.** Field dependence of the magnetization below 6 K for **2**.

**Table S2.** Fitting of the  $\tau$  vs.  $1/T$  dependences for **2** ( $H = 5$  kOe,  $T = 2-7$  K).

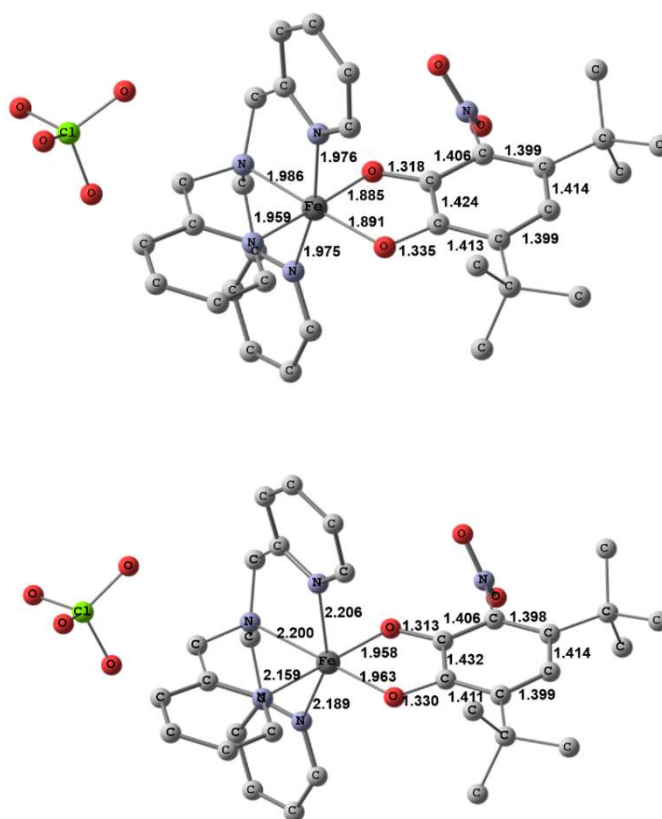
|                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
|  <p><b>Raman</b><br/> <math>\tau^{-1} = C_{\text{Raman}} T^{n_{\text{Raman}}}</math><br/> <math>C_{\text{Raman}} = 1310 \pm 41 \text{ s}^{-1} \text{K}^{-n_{\text{Raman}}}</math><br/> <math>n_{\text{Raman}} = 2.79 \pm 0.04</math><br/> <math>R^2 = 0.99904</math></p>                                                                                                                     |  <p><b>Direct</b><br/> <math>\tau^{-1} = A_{\text{direct}} T</math><br/> <math>A_{\text{direct}} = 6729 \pm 870 \text{ K}^{-1} \text{s}^{-1}</math><br/> <math>R^2 = 0.59215</math></p>                                                                                                                                                                                                     |
|  <p><b>Raman+Direct</b><br/> <math>\tau^{-1} = C_{\text{Raman}} T^{n_{\text{Raman}}} + A_{\text{direct}} T</math><br/> <math>C_{\text{Raman}} = 1311 \pm 540 \text{ s}^{-1} \text{K}^{-n_{\text{Raman}}}</math><br/> <math>n_{\text{Raman}} = 2.8 \pm 0.3</math><br/> <math>A_{\text{direct}} = 0 \pm 1006 \text{ K}^{-1} \text{s}^{-1}</math><br/> <math>R^2 = 0.99885</math></p>           |  <p><b>Raman+Direct</b><br/> <math>\tau^{-1} = C_{\text{Raman}} T^{n_{\text{Raman}}} + A_{\text{direct}} T</math><br/> <math>C_{\text{Raman}} = 2594 \pm 866 \text{ s}^{-1} \text{K}^{-n_{\text{Raman}}}</math><br/> <math>n_{\text{Raman}} = 2 \text{ (fixed)}</math><br/> <math>A_{\text{direct}} = 0 \pm 2003 \text{ K}^{-1} \text{s}^{-1}</math><br/> <math>R^2 = 0.91585</math></p>    |
|  <p><b>Raman+Direct</b><br/> <math>\tau^{-1} = C_{\text{Raman}} T^{n_{\text{Raman}}} + A_{\text{direct}} T</math><br/> <math>C_{\text{Raman}} = 73.3 \pm 9.1 \text{ s}^{-1} \text{K}^{-n_{\text{Raman}}}</math><br/> <math>n_{\text{Raman}} = 5 \text{ (fixed)}</math><br/> <math>A_{\text{direct}} = 3506 \pm 267 \text{ K}^{-1} \text{s}^{-1}</math><br/> <math>R^2 = 0.98069</math></p> |  <p><b>Raman+Direct</b><br/> <math>\tau^{-1} = C_{\text{Raman}} T^{n_{\text{Raman}}} + A_{\text{direct}} T</math><br/> <math>C_{\text{Raman}} = 6.7 \pm 1.5 \text{ s}^{-1} \text{K}^{-n_{\text{Raman}}}</math><br/> <math>n_{\text{Raman}} = 7 \text{ (fixed)}</math><br/> <math>A_{\text{direct}} = 4433 \pm 333 \text{ K}^{-1} \text{s}^{-1}</math><br/> <math>R^2 = 0.94673</math></p> |
|  <p><b>Raman+Direct</b><br/> <math>\tau^{-1} = C_{\text{Raman}} T^{n_{\text{Raman}}} + A_{\text{direct}} T</math><br/> <math>C_{\text{Raman}} = 0.6 \pm 0.2 \text{ s}^{-1} \text{K}^{-n_{\text{Raman}}}</math><br/> <math>n_{\text{Raman}} = 9 \text{ (fixed)}</math><br/> <math>A_{\text{direct}} = 4895 \pm 396 \text{ K}^{-1} \text{s}^{-1}</math><br/> <math>R^2 = 0.90482</math></p>  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |



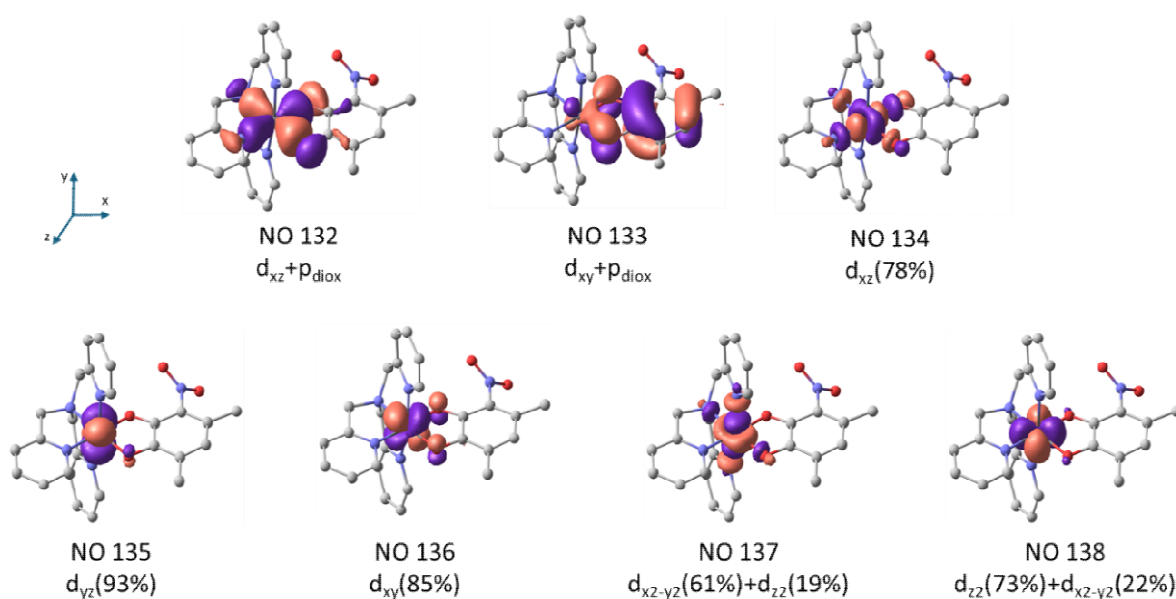
**Figure S5.** Variable temperature  $^{57}\text{Fe}$  Mössbauer spectra of **2** (*hs*-Fe(III) – red, *ls*-Fe(III) - blue).



**Figure S6** Variable temperature  $^{57}\text{Fe}$  Mössbauer spectra of **3** (*hs*-Fe(III) – red, *ls*-Fe(III) - blue).



**Figure S7.** Optimized geometries of **2** in the low-spin (top) and high-spin (bottom) states according to the DFT calculations (UTPSSh/6-311++G(d,p)). Bond lengths are given in Å. Hydrogen atoms are not shown.



**Figure S8.** Natural Orbitals of complex **2** included in the CAS(9,7) active space.

**Table S3.** Calculated SA-CASSCF(9,7)/NEVPT2 state energies for **2** including spin-orbit effects.

| Root | Multiplicity | $\Delta E/\text{cm}^{-1}$ |
|------|--------------|---------------------------|
| 0    | Doublet      | 0                         |
| 1    | Doublet      | 2860.6                    |
| 2    | Doublet      | 3120.5                    |
| 0    | Sextet       | 3223.0                    |
| 0    | Quartet      | 4824.2                    |

**Cartesian coordinates** of the isomers of the complexes **1-4** calculated by the DFT UTPSSh/6-  
311++G(d,p) method

**LS-1-cis** ( $E_{\text{total}} = -3712.21887181$  a.u.,  $E_{\text{ZPE}} = -3711.55597$  a.u.)

|    |              |              |              |
|----|--------------|--------------|--------------|
| 26 | -0.274904000 | 0.523085000  | 0.020233000  |
| 8  | 0.724950000  | -1.122332000 | -0.041701000 |
| 8  | 1.435790000  | 1.366169000  | 0.050086000  |
| 8  | 2.436971000  | -3.195449000 | -0.119286000 |
| 1  | 1.470863000  | -3.077398000 | -0.117234000 |
| 7  | -1.267079000 | 2.196411000  | 0.067827000  |
| 7  | -0.467797000 | 0.338906000  | 1.970021000  |
| 7  | -2.052782000 | -0.369958000 | -0.005860000 |
| 7  | -0.471604000 | 0.490001000  | -1.936487000 |
| 6  | 2.434021000  | 0.493721000  | 0.020520000  |
| 6  | 4.316216000  | -1.654038000 | -0.058798000 |
| 6  | 3.819852000  | 0.805364000  | 0.033893000  |
| 6  | 2.020202000  | -0.868061000 | -0.030510000 |
| 6  | 4.690128000  | -0.282661000 | -0.006064000 |
| 1  | 5.750410000  | -0.072299000 | 0.003333000  |
| 6  | 2.952457000  | -1.927079000 | -0.070202000 |
| 6  | -2.610572000 | 2.063092000  | 0.059711000  |
| 6  | -1.434718000 | -0.537648000 | 2.334934000  |
| 6  | -1.465045000 | -0.324300000 | -2.366649000 |
| 6  | 5.363386000  | -2.778160000 | -0.101849000 |
| 6  | -0.721939000 | 3.431063000  | 0.077337000  |
| 1  | 0.361138000  | 3.454596000  | 0.082286000  |
| 6  | 4.317826000  | 2.256251000  | 0.089185000  |
| 6  | -2.080360000 | -1.268062000 | 1.190182000  |
| 1  | -1.465924000 | -2.139696000 | 0.949903000  |
| 1  | -3.096335000 | -1.601291000 | 1.416528000  |
| 6  | -3.450783000 | 3.177784000  | 0.056269000  |
| 1  | -4.525588000 | 3.035013000  | 0.045969000  |
| 6  | -3.150443000 | 0.661134000  | 0.072450000  |
| 1  | -3.735853000 | 0.486092000  | 0.979662000  |
| 1  | -3.861102000 | 0.497420000  | -0.743247000 |
| 6  | 0.221746000  | 0.994188000  | 2.920351000  |
| 1  | 0.987886000  | 1.669257000  | 2.559269000  |
| 6  | 0.232477000  | 1.203009000  | -2.833468000 |
| 1  | 1.019767000  | 1.822776000  | -2.422133000 |
| 6  | -2.120357000 | -1.139492000 | -1.286755000 |
| 1  | -3.148071000 | -1.420088000 | -1.530488000 |
| 1  | -1.532661000 | -2.050320000 | -1.143802000 |
| 6  | -2.890455000 | 4.449968000  | 0.067016000  |
| 1  | -3.526552000 | 5.328388000  | 0.064938000  |
| 6  | -1.499962000 | 4.578692000  | 0.079375000  |
| 1  | -1.022908000 | 5.551474000  | 0.088122000  |
| 6  | 5.191736000  | -3.602656000 | -1.399778000 |
| 1  | 4.198509000  | -4.050156000 | -1.459333000 |
| 1  | 5.936204000  | -4.406449000 | -1.429613000 |
| 1  | 5.340652000  | -2.967787000 | -2.279388000 |
| 6  | 3.801322000  | 2.942757000  | 1.374854000  |
| 1  | 2.709478000  | 2.952048000  | 1.397991000  |
| 1  | 4.157695000  | 3.978435000  | 1.420179000  |
| 1  | 4.165705000  | 2.417408000  | 2.263552000  |
| 6  | -1.752115000 | -0.756851000 | 3.671568000  |
| 1  | -2.549528000 | -1.446029000 | 3.924482000  |
| 6  | -0.029092000 | 0.805656000  | 4.274183000  |
| 1  | 0.554216000  | 1.348559000  | 5.008261000  |

|    |              |              |              |
|----|--------------|--------------|--------------|
| 6  | 3.808399000  | 3.036139000  | -1.145069000 |
| 1  | 4.177925000  | 2.578102000  | -2.068227000 |
| 1  | 4.164447000  | 4.072390000  | -1.111600000 |
| 1  | 2.716667000  | 3.047163000  | -1.173674000 |
| 6  | -1.796319000 | -0.419366000 | -3.714767000 |
| 1  | -2.614335000 | -1.062137000 | -4.018964000 |
| 6  | -0.030629000 | 1.137229000  | -4.196318000 |
| 1  | 0.565050000  | 1.722831000  | -4.886319000 |
| 6  | -1.066059000 | 0.318824000  | -4.644092000 |
| 1  | -1.304119000 | 0.257755000  | -5.700379000 |
| 6  | -1.035922000 | -0.078841000 | 4.656347000  |
| 1  | -1.263531000 | -0.236449000 | 5.704913000  |
| 6  | 6.803664000  | -2.235168000 | -0.079477000 |
| 1  | 7.014602000  | -1.597216000 | -0.944072000 |
| 1  | 7.500725000  | -3.078465000 | -0.112016000 |
| 1  | 7.013239000  | -1.666874000 | 0.832736000  |
| 6  | 5.189979000  | -3.701816000 | 1.127272000  |
| 1  | 5.337060000  | -3.137719000 | 2.054148000  |
| 1  | 5.934887000  | -4.505100000 | 1.095278000  |
| 1  | 4.196938000  | -4.153090000 | 1.149956000  |
| 6  | 5.854166000  | 2.343539000  | 0.096712000  |
| 1  | 6.285888000  | 1.840289000  | 0.967712000  |
| 1  | 6.153833000  | 3.395838000  | 0.137302000  |
| 1  | 6.290956000  | 1.907395000  | -0.807325000 |
| 17 | -5.598587000 | -1.971325000 | -0.042724000 |
| 8  | -5.387784000 | -1.170915000 | 1.219898000  |
| 8  | -4.532043000 | -3.026429000 | -0.112300000 |
| 8  | -5.421267000 | -1.045251000 | -1.224463000 |
| 8  | -6.946213000 | -2.570182000 | -0.056876000 |

**HS-1-cis** ( $E_{\text{total}} = -3712.20228658$  a.u.,  $E_{\text{ZPE}} = -3711.542198$  a.u.)

|    |              |              |              |
|----|--------------|--------------|--------------|
| 26 | 0.077908000  | 0.243510000  | 0.196855000  |
| 8  | -1.170873000 | -1.201640000 | -0.376846000 |
| 8  | -1.611892000 | 1.227530000  | 0.473829000  |
| 8  | -3.087165000 | -2.932051000 | -1.095582000 |
| 1  | -2.113564000 | -2.925334000 | -1.049397000 |
| 7  | 1.282597000  | 1.960298000  | 0.740878000  |
| 7  | 0.634940000  | 0.734451000  | -1.879081000 |
| 7  | 2.101036000  | -0.637112000 | -0.007075000 |
| 7  | 0.431929000  | -0.754392000 | 2.120864000  |
| 6  | -2.693417000 | 0.516863000  | 0.166886000  |
| 6  | -4.796074000 | -1.281352000 | -0.581047000 |
| 6  | -4.032246000 | 0.959012000  | 0.262953000  |
| 6  | -2.427425000 | -0.808498000 | -0.297365000 |
| 6  | -5.016924000 | 0.038892000  | -0.115108000 |
| 1  | -6.046732000 | 0.361548000  | -0.047407000 |
| 6  | -3.467146000 | -1.691086000 | -0.665621000 |
| 6  | 2.609064000  | 1.755781000  | 0.647280000  |
| 6  | 1.775740000  | 0.161371000  | -2.313320000 |
| 6  | 1.456303000  | -1.631311000 | 2.137745000  |
| 6  | -5.954679000 | -2.211674000 | -0.972752000 |
| 6  | 0.816434000  | 3.207887000  | 0.941112000  |
| 1  | -0.263029000 | 3.296620000  | 0.997438000  |
| 6  | -4.372653000 | 2.372694000  | 0.754816000  |
| 6  | 2.325660000  | -0.942811000 | -1.446994000 |
| 1  | 1.758022000  | -1.852690000 | -1.672962000 |
| 1  | 3.382238000  | -1.144171000 | -1.658450000 |
| 6  | 3.518864000  | 2.812731000  | 0.735761000  |
| 1  | 4.579912000  | 2.610326000  | 0.636778000  |

|    |              |              |              |
|----|--------------|--------------|--------------|
| 6  | 3.109586000  | 0.338203000  | 0.515467000  |
| 1  | 4.023074000  | 0.321056000  | -0.085331000 |
| 1  | 3.417242000  | 0.002313000  | 1.510725000  |
| 6  | 0.038836000  | 1.665840000  | -2.641312000 |
| 1  | -0.878291000 | 2.087647000  | -2.243740000 |
| 6  | -0.255965000 | -0.526511000 | 3.252146000  |
| 1  | -1.072464000 | 0.183528000  | 3.174334000  |
| 6  | 2.131419000  | -1.880190000 | 0.809970000  |
| 1  | 3.159245000  | -2.238400000 | 0.932795000  |
| 1  | 1.557516000  | -2.641649000 | 0.270711000  |
| 6  | 3.036834000  | 4.099540000  | 0.948454000  |
| 1  | 3.725172000  | 4.934907000  | 1.021073000  |
| 6  | 1.659973000  | 4.303420000  | 1.059757000  |
| 1  | 1.246002000  | 5.291045000  | 1.225081000  |
| 6  | -5.931928000 | -3.478236000 | -0.084764000 |
| 1  | -4.994491000 | -4.025679000 | -0.194633000 |
| 1  | -6.756116000 | -4.143634000 | -0.366123000 |
| 1  | -6.056145000 | -3.209565000 | 0.969473000  |
| 6  | -3.731978000 | 3.419785000  | -0.185523000 |
| 1  | -2.647554000 | 3.296582000  | -0.222182000 |
| 1  | -3.957223000 | 4.433172000  | 0.166932000  |
| 1  | -4.128843000 | 3.316586000  | -1.200830000 |
| 6  | 2.370411000  | 0.527415000  | -3.519661000 |
| 1  | 3.302289000  | 0.061340000  | -3.819650000 |
| 6  | 0.559099000  | 2.069237000  | -3.865787000 |
| 1  | 0.043597000  | 2.821451000  | -4.451115000 |
| 6  | -3.832832000 | 2.571157000  | 2.190227000  |
| 1  | -4.299161000 | 1.856623000  | 2.876568000  |
| 1  | -4.063310000 | 3.582863000  | 2.544070000  |
| 1  | -2.750607000 | 2.429145000  | 2.222018000  |
| 6  | 1.833944000  | -2.293832000 | 3.304557000  |
| 1  | 2.677435000  | -2.974794000 | 3.286020000  |
| 6  | 0.052173000  | -1.159445000 | 4.450479000  |
| 1  | -0.529271000 | -0.947253000 | 5.339788000  |
| 6  | 1.119184000  | -2.056471000 | 4.475992000  |
| 1  | 1.394881000  | -2.559604000 | 5.396513000  |
| 6  | 1.750000000  | 1.494018000  | -4.307534000 |
| 1  | 2.192511000  | 1.797374000  | -5.250286000 |
| 6  | -7.327078000 | -1.538367000 | -0.793230000 |
| 1  | -7.510395000 | -1.253060000 | 0.247957000  |
| 1  | -8.109950000 | -2.245212000 | -1.085844000 |
| 1  | -7.432311000 | -0.648265000 | -1.422267000 |
| 6  | -5.819626000 | -2.617119000 | -2.459559000 |
| 1  | -5.862547000 | -1.732540000 | -3.103478000 |
| 1  | -6.644333000 | -3.282564000 | -2.739286000 |
| 1  | -4.878806000 | -3.136902000 | -2.647298000 |
| 6  | -5.889103000 | 2.631456000  | 0.782709000  |
| 1  | -6.336390000 | 2.542960000  | -0.212668000 |
| 1  | -6.072776000 | 3.649885000  | 1.140305000  |
| 1  | -6.407544000 | 1.943287000  | 1.458215000  |
| 17 | 6.129708000  | -1.374530000 | -0.511732000 |
| 8  | 6.155804000  | 0.126949000  | -0.392114000 |
| 8  | 5.413233000  | -1.736227000 | -1.785425000 |
| 8  | 5.336034000  | -1.927054000 | 0.647614000  |
| 8  | 7.500093000  | -1.922044000 | -0.510499000 |

**LS-1-trans** ( $E_{\text{total}} = -3712.21850477$  a.u.,  $E_{\text{ZPE}} = -3711.555708$  a.u.)

|    |              |             |             |
|----|--------------|-------------|-------------|
| 26 | 0.214590000  | 0.689561000 | 0.001105000 |
| 8  | -1.527795000 | 1.489345000 | 0.001582000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 8 | -0.733997000 | -0.976876000 | 0.001220000  |
| 8 | -4.111094000 | 2.253479000  | 0.000741000  |
| 1 | -3.240754000 | 2.688007000  | 0.001426000  |
| 7 | 1.189446000  | 2.378145000  | 0.000556000  |
| 7 | 0.406891000  | 0.586324000  | -1.952998000 |
| 7 | 1.998252000  | -0.182586000 | 0.000486000  |
| 7 | 0.408146000  | 0.586079000  | 1.955012000  |
| 6 | -2.041868000 | -0.808295000 | 0.000604000  |
| 6 | -4.807406000 | -0.081289000 | -0.000305000 |
| 6 | -3.018182000 | -1.843162000 | -0.000057000 |
| 6 | -2.466602000 | 0.551236000  | 0.000802000  |
| 6 | -4.347131000 | -1.428383000 | -0.000490000 |
| 1 | -5.106800000 | -2.197492000 | -0.001005000 |
| 6 | -3.829409000 | 0.907684000  | 0.000397000  |
| 6 | 2.534100000  | 2.256898000  | -0.000357000 |
| 6 | 1.394652000  | -0.250708000 | -2.352482000 |
| 6 | 1.396237000  | -0.250860000 | 2.353855000  |
| 6 | -6.304940000 | 0.263296000  | -0.000801000 |
| 6 | 0.635347000  | 3.608538000  | 0.000019000  |
| 1 | -0.447704000 | 3.625368000  | 0.000752000  |
| 6 | -2.611781000 | -3.322123000 | -0.000246000 |
| 6 | 2.053434000  | -1.017866000 | -1.239778000 |
| 1 | 1.460469000  | -1.915571000 | -1.046011000 |
| 1 | 3.078424000  | -1.314699000 | -1.475250000 |
| 6 | 3.364871000  | 3.378973000  | -0.001681000 |
| 1 | 4.440867000  | 3.245102000  | -0.002374000 |
| 6 | 3.086956000  | 0.860562000  | 0.000100000  |
| 1 | 3.739528000  | 0.697729000  | -0.862799000 |
| 1 | 3.739413000  | 0.698335000  | 0.863185000  |
| 6 | -0.298094000 | 1.264539000  | -2.875522000 |
| 1 | -1.080471000 | 1.905002000  | -2.486282000 |
| 6 | -0.296668000 | 1.263825000  | 2.878017000  |
| 1 | -1.079347000 | 1.904205000  | 2.489251000  |
| 6 | 2.054485000  | -1.017823000 | 1.240668000  |
| 1 | 3.079703000  | -1.314403000 | 1.475463000  |
| 1 | 1.461637000  | -1.915717000 | 1.047394000  |
| 6 | 2.794020000  | 4.646279000  | -0.002140000 |
| 1 | 3.422519000  | 5.530115000  | -0.003175000 |
| 6 | 1.402249000  | 4.763331000  | -0.001295000 |
| 1 | 0.916921000  | 5.732035000  | -0.001677000 |
| 6 | -6.652465000 | 1.084784000  | -1.264997000 |
| 1 | -6.082831000 | 2.014623000  | -1.304979000 |
| 1 | -7.720174000 | 1.332355000  | -1.264856000 |
| 1 | -6.437522000 | 0.505463000  | -2.168874000 |
| 6 | -1.776266000 | -3.634448000 | 1.263035000  |
| 1 | -0.880152000 | -3.012685000 | 1.301797000  |
| 1 | -1.470454000 | -4.686741000 | 1.261341000  |
| 1 | -2.365043000 | -3.450711000 | 2.167678000  |
| 6 | 1.717844000  | -0.404710000 | -3.697052000 |
| 1 | 2.531154000  | -1.063748000 | -3.978095000 |
| 6 | -0.042301000 | 1.140280000  | -4.235635000 |
| 1 | -0.638388000 | 1.699144000  | -4.947119000 |
| 6 | -1.775196000 | -3.633845000 | -1.262965000 |
| 1 | -2.363186000 | -3.449643000 | -2.168025000 |
| 1 | -1.469402000 | -4.686143000 | -1.261533000 |
| 1 | -0.879034000 | -3.012085000 | -1.300643000 |
| 6 | 1.720057000  | -0.405121000 | 3.698243000  |
| 1 | 2.533627000  | -1.064055000 | 3.978781000  |
| 6 | -0.040269000 | 1.139258000  | 4.237986000  |

|    |              |              |              |
|----|--------------|--------------|--------------|
| 1  | -0.636231000 | 1.697735000  | 4.949880000  |
| 6  | 0.988635000  | 0.296446000  | 4.654756000  |
| 1  | 1.221130000  | 0.188953000  | 5.708578000  |
| 6  | 0.986184000  | 0.297286000  | -4.653068000 |
| 1  | 1.218188000  | 0.190000000  | -5.707020000 |
| 6  | -7.193041000 | -0.994219000 | -0.001627000 |
| 1  | -7.028118000 | -1.611585000 | -0.890613000 |
| 1  | -8.243477000 | -0.686256000 | -0.001858000 |
| 1  | -7.028720000 | -1.612310000 | 0.886968000  |
| 6  | -6.653520000 | 1.083848000  | 1.263713000  |
| 1  | -6.439302000 | 0.503868000  | 2.167339000  |
| 1  | -7.721237000 | 1.331387000  | 1.262880000  |
| 1  | -6.083949000 | 2.013673000  | 1.304851000  |
| 6  | -3.832167000 | -4.259174000 | -0.000989000 |
| 1  | -4.456105000 | -4.116673000 | 0.887459000  |
| 1  | -3.485976000 | -5.297679000 | -0.001074000 |
| 1  | -4.455341000 | -4.116273000 | -0.889908000 |
| 17 | 5.579285000  | -1.712309000 | -0.001525000 |
| 8  | 5.381018000  | -0.849323000 | -1.225445000 |
| 8  | 4.517363000  | -2.774581000 | -0.001232000 |
| 8  | 5.382238000  | -0.849836000 | 1.222925000  |
| 8  | 6.929671000  | -2.305197000 | -0.002330000 |

**HS-1-trans** ( $E_{\text{total}} = -3712.20164899$  a.u.,  $E_{\text{ZPE}} = -3711.541606$  a.u.)

|    |              |              |              |
|----|--------------|--------------|--------------|
| 26 | 0.039315000  | 0.361966000  | 0.304010000  |
| 8  | -1.684352000 | 1.270913000  | 0.704551000  |
| 8  | -1.160270000 | -1.002925000 | -0.465283000 |
| 8  | -4.171336000 | 2.217453000  | 1.085558000  |
| 1  | -3.259536000 | 2.494910000  | 1.285421000  |
| 7  | 1.225711000  | 2.013538000  | 1.067822000  |
| 7  | 0.603435000  | 1.136730000  | -1.683270000 |
| 7  | 2.062398000  | -0.466544000 | 0.003320000  |
| 7  | 0.392597000  | -0.860955000 | 2.094739000  |
| 6  | -2.440185000 | -0.698374000 | -0.374120000 |
| 6  | -5.107861000 | 0.250911000  | -0.008048000 |
| 6  | -3.518358000 | -1.492348000 | -0.851405000 |
| 6  | -2.715053000 | 0.546043000  | 0.269139000  |
| 6  | -4.797397000 | -0.979613000 | -0.645565000 |
| 1  | -5.632954000 | -1.566477000 | -1.000557000 |
| 6  | -4.028365000 | 1.008395000  | 0.449288000  |
| 6  | 2.553707000  | 1.825620000  | 0.959110000  |
| 6  | 1.746836000  | 0.624735000  | -2.182273000 |
| 6  | 1.416493000  | -1.733359000 | 1.998704000  |
| 6  | -6.557135000 | 0.727219000  | 0.170780000  |
| 6  | 0.756177000  | 3.226431000  | 1.416202000  |
| 1  | -0.323633000 | 3.307596000  | 1.474475000  |
| 6  | -3.264299000 | -2.833808000 | -1.549972000 |
| 6  | 2.294789000  | -0.581806000 | -1.463564000 |
| 1  | 1.729530000  | -1.455169000 | -1.807959000 |
| 1  | 3.353364000  | -0.750516000 | -1.693020000 |
| 6  | 3.459845000  | 2.865561000  | 1.184588000  |
| 1  | 4.521987000  | 2.678622000  | 1.068256000  |
| 6  | 3.061611000  | 0.437774000  | 0.654096000  |
| 1  | 3.980365000  | 0.501771000  | 0.064731000  |
| 1  | 3.361981000  | -0.019834000 | 1.601945000  |
| 6  | 0.009613000  | 2.157758000  | -2.322196000 |
| 1  | -0.910171000 | 2.524201000  | -1.878397000 |
| 6  | -0.298909000 | -0.783641000 | 3.243778000  |
| 1  | -1.115387000 | -0.069414000 | 3.256806000  |

|    |              |              |              |
|----|--------------|--------------|--------------|
| 6  | 2.095111000  | -1.805688000 | 0.651421000  |
| 1  | 3.124017000  | -2.173055000 | 0.729087000  |
| 1  | 1.523997000  | -2.491172000 | 0.016097000  |
| 6  | 2.972998000  | 4.115183000  | 1.551043000  |
| 1  | 3.658228000  | 4.936575000  | 1.731626000  |
| 6  | 1.594629000  | 4.301138000  | 1.675559000  |
| 1  | 1.176473000  | 5.260081000  | 1.957782000  |
| 6  | -6.755407000 | 2.080318000  | -0.553357000 |
| 1  | -6.087146000 | 2.846266000  | -0.156799000 |
| 1  | -7.789034000 | 2.421243000  | -0.424573000 |
| 1  | -6.563984000 | 1.971969000  | -1.625954000 |
| 6  | -2.524408000 | -3.791642000 | -0.586796000 |
| 1  | -1.570308000 | -3.366172000 | -0.270541000 |
| 1  | -2.332867000 | -4.749311000 | -1.084356000 |
| 1  | -3.131622000 | -3.985340000 | 0.303585000  |
| 6  | 2.346649000  | 1.143792000  | -3.328568000 |
| 1  | 3.280751000  | 0.721148000  | -3.681272000 |
| 6  | 0.534281000  | 2.715377000  | -3.482545000 |
| 1  | 0.019863000  | 3.535518000  | -3.969293000 |
| 6  | -2.403210000 | -2.608595000 | -2.815052000 |
| 1  | -2.924118000 | -1.955071000 | -3.522502000 |
| 1  | -2.211098000 | -3.565978000 | -3.312906000 |
| 1  | -1.446005000 | -2.150494000 | -2.559678000 |
| 6  | 1.790127000  | -2.544005000 | 3.069418000  |
| 1  | 2.633222000  | -3.217495000 | 2.964040000  |
| 6  | 0.004976000  | -1.569035000 | 4.349311000  |
| 1  | -0.579512000 | -1.475743000 | 5.256864000  |
| 6  | 1.071624000  | -2.462414000 | 4.259600000  |
| 1  | 1.344045000  | -3.082798000 | 5.106611000  |
| 6  | 1.728106000  | 2.202714000  | -3.988750000 |
| 1  | 2.174306000  | 2.624945000  | -4.882760000 |
| 6  | -7.575330000 | -0.269322000 | -0.412031000 |
| 1  | -7.438086000 | -0.412462000 | -1.488734000 |
| 1  | -8.585015000 | 0.123424000  | -0.255542000 |
| 1  | -7.519435000 | -1.246160000 | 0.079169000  |
| 6  | -6.870387000 | 0.893218000  | 1.677102000  |
| 1  | -6.761692000 | -0.063552000 | 2.198298000  |
| 1  | -7.903815000 | 1.235141000  | 1.804848000  |
| 1  | -6.205488000 | 1.621088000  | 2.144664000  |
| 6  | -4.572149000 | -3.517888000 | -1.984209000 |
| 1  | -5.219625000 | -3.739791000 | -1.129523000 |
| 1  | -4.333879000 | -4.466434000 | -2.476047000 |
| 1  | -5.134951000 | -2.905970000 | -2.696739000 |
| 17 | 6.103504000  | -1.080906000 | -0.577071000 |
| 8  | 6.118106000  | 0.387507000  | -0.240331000 |
| 8  | 5.397095000  | -1.257434000 | -1.894959000 |
| 8  | 5.306899000  | -1.800870000 | 0.483629000  |
| 8  | 7.477828000  | -1.614028000 | -0.646116000 |

**LS-2-cis** ( $E_{\text{total}} = -3841.5313877$  a.u.,  $E_{\text{ZPE}} = -3840.870226$  a.u.)

|    |              |              |              |
|----|--------------|--------------|--------------|
| 26 | -0.357333000 | 0.542043000  | -0.032130000 |
| 8  | 1.224010000  | 1.558259000  | -0.237875000 |
| 8  | 0.756628000  | -0.965029000 | -0.238427000 |
| 7  | -1.543502000 | 2.079597000  | 0.227671000  |
| 7  | -0.886057000 | 0.485601000  | -1.934278000 |
| 7  | -0.224377000 | 0.340539000  | 1.929298000  |
| 6  | 2.308410000  | 0.779706000  | -0.201846000 |
| 7  | 2.617848000  | -2.952208000 | -0.136113000 |
| 7  | -1.978432000 | -0.583570000 | 0.194073000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | 4.640995000  | 0.241583000  | -0.179474000 |
| 1 | 5.667652000  | 0.574740000  | -0.167689000 |
| 6 | 2.025769000  | -0.615917000 | -0.176482000 |
| 8 | 2.011624000  | -3.334211000 | 0.859716000  |
| 6 | 3.648640000  | 1.226366000  | -0.220037000 |
| 6 | 3.078386000  | -1.547030000 | -0.149102000 |
| 6 | 4.420983000  | -1.154339000 | -0.144462000 |
| 8 | 2.831182000  | -3.640625000 | -1.131321000 |
| 6 | -2.836825000 | 1.752622000  | 0.429242000  |
| 6 | 3.993917000  | 2.721245000  | -0.287843000 |
| 6 | -3.189633000 | 0.294240000  | 0.363746000  |
| 1 | -3.751439000 | -0.010135000 | 1.249028000  |
| 1 | -3.869773000 | 0.121915000  | -0.477375000 |
| 6 | -1.010829000 | -0.643175000 | 2.426497000  |
| 6 | -1.172195000 | 3.376362000  | 0.249643000  |
| 1 | -0.117417000 | 3.557672000  | 0.080505000  |
| 6 | -0.481739000 | 1.316043000  | -2.910284000 |
| 1 | 0.250030000  | 2.059725000  | -2.618614000 |
| 6 | -3.807994000 | 2.729106000  | 0.660100000  |
| 1 | -4.837866000 | 2.425492000  | 0.812294000  |
| 6 | 5.625361000  | -2.120760000 | -0.109706000 |
| 6 | -1.785002000 | -0.488221000 | -2.213959000 |
| 6 | 0.537516000  | 1.067958000  | 2.764657000  |
| 1 | 1.150222000  | 1.828259000  | 2.296846000  |
| 6 | -1.742617000 | -1.447628000 | 1.388391000  |
| 1 | -1.081630000 | -2.260562000 | 1.072485000  |
| 1 | -2.684417000 | -1.870146000 | 1.747863000  |
| 6 | -2.334667000 | -0.628901000 | -3.483786000 |
| 1 | -3.084181000 | -1.391765000 | -3.657574000 |
| 6 | -2.084955000 | 4.395391000  | 0.472587000  |
| 1 | -1.749555000 | 5.425546000  | 0.480939000  |
| 6 | -3.426618000 | 4.064945000  | 0.682015000  |
| 1 | -4.163621000 | 4.840716000  | 0.858720000  |
| 6 | -0.968971000 | 1.213355000  | -4.207221000 |
| 1 | -0.615102000 | 1.897575000  | -4.968982000 |
| 6 | 3.406077000  | 3.325687000  | -1.584405000 |
| 1 | 3.834354000  | 2.836609000  | -2.464896000 |
| 1 | 3.640261000  | 4.394786000  | -1.639212000 |
| 1 | 2.321672000  | 3.204135000  | -1.611483000 |
| 6 | -1.916167000 | 0.231754000  | -4.495992000 |
| 1 | -2.328804000 | 0.141649000  | -5.494768000 |
| 6 | -2.090912000 | -1.396087000 | -1.057719000 |
| 1 | -3.076920000 | -1.859555000 | -1.134873000 |
| 1 | -1.314846000 | -2.165141000 | -1.010751000 |
| 6 | -1.067690000 | -0.904543000 | 3.791866000  |
| 1 | -1.719106000 | -1.688598000 | 4.159810000  |
| 6 | 3.401866000  | 3.457646000  | 0.935602000  |
| 1 | 2.314631000  | 3.359554000  | 0.958606000  |
| 1 | 3.651916000  | 4.523581000  | 0.889341000  |
| 1 | 3.812932000  | 3.052678000  | 1.866229000  |
| 6 | 0.542004000  | 0.846036000  | 4.135981000  |
| 1 | 1.175722000  | 1.448800000  | 4.775150000  |
| 6 | 5.511997000  | 2.973617000  | -0.296774000 |
| 1 | 5.993267000  | 2.604674000  | 0.614622000  |
| 1 | 5.694243000  | 4.051356000  | -0.355870000 |
| 1 | 5.997678000  | 2.507355000  | -1.159685000 |
| 6 | -0.277661000 | -0.152672000 | 4.658219000  |
| 1 | -0.302990000 | -0.343276000 | 5.725470000  |
| 6 | 5.888048000  | -2.668882000 | -1.533336000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| 1  | 5.027773000  | -3.222666000 | -1.911089000 |
| 1  | 6.756070000  | -3.337615000 | -1.515272000 |
| 1  | 6.103669000  | -1.848119000 | -2.224885000 |
| 6  | 5.403685000  | -3.295261000 | 0.872542000  |
| 1  | 5.122805000  | -2.930930000 | 1.865277000  |
| 1  | 6.338992000  | -3.855671000 | 0.970141000  |
| 1  | 4.647036000  | -4.002751000 | 0.533528000  |
| 6  | 6.908260000  | -1.399181000 | 0.357822000  |
| 1  | 7.243867000  | -0.638483000 | -0.352929000 |
| 1  | 7.711939000  | -2.136839000 | 0.441120000  |
| 1  | 6.776603000  | -0.929437000 | 1.337774000  |
| 8  | -4.654536000 | -2.383875000 | 0.678225000  |
| 8  | -6.227274000 | -0.516130000 | 0.772387000  |
| 17 | -5.829871000 | -1.728939000 | -0.012597000 |
| 8  | -5.353716000 | -1.287358000 | -1.379564000 |
| 8  | -6.952942000 | -2.676331000 | -0.136105000 |

**HS-2-cis** ( $E_{\text{total}} = -3841.51320647$  a.u.,  $E_{\text{ZPE}} = -3840.855061$  a.u.)

|    |              |              |              |
|----|--------------|--------------|--------------|
| 26 | -0.229088000 | 0.386102000  | -0.130495000 |
| 8  | 1.390028000  | 1.430227000  | -0.506575000 |
| 8  | 1.077118000  | -1.052485000 | 0.108095000  |
| 7  | -1.574417000 | 2.066379000  | -0.299615000 |
| 7  | -0.962550000 | -0.387152000 | -2.042715000 |
| 7  | -0.376465000 | 0.676341000  | 2.051441000  |
| 6  | 2.513716000  | 0.736621000  | -0.344873000 |
| 7  | 3.068328000  | -2.865005000 | 0.552314000  |
| 7  | -2.111970000 | -0.618220000 | 0.404776000  |
| 6  | 4.875405000  | 0.352852000  | -0.272726000 |
| 1  | 5.878616000  | 0.739944000  | -0.368725000 |
| 6  | 2.318668000  | -0.637525000 | 0.007236000  |
| 8  | 2.579587000  | -3.050447000 | 1.660131000  |
| 6  | 3.821759000  | 1.247346000  | -0.486088000 |
| 6  | 3.432644000  | -1.473501000 | 0.199614000  |
| 6  | 4.746233000  | -1.014554000 | 0.064215000  |
| 8  | 3.242260000  | -3.738032000 | -0.294351000 |
| 6  | -2.857366000 | 1.774048000  | -0.023830000 |
| 6  | 4.066462000  | 2.717466000  | -0.855231000 |
| 6  | -3.248495000 | 0.338511000  | 0.223679000  |
| 1  | -3.923361000 | 0.281918000  | 1.080314000  |
| 1  | -3.852552000 | 0.001587000  | -0.626910000 |
| 6  | -1.330599000 | -0.048815000 | 2.666156000  |
| 6  | -1.225615000 | 3.339689000  | -0.574306000 |
| 1  | -0.173275000 | 3.500031000  | -0.782325000 |
| 6  | -0.592762000 | 0.036091000  | -3.263165000 |
| 1  | 0.212598000  | 0.762351000  | -3.291907000 |
| 6  | -3.845086000 | 2.765234000  | -0.015361000 |
| 1  | -4.870610000 | 2.486481000  | 0.203130000  |
| 6  | 6.008368000  | -1.887124000 | 0.235729000  |
| 6  | -1.953539000 | -1.297286000 | -1.933560000 |
| 6  | 0.338310000  | 1.562854000  | 2.763038000  |
| 1  | 1.096392000  | 2.109376000  | 2.212605000  |
| 6  | -2.015454000 | -1.086747000 | 1.810632000  |
| 1  | -1.389808000 | -1.985970000 | 1.814345000  |
| 1  | -3.004785000 | -1.354512000 | 2.194986000  |
| 6  | -2.631693000 | -1.783735000 | -3.048944000 |
| 1  | -3.459127000 | -2.469768000 | -2.911327000 |
| 6  | -2.149493000 | 4.372515000  | -0.587856000 |
| 1  | -1.830918000 | 5.382733000  | -0.815754000 |
| 6  | -3.485142000 | 4.075542000  | -0.301324000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| 1  | -4.235335000 | 4.859195000  | -0.302622000 |
| 6  | -1.202019000 | -0.424471000 | -4.423702000 |
| 1  | -0.871505000 | -0.059183000 | -5.388796000 |
| 6  | 3.424990000  | 3.019534000  | -2.229572000 |
| 1  | 3.874180000  | 2.394674000  | -3.008137000 |
| 1  | 3.591450000  | 4.069169000  | -2.497414000 |
| 1  | 2.350171000  | 2.830389000  | -2.208658000 |
| 6  | -2.245461000 | -1.343007000 | -4.311898000 |
| 1  | -2.758821000 | -1.703796000 | -5.196580000 |
| 6  | -2.252511000 | -1.768339000 | -0.533710000 |
| 1  | -3.249321000 | -2.211102000 | -0.465357000 |
| 1  | -1.501684000 | -2.514002000 | -0.250153000 |
| 6  | -1.611762000 | 0.113399000  | 4.021770000  |
| 1  | -2.397747000 | -0.474563000 | 4.482194000  |
| 6  | 3.441077000  | 3.635152000  | 0.220963000  |
| 1  | 2.366500000  | 3.460598000  | 0.303825000  |
| 1  | 3.604949000  | 4.686274000  | -0.042295000 |
| 1  | 3.903435000  | 3.453426000  | 1.196842000  |
| 6  | 0.126826000  | 1.769101000  | 4.120936000  |
| 1  | 0.728383000  | 2.491821000  | 4.659205000  |
| 6  | 5.564603000  | 3.056016000  | -0.949428000 |
| 1  | 6.081431000  | 2.894263000  | 0.002014000  |
| 1  | 5.675558000  | 4.112830000  | -1.212124000 |
| 1  | 6.067730000  | 2.467399000  | -1.723191000 |
| 6  | -0.870873000 | 1.033741000  | 4.758837000  |
| 1  | -1.071155000 | 1.176351000  | 5.815279000  |
| 6  | 6.230341000  | -2.721067000 | -1.049851000 |
| 1  | 5.389141000  | -3.388651000 | -1.241636000 |
| 1  | 7.139782000  | -3.323256000 | -0.944216000 |
| 1  | 6.355517000  | -2.062862000 | -1.915639000 |
| 6  | 5.908642000  | -2.828840000 | 1.459041000  |
| 1  | 5.646039000  | -2.274298000 | 2.364784000  |
| 1  | 6.883194000  | -3.300249000 | 1.620943000  |
| 1  | 5.187682000  | -3.635189000 | 1.322887000  |
| 6  | 7.266067000  | -1.018369000 | 0.452613000  |
| 1  | 7.514545000  | -0.415952000 | -0.425908000 |
| 1  | 8.117512000  | -1.679420000 | 0.639510000  |
| 1  | 7.158452000  | -0.353549000 | 1.315630000  |
| 8  | -5.041332000 | -2.002377000 | 1.148362000  |
| 8  | -6.359562000 | -0.037701000 | 0.534885000  |
| 17 | -6.068090000 | -1.464659000 | 0.177668000  |
| 8  | -5.445249000 | -1.500680000 | -1.200445000 |
| 8  | -7.295020000 | -2.282798000 | 0.213159000  |

**LS-2-trans** ( $E_{\text{total}} = -3841.534996$  a.u.,  $E_{\text{ZPE}} = -3840.873862$  a.u.)

|    |              |              |              |
|----|--------------|--------------|--------------|
| 26 | 0.333985000  | -0.475631000 | 0.212013000  |
| 8  | -0.644423000 | 1.098889000  | 0.637968000  |
| 8  | -1.339692000 | -1.310181000 | 0.099682000  |
| 7  | 1.318879000  | -2.116185000 | -0.203904000 |
| 7  | 0.388912000  | 0.049766000  | -1.684539000 |
| 7  | 0.691050000  | -0.809133000 | 2.119571000  |
| 6  | -1.940521000 | 0.926510000  | 0.399879000  |
| 7  | -3.839742000 | -2.147274000 | -0.571312000 |
| 7  | 2.113796000  | 0.408199000  | 0.271824000  |
| 6  | -4.249960000 | 1.531356000  | 0.198834000  |
| 1  | -5.011907000 | 2.295012000  | 0.238642000  |
| 6  | -2.309238000 | -0.407080000 | 0.070358000  |
| 8  | -3.301065000 | -2.537200000 | -1.605955000 |
| 6  | -2.938497000 | 1.924771000  | 0.484289000  |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -3.647473000 | -0.726835000 | -0.210292000 |
| 6 | -4.669331000 | 0.229385000  | -0.155594000 |
| 8 | -4.479597000 | -2.868021000 | 0.189686000  |
| 6 | 2.659229000  | -1.976038000 | -0.245289000 |
| 6 | -2.587884000 | 3.368893000  | 0.864954000  |
| 6 | 3.198008000  | -0.586270000 | -0.058887000 |
| 1 | 3.971603000  | -0.562326000 | 0.711133000  |
| 1 | 3.699722000  | -0.262236000 | -0.976700000 |
| 6 | 1.706242000  | -0.067326000 | 2.620880000  |
| 6 | 0.763477000  | -3.328071000 | -0.413762000 |
| 1 | -0.319299000 | -3.354751000 | -0.375304000 |
| 6 | -0.373697000 | -0.441841000 | -2.678269000 |
| 1 | -1.125305000 | -1.167467000 | -2.387343000 |
| 6 | 3.497338000  | -3.065131000 | -0.489228000 |
| 1 | 4.570630000  | -2.913488000 | -0.517993000 |
| 6 | -6.158458000 | -0.047438000 | -0.455346000 |
| 6 | 1.345264000  | 0.970050000  | -1.958997000 |
| 6 | 0.051334000  | -1.687377000 | 2.910184000  |
| 1 | -0.758965000 | -2.233612000 | 2.441421000  |
| 6 | 2.269198000  | 0.941873000  | 1.657352000  |
| 1 | 1.656955000  | 1.846122000  | 1.721664000  |
| 1 | 3.312460000  | 1.202216000  | 1.854015000  |
| 6 | 1.586228000  | 1.399114000  | -3.259454000 |
| 1 | 2.386232000  | 2.104934000  | -3.449152000 |
| 6 | 1.538832000  | -4.449999000 | -0.663660000 |
| 1 | 1.058724000  | -5.407084000 | -0.828177000 |
| 6 | 2.928854000  | -4.316380000 | -0.698191000 |
| 1 | 3.560124000  | -5.177175000 | -0.890174000 |
| 6 | -0.202256000 | -0.031600000 | -3.995408000 |
| 1 | -0.838459000 | -0.443924000 | -4.769209000 |
| 6 | -1.935799000 | 3.386390000  | 2.267704000  |
| 1 | -2.636577000 | 3.010914000  | 3.020320000  |
| 1 | -1.662013000 | 4.412377000  | 2.538217000  |
| 1 | -1.037745000 | 2.766637000  | 2.290888000  |
| 6 | 0.796611000  | 0.893885000  | -4.291165000 |
| 1 | 0.965606000  | 1.213826000  | -5.313580000 |
| 6 | 2.074797000  | 1.497332000  | -0.752892000 |
| 1 | 3.082204000  | 1.847416000  | -0.991120000 |
| 1 | 1.488815000  | 2.316743000  | -0.327645000 |
| 6 | 2.126702000  | -0.213142000 | 3.938957000  |
| 1 | 2.956530000  | 0.379568000  | 4.306177000  |
| 6 | -1.603657000 | 3.955941000  | -0.172719000 |
| 1 | -0.690742000 | 3.360591000  | -0.222255000 |
| 1 | -1.337410000 | 4.982115000  | 0.103575000  |
| 1 | -2.058978000 | 3.977118000  | -1.168064000 |
| 6 | 0.407292000  | -1.866876000 | 4.241431000  |
| 1 | -0.134820000 | -2.580113000 | 4.850416000  |
| 6 | -3.826633000 | 4.280429000  | 0.909618000  |
| 1 | -4.320164000 | 4.348146000  | -0.065346000 |
| 1 | -3.516101000 | 5.290464000  | 1.194593000  |
| 1 | -4.558556000 | 3.937094000  | 1.647891000  |
| 6 | 1.465385000  | -1.123526000 | 4.761461000  |
| 1 | 1.773971000  | -1.251816000 | 5.793143000  |
| 6 | -6.816258000 | -0.737001000 | 0.764930000  |
| 1 | -6.344994000 | -1.695440000 | 0.984657000  |
| 1 | -7.879735000 | -0.906825000 | 0.561859000  |
| 1 | -6.736079000 | -0.099808000 | 1.651410000  |
| 6 | -6.341214000 | -0.922843000 | -1.717445000 |
| 1 | -5.815824000 | -0.490085000 | -2.574244000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| 1  | -7.406614000 | -0.972515000 | -1.964313000 |
| 1  | -6.000604000 | -1.949605000 | -1.581666000 |
| 6  | -6.930927000 | 1.263436000  | -0.717975000 |
| 1  | -6.986085000 | 1.900196000  | 0.169675000  |
| 1  | -7.958035000 | 1.011287000  | -0.998280000 |
| 1  | -6.488220000 | 1.840059000  | -1.536247000 |
| 8  | 5.015016000  | 1.846055000  | 0.572297000  |
| 8  | 6.339419000  | -0.092642000 | -0.102796000 |
| 17 | 5.952460000  | 1.302864000  | -0.484568000 |
| 8  | 5.178779000  | 1.256568000  | -1.783023000 |
| 8  | 7.138566000  | 2.168784000  | -0.617433000 |

**HS-2-trans** ( $E_{\text{total}} = -3841.51592107$  a.u.,  $E_{\text{ZPE}} = -3840.857764$  a.u.)

|    |              |              |              |
|----|--------------|--------------|--------------|
| 26 | 0.203100000  | 0.166493000  | -0.125724000 |
| 8  | -1.031420000 | -1.350967000 | 0.003938000  |
| 8  | -1.482906000 | 1.168641000  | -0.218324000 |
| 7  | 1.307810000  | 2.012105000  | -0.278571000 |
| 7  | 0.619438000  | 0.199999000  | 2.022057000  |
| 7  | 0.742459000  | -0.265952000 | -2.204859000 |
| 6  | -2.308262000 | -1.008379000 | 0.031792000  |
| 7  | -3.931616000 | 2.363010000  | -0.170705000 |
| 7  | 2.256108000  | -0.627347000 | 0.016450000  |
| 6  | -4.676756000 | -1.331519000 | 0.171249000  |
| 1  | -5.514039000 | -2.003980000 | 0.281806000  |
| 6  | -2.545401000 | 0.398262000  | -0.077118000 |
| 8  | -3.510533000 | 3.017935000  | 0.777194000  |
| 6  | -3.399144000 | -1.898096000 | 0.159512000  |
| 6  | -3.859352000 | 0.889134000  | -0.056151000 |
| 6  | -4.972617000 | 0.046548000  | 0.062112000  |
| 8  | -4.361229000 | 2.845251000  | -1.216217000 |
| 6  | 2.643335000  | 1.878028000  | -0.223973000 |
| 6  | -3.172569000 | -3.409952000 | 0.284978000  |
| 6  | 3.241420000  | 0.499169000  | -0.084894000 |
| 1  | 3.911213000  | 0.313466000  | -0.928417000 |
| 1  | 3.892602000  | 0.479047000  | 0.793236000  |
| 6  | 1.856295000  | -1.008014000 | -2.368786000 |
| 6  | 0.762938000  | 3.241552000  | -0.394707000 |
| 1  | -0.321006000 | 3.268962000  | -0.419152000 |
| 6  | -0.055952000 | 0.931756000  | 2.924251000  |
| 1  | -0.933902000 | 1.451028000  | 2.554318000  |
| 6  | 3.492578000  | 2.987376000  | -0.290484000 |
| 1  | 4.565710000  | 2.834716000  | -0.240755000 |
| 6  | -6.441077000 | 0.522372000  | 0.068272000  |
| 6  | 1.726447000  | -0.468822000 | 2.403799000  |
| 6  | 0.121721000  | 0.239853000  | -3.283591000 |
| 1  | -0.768691000 | 0.827682000  | -3.087092000 |
| 6  | 2.444382000  | -1.587048000 | -1.105431000 |
| 1  | 1.889998000  | -2.498538000 | -0.855475000 |
| 1  | 3.503588000  | -1.838133000 | -1.223502000 |
| 6  | 2.203769000  | -0.407924000 | 3.711114000  |
| 1  | 3.114409000  | -0.933265000 | 3.975443000  |
| 6  | 1.542261000  | 4.385381000  | -0.468900000 |
| 1  | 1.069564000  | 5.355792000  | -0.561965000 |
| 6  | 2.932604000  | 4.252299000  | -0.416727000 |
| 1  | 3.571324000  | 5.127587000  | -0.470647000 |
| 6  | 0.349057000  | 1.024736000  | 4.250867000  |
| 1  | -0.222995000 | 1.624368000  | 4.948759000  |
| 6  | -2.438383000 | -3.927224000 | -0.974585000 |
| 1  | -3.043269000 | -3.754061000 | -1.870589000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| 1  | -2.263101000 | -5.005183000 | -0.885164000 |
| 1  | -1.476962000 | -3.426408000 | -1.100708000 |
| 6  | 1.500651000  | 0.346676000  | 4.647738000  |
| 1  | 1.853141000  | 0.412183000  | 5.671451000  |
| 6  | 2.380058000  | -1.310181000 | 1.334647000  |
| 1  | 3.430099000  | -1.514627000 | 1.569982000  |
| 1  | 1.837446000  | -2.259606000 | 1.264757000  |
| 6  | 2.395186000  | -1.249294000 | -3.630905000 |
| 1  | 3.307368000  | -1.827737000 | -3.723573000 |
| 6  | -2.316735000 | -3.702755000 | 1.539977000  |
| 1  | -1.350702000 | -3.198513000 | 1.480419000  |
| 1  | -2.144989000 | -4.781381000 | 1.628260000  |
| 1  | -2.831733000 | -3.364703000 | 2.445106000  |
| 6  | 0.589929000  | 0.027811000  | -4.574806000 |
| 1  | 0.059559000  | 0.452704000  | -5.418599000 |
| 6  | -4.492331000 | -4.189344000 | 0.417430000  |
| 1  | -5.052821000 | -3.897199000 | 1.311484000  |
| 1  | -4.268361000 | -5.257385000 | 0.500415000  |
| 1  | -5.135897000 | -4.052138000 | -0.457624000 |
| 6  | 1.749792000  | -0.726009000 | -4.748898000 |
| 1  | 2.151308000  | -0.897698000 | -5.741768000 |
| 6  | -6.886739000 | 0.831918000  | -1.382151000 |
| 1  | -6.282316000 | 1.625028000  | -1.824429000 |
| 1  | -7.935980000 | 1.148044000  | -1.383708000 |
| 1  | -6.798373000 | -0.061996000 | -2.007681000 |
| 6  | -6.645266000 | 1.771965000  | 0.956996000  |
| 1  | -6.250680000 | 1.608432000  | 1.964224000  |
| 1  | -7.717798000 | 1.973599000  | 1.042173000  |
| 1  | -6.187456000 | 2.671591000  | 0.545279000  |
| 6  | -7.382548000 | -0.568927000 | 0.622284000  |
| 1  | -7.421809000 | -1.452161000 | -0.021576000 |
| 1  | -8.396505000 | -0.161129000 | 0.671594000  |
| 1  | -7.094255000 | -0.882161000 | 1.630674000  |
| 8  | 5.612101000  | -1.537192000 | -0.805764000 |
| 8  | 6.373939000  | 0.667805000  | -0.078769000 |
| 17 | 6.348240000  | -0.788685000 | 0.280311000  |
| 8  | 5.567858000  | -0.950722000 | 1.565715000  |
| 8  | 7.714750000  | -1.321774000 | 0.438041000  |

**LS-3-cis** ( $E_{\text{total}} = -3790.84434935$  a.u.,  $E_{\text{ZPE}} = -3790.124973$  a.u.)

|    |              |              |              |
|----|--------------|--------------|--------------|
| 26 | 0.340235000  | 0.662692000  | 0.076352000  |
| 8  | -1.271525000 | 1.604999000  | -0.240513000 |
| 8  | -0.787843000 | -0.739261000 | 0.671021000  |
| 7  | 1.521203000  | 2.098535000  | -0.533194000 |
| 7  | 2.003570000  | -0.375898000 | 0.402510000  |
| 7  | 0.438456000  | -0.194217000 | -1.697915000 |
| 8  | -2.062054000 | -3.562558000 | 0.018170000  |
| 7  | 0.624998000  | 1.278945000  | 1.923146000  |
| 6  | 1.544789000  | 0.554679000  | 2.603725000  |
| 6  | 1.925338000  | 0.895165000  | 3.898053000  |
| 1  | 2.680140000  | 0.306373000  | 4.406584000  |
| 6  | 1.323761000  | 1.990871000  | 4.514364000  |
| 1  | 1.603431000  | 2.273173000  | 5.523428000  |
| 6  | 0.362166000  | 2.717752000  | 3.814857000  |
| 1  | -0.133626000 | 3.572271000  | 4.259652000  |
| 6  | 0.042908000  | 2.334697000  | 2.517745000  |
| 1  | -0.693939000 | 2.856879000  | 1.919469000  |
| 6  | -2.334882000 | 0.818394000  | -0.099433000 |
| 6  | 2.837564000  | 1.804523000  | -0.483227000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -3.070739000 | -1.458869000 | 0.604597000  |
| 6 | -2.055561000 | -0.494203000 | 0.394044000  |
| 6 | -3.670923000 | 1.198378000  | -0.365136000 |
| 6 | -4.397725000 | -1.095001000 | 0.317880000  |
| 6 | 1.280120000  | -1.255335000 | -1.733656000 |
| 6 | -4.642546000 | 0.222222000  | -0.146765000 |
| 1 | -5.666475000 | 0.492977000  | -0.355208000 |
| 6 | -0.199888000 | 0.180192000  | -2.819857000 |
| 1 | -0.868032000 | 1.026190000  | -2.718424000 |
| 6 | -4.026480000 | 2.607336000  | -0.861440000 |
| 6 | 1.129423000  | 3.320429000  | -0.949902000 |
| 1 | 0.057860000  | 3.480662000  | -0.962751000 |
| 6 | 3.203601000  | 0.413857000  | -0.047624000 |
| 1 | 3.955984000  | 0.436832000  | 0.743421000  |
| 1 | 3.681853000  | -0.116986000 | -0.877412000 |
| 6 | 2.048786000  | -0.656053000 | 1.866975000  |
| 1 | 3.051747000  | -0.967578000 | 2.170080000  |
| 1 | 1.349563000  | -1.476195000 | 2.054735000  |
| 6 | 1.867204000  | -1.629660000 | -0.401864000 |
| 1 | 1.142665000  | -2.263720000 | 0.116630000  |
| 1 | 2.826008000  | -2.145185000 | -0.494638000 |
| 6 | -2.579260000 | -2.789092000 | 1.112761000  |
| 1 | -1.767599000 | -2.614277000 | 1.832308000  |
| 1 | -3.362216000 | -3.363098000 | 1.617254000  |
| 6 | 3.808451000  | 2.738040000  | -0.850371000 |
| 1 | 4.855799000  | 2.461524000  | -0.799241000 |
| 6 | 2.040504000  | 4.293454000  | -1.331471000 |
| 1 | 1.685640000  | 5.262646000  | -1.661323000 |
| 6 | -5.599963000 | -2.050466000 | 0.502817000  |
| 6 | -3.319228000 | 2.889747000  | -2.206765000 |
| 1 | -2.234645000 | 2.834893000  | -2.093776000 |
| 1 | -3.580025000 | 3.891993000  | -2.565776000 |
| 1 | -3.631480000 | 2.164794000  | -2.965584000 |
| 6 | -0.016227000 | -0.483996000 | -4.026536000 |
| 1 | -0.555110000 | -0.154842000 | -4.906931000 |
| 6 | 1.532374000  | -1.946485000 | -2.913710000 |
| 1 | 2.244238000  | -2.763426000 | -2.910645000 |
| 6 | 3.404749000  | 3.997068000  | -1.279455000 |
| 1 | 4.141542000  | 4.737707000  | -1.570854000 |
| 6 | -5.827693000 | -2.343914000 | 2.006825000  |
| 1 | -4.975449000 | -2.833275000 | 2.481637000  |
| 1 | -6.700011000 | -2.995948000 | 2.129851000  |
| 1 | -6.020210000 | -1.412115000 | 2.547953000  |
| 6 | -6.922150000 | -1.444020000 | -0.015663000 |
| 1 | -7.220104000 | -0.552963000 | 0.545748000  |
| 1 | -7.716977000 | -2.187240000 | 0.103464000  |
| 1 | -6.864296000 | -1.186527000 | -1.077755000 |
| 6 | 0.870151000  | -1.558032000 | -4.076444000 |
| 1 | 1.048624000  | -2.082949000 | -5.008520000 |
| 6 | -3.576078000 | 3.655459000  | 0.182695000  |
| 1 | -4.081435000 | 3.486974000  | 1.139065000  |
| 1 | -3.828195000 | 4.664401000  | -0.163866000 |
| 1 | -2.497655000 | 3.602033000  | 0.344054000  |
| 6 | -5.394339000 | -3.361338000 | -0.293313000 |
| 1 | -5.343920000 | -3.142733000 | -1.364692000 |
| 1 | -6.245009000 | -4.031228000 | -0.122813000 |
| 1 | -4.478645000 | -3.889650000 | -0.030802000 |
| 6 | -5.539156000 | 2.785299000  | -1.082363000 |
| 1 | -5.924345000 | 2.096131000  | -1.840595000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| 1  | -5.732367000 | 3.805310000  | -1.430250000 |
| 1  | -6.106069000 | 2.635877000  | -0.158043000 |
| 6  | -1.470416000 | -4.767730000 | 0.473107000  |
| 1  | -2.201970000 | -5.405751000 | 0.991969000  |
| 1  | -0.633378000 | -4.568744000 | 1.159236000  |
| 1  | -1.098128000 | -5.293628000 | -0.407333000 |
| 17 | 5.742558000  | -1.812741000 | 0.025340000  |
| 8  | 6.279466000  | -0.419658000 | 0.150942000  |
| 8  | 6.825270000  | -2.810936000 | 0.118991000  |
| 8  | 4.723053000  | -2.034250000 | 1.121216000  |
| 8  | 5.015785000  | -1.939176000 | -1.293547000 |

**HS-3-cis** ( $E_{\text{total}} = -3790.82661134$  a.u.,  $E_{\text{ZPE}} = -3790.110197$  a.u.)

|    |              |              |              |
|----|--------------|--------------|--------------|
| 26 | 0.206272000  | 0.468203000  | -0.002248000 |
| 8  | -1.406357000 | 1.470046000  | -0.500364000 |
| 8  | -1.117805000 | -0.868242000 | 0.534653000  |
| 7  | 1.559371000  | 2.062256000  | -0.578616000 |
| 7  | 2.143769000  | -0.473625000 | 0.504799000  |
| 7  | 0.741692000  | -0.639246000 | -1.824430000 |
| 8  | -2.723615000 | -3.587393000 | 0.068874000  |
| 7  | 0.572357000  | 1.107985000  | 2.082492000  |
| 6  | 1.598239000  | 0.491391000  | 2.701112000  |
| 6  | 2.040820000  | 0.892482000  | 3.960843000  |
| 1  | 2.881631000  | 0.386338000  | 4.421843000  |
| 6  | 1.390604000  | 1.944745000  | 4.600804000  |
| 1  | 1.718011000  | 2.275551000  | 5.580600000  |
| 6  | 0.319292000  | 2.568674000  | 3.963229000  |
| 1  | -0.215036000 | 3.388902000  | 4.427764000  |
| 6  | -0.054729000 | 2.121238000  | 2.701282000  |
| 1  | -0.876430000 | 2.572159000  | 2.155045000  |
| 6  | -2.531449000 | 0.794506000  | -0.280379000 |
| 6  | 2.862271000  | 1.789428000  | -0.392605000 |
| 6  | -3.461635000 | -1.359677000 | 0.576578000  |
| 6  | -2.363931000 | -0.512234000 | 0.289827000  |
| 6  | -3.828664000 | 1.270535000  | -0.563137000 |
| 6  | -4.756607000 | -0.887901000 | 0.295707000  |
| 6  | 1.740094000  | -1.531600000 | -1.660165000 |
| 6  | -4.884872000 | 0.409087000  | -0.258466000 |
| 1  | -5.882592000 | 0.762924000  | -0.470532000 |
| 6  | 0.254344000  | -0.422590000 | -3.056562000 |
| 1  | -0.553427000 | 0.297906000  | -3.128049000 |
| 6  | -4.055492000 | 2.659403000  | -1.176722000 |
| 6  | 1.192691000  | 3.280252000  | -1.024989000 |
| 1  | 0.125219000  | 3.427057000  | -1.149006000 |
| 6  | 3.266020000  | 0.405183000  | 0.053209000  |
| 1  | 4.024133000  | 0.475157000  | 0.836558000  |
| 1  | 3.777283000  | -0.086497000 | -0.781867000 |
| 6  | 2.186780000  | -0.692864000 | 1.971840000  |
| 1  | 3.207094000  | -0.915847000 | 2.299232000  |
| 1  | 1.560581000  | -1.564988000 | 2.189733000  |
| 6  | 2.171178000  | -1.767817000 | -0.234984000 |
| 1  | 1.437618000  | -2.427940000 | 0.240818000  |
| 1  | 3.161314000  | -2.227981000 | -0.187521000 |
| 6  | -3.083541000 | -2.704324000 | 1.142136000  |
| 1  | -2.212385000 | -2.576106000 | 1.798022000  |
| 1  | -3.888774000 | -3.159959000 | 1.727077000  |
| 6  | 3.851709000  | 2.744320000  | -0.651071000 |
| 1  | 4.893007000  | 2.483170000  | -0.494652000 |
| 6  | 2.116496000  | 4.275102000  | -1.305732000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| 1  | 1.781792000  | 5.240940000  | -1.665181000 |
| 6  | -6.040008000 | -1.702025000 | 0.582592000  |
| 6  | -3.345430000 | 2.744499000  | -2.547930000 |
| 1  | -2.273264000 | 2.569115000  | -2.441746000 |
| 1  | -3.497264000 | 3.736732000  | -2.988497000 |
| 1  | -3.754849000 | 1.999654000  | -3.238088000 |
| 6  | 0.750686000  | -1.078930000 | -4.177043000 |
| 1  | 0.326528000  | -0.876668000 | -5.153465000 |
| 6  | 2.310214000  | -2.207162000 | -2.736649000 |
| 1  | 3.148591000  | -2.872061000 | -2.564764000 |
| 6  | 3.472678000  | 3.998256000  | -1.112661000 |
| 1  | 4.223763000  | 4.752792000  | -1.321219000 |
| 6  | -6.236491000 | -1.869011000 | 2.110164000  |
| 1  | -5.417292000 | -2.407696000 | 2.589797000  |
| 1  | -7.162283000 | -2.421545000 | 2.307117000  |
| 1  | -6.316611000 | -0.888391000 | 2.590000000  |
| 6  | -7.313586000 | -0.998892000 | 0.064752000  |
| 1  | -7.496107000 | -0.044233000 | 0.568057000  |
| 1  | -8.174261000 | -1.644914000 | 0.265078000  |
| 1  | -7.273297000 | -0.824428000 | -1.014902000 |
| 6  | 1.803140000  | -1.978528000 | -4.013700000 |
| 1  | 2.230214000  | -2.488623000 | -4.870397000 |
| 6  | -3.487845000 | 3.745257000  | -0.233186000 |
| 1  | -4.000341000 | 3.718749000  | 0.734160000  |
| 1  | -3.637961000 | 4.739104000  | -0.670665000 |
| 1  | -2.419618000 | 3.594186000  | -0.066579000 |
| 6  | -5.997201000 | -3.078193000 | -0.123098000 |
| 1  | -5.962795000 | -2.940440000 | -1.208416000 |
| 1  | -6.905158000 | -3.642229000 | 0.119663000  |
| 1  | -5.131026000 | -3.678831000 | 0.151136000  |
| 6  | -5.547246000 | 2.964652000  | -1.400014000 |
| 1  | -6.010576000 | 2.251591000  | -2.089341000 |
| 1  | -5.646618000 | 3.963272000  | -1.837800000 |
| 1  | -6.110441000 | 2.955474000  | -0.461228000 |
| 6  | -2.166438000 | -4.795259000 | 0.557319000  |
| 1  | -2.880531000 | -5.343100000 | 1.191174000  |
| 1  | -1.253978000 | -4.604567000 | 1.141847000  |
| 1  | -1.917713000 | -5.406036000 | -0.311815000 |
| 17 | 6.037899000  | -1.521889000 | 0.143635000  |
| 8  | 6.401284000  | -0.070149000 | 0.227353000  |
| 8  | 7.237467000  | -2.376024000 | 0.243248000  |
| 8  | 5.068123000  | -1.839463000 | 1.259929000  |
| 8  | 5.317605000  | -1.769087000 | -1.161924000 |

**LS-3-trans** ( $E_{\text{total}} = -3790.84693384$  a.u.,  $E_{\text{ZPE}} = -3790.127403$  a.u.)

|    |              |              |              |
|----|--------------|--------------|--------------|
| 26 | -0.337595000 | 0.333680000  | 0.267953000  |
| 8  | 0.580657000  | -1.323698000 | 0.100964000  |
| 8  | 1.333230000  | 1.031635000  | 0.767433000  |
| 7  | -1.263955000 | 2.052063000  | 0.413884000  |
| 7  | -2.097231000 | -0.391728000 | -0.319200000 |
| 7  | -0.996817000 | -0.173217000 | 2.052688000  |
| 8  | 3.613345000  | 2.811411000  | -0.354093000 |
| 7  | -0.069939000 | 0.668388000  | -1.651437000 |
| 6  | -0.975517000 | 0.043406000  | -2.441641000 |
| 6  | -0.973927000 | 0.214383000  | -3.821801000 |
| 1  | -1.725367000 | -0.282528000 | -4.424687000 |
| 6  | 0.003381000  | 1.022557000  | -4.401305000 |
| 1  | 0.026091000  | 1.166665000  | -5.476108000 |
| 6  | 0.945706000  | 1.640108000  | -3.582663000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 1 | 1.727884000  | 2.266853000  | -3.993865000 |
| 6 | 0.876514000  | 1.448437000  | -2.206597000 |
| 1 | 1.583031000  | 1.906283000  | -1.521736000 |
| 6 | 1.893266000  | -1.134727000 | 0.123557000  |
| 6 | -2.575006000 | 2.021920000  | 0.098302000  |
| 6 | 3.673210000  | 0.567778000  | 0.506376000  |
| 6 | 2.314011000  | 0.183808000  | 0.470001000  |
| 6 | 2.866177000  | -2.129478000 | -0.131496000 |
| 6 | 4.645813000  | -0.409210000 | 0.223124000  |
| 6 | -2.050760000 | -1.023372000 | 2.015470000  |
| 6 | 4.198822000  | -1.721228000 | -0.067217000 |
| 1 | 4.949872000  | -2.469749000 | -0.270378000 |
| 6 | -0.538661000 | 0.263320000  | 3.237864000  |
| 1 | 0.316385000  | 0.927473000  | 3.190916000  |
| 6 | 2.465016000  | -3.571894000 | -0.466214000 |
| 6 | -0.686911000 | 3.223658000  | 0.751838000  |
| 1 | 0.370726000  | 3.163519000  | 0.979953000  |
| 6 | -3.153509000 | 0.678756000  | -0.243600000 |
| 1 | -3.712638000 | 0.719585000  | -1.180365000 |
| 1 | -3.889577000 | 0.392333000  | 0.514788000  |
| 6 | -1.912000000 | -0.885526000 | -1.714558000 |
| 1 | -2.877092000 | -1.009007000 | -2.212707000 |
| 1 | -1.426858000 | -1.863408000 | -1.644600000 |
| 6 | -2.412588000 | -1.499353000 | 0.635649000  |
| 1 | -1.758134000 | -2.337259000 | 0.379939000  |
| 1 | -3.459245000 | -1.801965000 | 0.556788000  |
| 6 | 3.904014000  | 2.021717000  | 0.818032000  |
| 1 | 3.220790000  | 2.332903000  | 1.620385000  |
| 1 | 4.926825000  | 2.232849000  | 1.139628000  |
| 6 | -3.356894000 | 3.178137000  | 0.116730000  |
| 1 | -4.408353000 | 3.111931000  | -0.140109000 |
| 6 | -1.406174000 | 4.408348000  | 0.794193000  |
| 1 | -0.908913000 | 5.329789000  | 1.073186000  |
| 6 | 6.164719000  | -0.120795000 | 0.226145000  |
| 6 | 1.614914000  | -3.590172000 | -1.757635000 |
| 1 | 0.718104000  | -2.980146000 | -1.638781000 |
| 1 | 1.312075000  | -4.616724000 | -1.993028000 |
| 1 | 2.191020000  | -3.200945000 | -2.603438000 |
| 6 | -1.123723000 | -0.123852000 | 4.437482000  |
| 1 | -0.723178000 | 0.245518000  | 5.374029000  |
| 6 | -2.701760000 | -1.428120000 | 3.176110000  |
| 1 | -3.569699000 | -2.072724000 | 3.102934000  |
| 6 | -2.765036000 | 4.385050000  | 0.470658000  |
| 1 | -3.353139000 | 5.296092000  | 0.493617000  |
| 6 | 6.647685000  | 0.228790000  | 1.655951000  |
| 1 | 6.167147000  | 1.118766000  | 2.066602000  |
| 1 | 7.729538000  | 0.404359000  | 1.651023000  |
| 1 | 6.441082000  | -0.603162000 | 2.336373000  |
| 6 | 6.998299000  | -1.343564000 | -0.214469000 |
| 1 | 6.888763000  | -2.188715000 | 0.471990000  |
| 1 | 8.055998000  | -1.061250000 | -0.222461000 |
| 1 | 6.734882000  | -1.675347000 | -1.223370000 |
| 6 | -2.227553000 | -0.974771000 | 4.405670000  |
| 1 | -2.717463000 | -1.276318000 | 5.325014000  |
| 6 | 1.643664000  | -4.164329000 | 0.702859000  |
| 1 | 2.245032000  | -4.193749000 | 1.617284000  |
| 1 | 1.336657000  | -5.188756000 | 0.463028000  |
| 1 | 0.751158000  | -3.566650000 | 0.895354000  |
| 6 | 6.513279000  | 1.011191000  | -0.770469000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| 1  | 6.264144000  | 0.699386000  | -1.789705000 |
| 1  | 7.588915000  | 1.218552000  | -0.731881000 |
| 1  | 5.976393000  | 1.939679000  | -0.577135000 |
| 6  | 3.685286000  | -4.481386000 | -0.693780000 |
| 1  | 4.295644000  | -4.142989000 | -1.537452000 |
| 1  | 3.338226000  | -5.494742000 | -0.919960000 |
| 1  | 4.322067000  | -4.538508000 | 0.194999000  |
| 6  | 3.729784000  | 4.198113000  | -0.081883000 |
| 1  | 4.751435000  | 4.462039000  | 0.228776000  |
| 1  | 3.033071000  | 4.509925000  | 0.711148000  |
| 1  | 3.488469000  | 4.729262000  | -1.004213000 |
| 17 | -6.066603000 | -0.990308000 | -0.565134000 |
| 8  | -6.255436000 | 0.440577000  | -0.964444000 |
| 8  | -7.304070000 | -1.768326000 | -0.767256000 |
| 8  | -4.935588000 | -1.572336000 | -1.384391000 |
| 8  | -5.639350000 | -1.039800000 | 0.884674000  |

**HS-3-trans** ( $E_{\text{total}} = -3790.82880709$  a.u.,  $E_{\text{ZPE}} = -3790.112285$  a.u.)

|    |              |              |              |
|----|--------------|--------------|--------------|
| 26 | 0.223707000  | 0.081322000  | -0.335760000 |
| 8  | -0.920183000 | -1.424662000 | 0.181966000  |
| 8  | -1.487320000 | 0.825381000  | -0.930610000 |
| 7  | 1.305034000  | 1.874705000  | -0.898310000 |
| 7  | 2.220598000  | -0.383730000 | 0.511487000  |
| 7  | 1.226284000  | -1.042373000 | -1.931823000 |
| 8  | -3.695522000 | 2.901340000  | -0.152218000 |
| 7  | 0.139923000  | 0.943279000  | 1.686063000  |
| 6  | 1.168134000  | 0.629612000  | 2.497689000  |
| 6  | 1.316829000  | 1.220548000  | 3.750720000  |
| 1  | 2.165965000  | 0.960231000  | 4.372815000  |
| 6  | 0.361539000  | 2.140899000  | 4.177830000  |
| 1  | 0.454829000  | 2.613502000  | 5.149856000  |
| 6  | -0.708487000 | 2.448442000  | 3.339844000  |
| 1  | -1.473931000 | 3.155650000  | 3.636497000  |
| 6  | -0.781723000 | 1.832554000  | 2.094338000  |
| 1  | -1.586013000 | 2.043643000  | 1.395682000  |
| 6  | -2.210457000 | -1.164584000 | 0.061562000  |
| 6  | 2.596592000  | 1.899430000  | -0.528361000 |
| 6  | -3.855784000 | 0.561469000  | -0.658160000 |
| 6  | -2.527991000 | 0.102610000  | -0.530687000 |
| 6  | -3.253489000 | -2.026549000 | 0.471664000  |
| 6  | -4.899796000 | -0.288514000 | -0.237195000 |
| 6  | 2.342021000  | -1.694726000 | -1.543086000 |
| 6  | -4.553911000 | -1.553174000 | 0.295016000  |
| 1  | -5.359299000 | -2.201619000 | 0.605443000  |
| 6  | 0.890552000  | -1.038029000 | -3.232495000 |
| 1  | -0.019015000 | -0.504211000 | -3.487412000 |
| 6  | -2.953051000 | -3.399386000 | 1.086565000  |
| 6  | 0.760025000  | 2.957889000  | -1.486424000 |
| 1  | -0.290877000 | 2.865602000  | -1.738358000 |
| 6  | 3.201868000  | 0.663406000  | 0.089700000  |
| 1  | 3.835696000  | 0.942935000  | 0.934130000  |
| 1  | 3.890440000  | 0.218866000  | -0.637353000 |
| 6  | 2.098063000  | -0.447990000 | 1.989718000  |
| 1  | 3.085044000  | -0.399683000 | 2.460266000  |
| 1  | 1.653561000  | -1.417957000 | 2.238201000  |
| 6  | 2.605558000  | -1.705553000 | -0.058446000 |
| 1  | 1.959042000  | -2.459784000 | 0.403571000  |
| 1  | 3.650220000  | -1.942012000 | 0.158490000  |
| 6  | -3.983409000 | 1.958322000  | -1.204098000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| 1  | -3.246811000 | 2.098810000  | -2.006459000 |
| 1  | -4.976331000 | 2.172759000  | -1.608094000 |
| 6  | 3.396988000  | 3.025623000  | -0.747725000 |
| 1  | 4.437442000  | 3.004120000  | -0.441425000 |
| 6  | 1.492018000  | 4.107925000  | -1.739674000 |
| 1  | 1.019771000  | 4.958397000  | -2.217034000 |
| 6  | -6.394587000 | 0.089954000  | -0.345647000 |
| 6  | -2.134283000 | -3.218171000 | 2.386454000  |
| 1  | -1.192530000 | -2.705584000 | 2.184013000  |
| 1  | -1.913964000 | -4.196964000 | 2.827664000  |
| 1  | -2.700055000 | -2.633280000 | 3.119062000  |
| 6  | 1.658174000  | -1.675912000 | -4.199392000 |
| 1  | 1.350478000  | -1.649237000 | -5.238047000 |
| 6  | 3.178559000  | -2.333132000 | -2.456311000 |
| 1  | 4.095661000  | -2.792139000 | -2.106237000 |
| 6  | 2.837292000  | 4.138471000  | -1.362361000 |
| 1  | 3.440106000  | 5.021959000  | -1.544148000 |
| 6  | -6.811911000 | 0.215121000  | -1.832515000 |
| 1  | -6.258672000 | 0.986535000  | -2.371194000 |
| 1  | -7.878371000 | 0.458579000  | -1.899418000 |
| 1  | -6.646540000 | -0.734711000 | -2.350469000 |
| 6  | -7.322055000 | -0.983043000 | 0.264678000  |
| 1  | -7.250359000 | -1.940246000 | -0.260778000 |
| 1  | -8.357601000 | -0.638165000 | 0.180584000  |
| 1  | -7.112390000 | -1.149080000 | 1.325735000  |
| 6  | 2.826981000  | -2.325861000 | -3.803664000 |
| 1  | 3.462528000  | -2.811104000 | -4.536518000 |
| 6  | -2.144109000 | -4.252537000 | 0.081384000  |
| 1  | -2.720514000 | -4.415381000 | -0.835216000 |
| 1  | -1.918474000 | -5.231120000 | 0.520374000  |
| 1  | -1.205519000 | -3.761520000 | -0.180811000 |
| 6  | -6.691667000 | 1.397456000  | 0.427852000  |
| 1  | -6.491712000 | 1.252594000  | 1.494223000  |
| 1  | -7.749636000 | 1.659996000  | 0.313210000  |
| 1  | -6.088210000 | 2.242866000  | 0.098893000  |
| 6  | -4.235033000 | -4.173595000 | 1.440087000  |
| 1  | -4.840308000 | -3.644402000 | 2.183331000  |
| 1  | -3.960173000 | -5.144038000 | 1.865609000  |
| 1  | -4.854517000 | -4.360984000 | 0.556938000  |
| 6  | -3.691450000 | 4.231631000  | -0.640903000 |
| 1  | -4.670677000 | 4.510738000  | -1.057858000 |
| 1  | -2.928328000 | 4.368199000  | -1.422203000 |
| 1  | -3.463938000 | 4.884439000  | 0.203556000  |
| 17 | 6.265020000  | -0.653938000 | 0.636527000  |
| 8  | 6.339015000  | 0.841496000  | 0.578585000  |
| 8  | 7.583615000  | -1.239902000 | 0.946080000  |
| 8  | 5.251599000  | -1.045239000 | 1.688304000  |
| 8  | 5.756472000  | -1.167343000 | -0.692107000 |

**LS-4-cis** ( $E_{\text{total}} = -3636.97218614$  a.u.,  $E_{\text{ZPE}} = -3636.314037$  a.u.)

|    |              |              |              |
|----|--------------|--------------|--------------|
| 26 | 0.200126000  | 0.464615000  | 0.010959000  |
| 8  | -0.735806000 | -1.191112000 | -0.032946000 |
| 8  | -1.526434000 | 1.256036000  | 0.030161000  |
| 7  | 1.169606000  | 2.156971000  | 0.048401000  |
| 7  | 0.404345000  | 0.417834000  | -1.946800000 |
| 7  | 1.990133000  | -0.403907000 | -0.006718000 |
| 7  | 0.400307000  | 0.310432000  | 1.963621000  |
| 6  | -2.494859000 | 0.348042000  | 0.011395000  |
| 6  | -4.327637000 | -1.803721000 | -0.041560000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 6 | -3.884310000 | 0.639483000  | 0.022800000  |
| 6 | -2.042233000 | -1.012694000 | -0.024809000 |
| 6 | -4.752294000 | -0.453158000 | -0.003373000 |
| 1 | -5.815385000 | -0.257812000 | 0.005129000  |
| 6 | -2.962860000 | -2.071525000 | -0.051615000 |
| 6 | 2.514403000  | 2.039112000  | 0.047559000  |
| 6 | 1.403415000  | -0.395165000 | -2.365815000 |
| 6 | 1.379900000  | -0.547572000 | 2.337252000  |
| 6 | -5.329596000 | -2.969167000 | -0.077943000 |
| 6 | 0.609807000  | 3.384754000  | 0.057473000  |
| 1 | -0.473625000 | 3.395571000  | 0.057219000  |
| 6 | -4.400327000 | 2.085823000  | 0.060834000  |
| 6 | 2.059380000  | -1.193549000 | -1.274650000 |
| 1 | 1.467351000  | -2.099309000 | -1.116742000 |
| 1 | 3.087265000  | -1.478576000 | -1.512188000 |
| 6 | 3.341138000  | 3.164095000  | 0.052517000  |
| 1 | 4.417663000  | 3.034561000  | 0.049113000  |
| 6 | 3.073361000  | 0.642840000  | 0.052128000  |
| 1 | 3.768565000  | 0.492912000  | -0.779382000 |
| 1 | 3.680793000  | 0.475242000  | 0.946361000  |
| 6 | -0.302951000 | 1.116242000  | -2.852246000 |
| 1 | -1.095945000 | 1.734087000  | -2.449004000 |
| 6 | -0.294719000 | 0.970668000  | 2.906184000  |
| 1 | -1.072279000 | 1.628533000  | 2.537920000  |
| 6 | 2.027929000  | -1.286892000 | 1.200325000  |
| 1 | 3.046709000  | -1.610854000 | 1.425948000  |
| 1 | 1.414707000  | -2.162735000 | 0.971052000  |
| 6 | 2.765387000  | 4.429431000  | 0.062313000  |
| 1 | 3.391043000  | 5.315318000  | 0.066534000  |
| 6 | 1.373407000  | 4.541915000  | 0.065901000  |
| 1 | 0.884961000  | 5.509027000  | 0.073678000  |
| 6 | -5.095868000 | -3.888429000 | 1.142762000  |
| 1 | -4.082386000 | -4.299064000 | 1.147178000  |
| 1 | -5.800814000 | -4.727247000 | 1.125195000  |
| 1 | -5.240703000 | -3.337061000 | 2.077070000  |
| 6 | -3.902185000 | 2.856321000  | -1.183670000 |
| 1 | -2.811148000 | 2.883696000  | -1.211923000 |
| 1 | -4.275512000 | 3.886804000  | -1.162569000 |
| 1 | -4.264870000 | 2.381399000  | -2.101009000 |
| 6 | 1.737733000  | -0.502386000 | -3.712371000 |
| 1 | 2.560553000  | -1.143068000 | -4.007792000 |
| 6 | -0.036824000 | 1.037898000  | -4.213789000 |
| 1 | -0.635012000 | 1.612160000  | -4.911117000 |
| 6 | -3.893148000 | 2.793818000  | 1.338373000  |
| 1 | -4.245710000 | 2.270998000  | 2.233353000  |
| 1 | -4.270358000 | 3.822468000  | 1.373536000  |
| 1 | -2.802077000 | 2.824160000  | 1.358117000  |
| 6 | 1.705268000  | -0.741823000 | 3.676064000  |
| 1 | 2.512712000  | -1.416531000 | 3.935918000  |
| 6 | -0.036029000 | 0.806879000  | 4.261617000  |
| 1 | -0.623782000 | 1.353116000  | 4.989650000  |
| 6 | 0.984361000  | -0.057944000 | 4.653125000  |
| 1 | 1.218528000  | -0.195797000 | 5.703038000  |
| 6 | 1.004826000  | 0.221328000  | -4.650784000 |
| 1 | 1.245504000  | 0.150847000  | -5.705897000 |
| 6 | -6.793303000 | -2.495414000 | -0.045838000 |
| 1 | -7.018148000 | -1.932521000 | 0.865843000  |
| 1 | -7.456560000 | -3.365908000 | -0.071495000 |
| 1 | -7.036048000 | -1.867934000 | -0.909427000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| 6  | -5.116981000 | -3.784869000 | -1.373852000 |
| 1  | -5.283349000 | -3.159719000 | -2.256752000 |
| 1  | -5.817174000 | -4.627103000 | -1.411571000 |
| 1  | -4.101260000 | -4.185958000 | -1.431116000 |
| 6  | -5.937978000 | 2.155640000  | 0.068374000  |
| 1  | -6.370729000 | 1.703227000  | -0.829462000 |
| 1  | -6.248019000 | 3.205386000  | 0.095261000  |
| 1  | -6.363832000 | 1.659650000  | 0.946288000  |
| 17 | 5.567836000  | -1.940477000 | -0.031904000 |
| 8  | 5.385820000  | -1.046362000 | -1.236151000 |
| 8  | 4.499616000  | -2.996481000 | -0.067057000 |
| 8  | 5.364997000  | -1.107283000 | 1.210940000  |
| 8  | 6.914198000  | -2.543333000 | -0.036840000 |
| 1  | -2.575261000 | -3.084745000 | -0.080982000 |

**HS-4-cis** ( $E_{\text{total}} = -3636.95526271$  a.u.,  $E_{\text{ZPE}} = -3636.299739$  a.u.)

|    |              |              |              |
|----|--------------|--------------|--------------|
| 26 | -0.018704000 | 0.207734000  | 0.001310000  |
| 8  | -1.231490000 | -1.312186000 | -0.240636000 |
| 8  | -1.702320000 | 1.200708000  | 0.144182000  |
| 7  | 1.265675000  | 1.925591000  | 0.307786000  |
| 7  | 0.477880000  | 0.315792000  | -2.143829000 |
| 7  | 1.949392000  | -0.780322000 | -0.130596000 |
| 7  | 0.422946000  | -0.367201000 | 2.086842000  |
| 6  | -2.778980000 | 0.425174000  | 0.032340000  |
| 6  | -4.876896000 | -1.456879000 | -0.229409000 |
| 6  | -4.115320000 | 0.882560000  | 0.108641000  |
| 6  | -2.505582000 | -0.971420000 | -0.179078000 |
| 6  | -5.121806000 | -0.080446000 | -0.026456000 |
| 1  | -6.149942000 | 0.250032000  | 0.029441000  |
| 6  | -3.555308000 | -1.890815000 | -0.305512000 |
| 6  | 2.580125000  | 1.647588000  | 0.296358000  |
| 6  | 1.520235000  | -0.451698000 | -2.521018000 |
| 6  | 1.447426000  | -1.232171000 | 2.226448000  |
| 6  | -6.017341000 | -2.479699000 | -0.359332000 |
| 6  | 0.857960000  | 3.194192000  | 0.516810000  |
| 1  | -0.216265000 | 3.344705000  | 0.513187000  |
| 6  | -4.433121000 | 2.368314000  | 0.333722000  |
| 6  | 2.039976000  | -1.408699000 | -1.476172000 |
| 1  | 1.389150000  | -2.289832000 | -1.469066000 |
| 1  | 3.067775000  | -1.719741000 | -1.691604000 |
| 6  | 3.541525000  | 2.644584000  | 0.498271000  |
| 1  | 4.592142000  | 2.373172000  | 0.480255000  |
| 6  | 3.038009000  | 0.230032000  | 0.054013000  |
| 1  | 3.692101000  | 0.215316000  | -0.822235000 |
| 1  | 3.682313000  | -0.083188000 | 0.879925000  |
| 6  | -0.084563000 | 1.143755000  | -3.038869000 |
| 1  | -0.924476000 | 1.729301000  | -2.680193000 |
| 6  | -0.165184000 | 0.135155000  | 3.184321000  |
| 1  | -0.989339000 | 0.818599000  | 3.009608000  |
| 6  | 1.997619000  | -1.807762000 | 0.944482000  |
| 1  | 3.017950000  | -2.182618000 | 1.077764000  |
| 1  | 1.346067000  | -2.632557000 | 0.635951000  |
| 6  | 3.119540000  | 3.949643000  | 0.713401000  |
| 1  | 3.846698000  | 4.738962000  | 0.872078000  |
| 6  | 1.750603000  | 4.234069000  | 0.722876000  |
| 1  | 1.383041000  | 5.240077000  | 0.887109000  |
| 6  | -5.895374000 | -3.526740000 | 0.771424000  |
| 1  | -4.937896000 | -4.053192000 | 0.726421000  |
| 1  | -6.695975000 | -4.270323000 | 0.687360000  |

|    |              |              |              |
|----|--------------|--------------|--------------|
| 1  | -5.971848000 | -3.048324000 | 1.752813000  |
| 6  | -3.837343000 | 3.210604000  | -0.818405000 |
| 1  | -2.754065000 | 3.086231000  | -0.869849000 |
| 1  | -4.062268000 | 4.272238000  | -0.663012000 |
| 1  | -4.270261000 | 2.908306000  | -1.777648000 |
| 6  | 2.048786000  | -0.389508000 | -3.809153000 |
| 1  | 2.906649000  | -1.000178000 | -4.066805000 |
| 6  | 0.374595000  | 1.248253000  | -4.346747000 |
| 1  | -0.109376000 | 1.928539000  | -5.037486000 |
| 6  | -3.828955000 | 2.833193000  | 1.679196000  |
| 1  | -4.262593000 | 2.266603000  | 2.509826000  |
| 1  | -4.046218000 | 3.895360000  | 1.841459000  |
| 1  | -2.746495000 | 2.692235000  | 1.687618000  |
| 6  | 1.932061000  | -1.599420000 | 3.480649000  |
| 1  | 2.777484000  | -2.274264000 | 3.552434000  |
| 6  | 0.249007000  | -0.197582000 | 4.468922000  |
| 1  | -0.254903000 | 0.229662000  | 5.327797000  |
| 6  | 1.321434000  | -1.075853000 | 4.617558000  |
| 1  | 1.681587000  | -1.344568000 | 5.604787000  |
| 6  | 1.465277000  | 0.471646000  | -4.735033000 |
| 1  | 1.860117000  | 0.539997000  | -5.742987000 |
| 6  | -7.409498000 | -1.831668000 | -0.262828000 |
| 1  | -7.558930000 | -1.333474000 | 0.700492000  |
| 1  | -8.177225000 | -2.606120000 | -0.358653000 |
| 1  | -7.573306000 | -1.099924000 | -1.060529000 |
| 6  | -5.914721000 | -3.196257000 | -1.725226000 |
| 1  | -6.003131000 | -2.478881000 | -2.547033000 |
| 1  | -6.717029000 | -3.935895000 | -1.825770000 |
| 1  | -4.959341000 | -3.717238000 | -1.833633000 |
| 6  | -5.947047000 | 2.641556000  | 0.380066000  |
| 1  | -6.439583000 | 2.367401000  | -0.558397000 |
| 1  | -6.112234000 | 3.711522000  | 0.543168000  |
| 1  | -6.434171000 | 2.101046000  | 1.197989000  |
| 17 | 6.035294000  | -1.307404000 | -0.170556000 |
| 8  | 6.175503000  | 0.164389000  | 0.090417000  |
| 8  | 5.264387000  | -1.493608000 | -1.456263000 |
| 8  | 5.226472000  | -1.916944000 | 0.950344000  |
| 8  | 7.357101000  | -1.957240000 | -0.263818000 |
| 1  | -3.301224000 | -2.934380000 | -0.459987000 |

**LS-4-trans** ( $E_{\text{total}} = -3636.97399217$  a.u.,  $E_{\text{ZPE}} = -3636.315648$  a.u.)

|    |              |              |              |
|----|--------------|--------------|--------------|
| 26 | 0.112323000  | 0.601100000  | 0.102461000  |
| 8  | -1.521897000 | 1.452727000  | 0.520226000  |
| 8  | -0.980988000 | -0.861981000 | -0.463832000 |
| 7  | 1.217205000  | 2.107926000  | 0.668827000  |
| 7  | 0.240970000  | 1.255999000  | -1.747151000 |
| 7  | 1.826716000  | -0.307971000 | -0.338197000 |
| 7  | 0.380114000  | -0.261796000 | 1.851362000  |
| 6  | -2.264880000 | -0.622337000 | -0.259915000 |
| 6  | -4.930343000 | 0.170662000  | 0.272572000  |
| 6  | -3.318315000 | -1.531511000 | -0.550188000 |
| 6  | -2.564902000 | 0.667115000  | 0.288884000  |
| 6  | -4.614985000 | -1.098403000 | -0.270681000 |
| 1  | -5.431511000 | -1.775237000 | -0.481091000 |
| 6  | -3.887573000 | 1.050485000  | 0.548279000  |
| 6  | 2.546532000  | 1.918979000  | 0.533562000  |
| 6  | 1.162846000  | 0.602911000  | -2.494270000 |
| 6  | 1.305985000  | -1.251394000 | 1.828773000  |
| 6  | -6.378433000 | 0.595046000  | 0.566761000  |

|    |              |              |              |
|----|--------------|--------------|--------------|
| 6  | 0.756473000  | 3.288084000  | 1.132916000  |
| 1  | -0.322138000 | 3.360036000  | 1.212333000  |
| 6  | -3.028284000 | -2.919099000 | -1.138308000 |
| 6  | 1.804645000  | -0.571099000 | -1.806065000 |
| 1  | 1.165767000  | -1.444929000 | -1.964389000 |
| 1  | 2.808722000  | -0.796754000 | -2.175050000 |
| 6  | 3.462774000  | 2.920395000  | 0.859026000  |
| 1  | 4.523308000  | 2.728448000  | 0.738947000  |
| 6  | 2.989317000  | 0.566847000  | 0.050894000  |
| 1  | 3.686674000  | 0.656551000  | -0.784262000 |
| 1  | 3.556528000  | 0.063872000  | 0.841005000  |
| 6  | -0.451392000 | 2.273171000  | -2.289315000 |
| 1  | -1.179479000 | 2.739630000  | -1.636068000 |
| 6  | -0.215371000 | 0.061332000  | 3.012410000  |
| 1  | -0.952906000 | 0.852875000  | 2.953732000  |
| 6  | 1.839246000  | -1.572199000 | 0.459561000  |
| 1  | 2.839209000  | -2.011591000 | 0.488947000  |
| 1  | 1.142409000  | -2.262228000 | -0.024331000 |
| 6  | 2.989128000  | 4.137128000  | 1.336480000  |
| 1  | 3.682644000  | 4.929368000  | 1.596785000  |
| 6  | 1.611784000  | 4.323682000  | 1.477767000  |
| 1  | 1.204174000  | 5.256874000  | 1.848097000  |
| 6  | -6.715900000 | 1.870836000  | -0.238502000 |
| 1  | -6.047129000 | 2.696477000  | 0.020941000  |
| 1  | -7.743555000 | 2.189176000  | -0.030069000 |
| 1  | -6.624172000 | 1.686166000  | -1.313323000 |
| 6  | -2.124613000 | -3.716709000 | -0.169339000 |
| 1  | -1.181898000 | -3.195092000 | 0.002534000  |
| 1  | -1.907772000 | -4.706310000 | -0.587307000 |
| 1  | -2.624774000 | -3.855390000 | 0.794667000  |
| 6  | 1.430637000  | 0.976867000  | -3.807234000 |
| 1  | 2.189318000  | 0.446366000  | -4.371148000 |
| 6  | -0.246880000 | 2.684925000  | -3.600870000 |
| 1  | -0.829083000 | 3.505451000  | -4.002866000 |
| 6  | -2.319817000 | -2.768158000 | -2.504495000 |
| 1  | -2.963149000 | -2.237269000 | -3.213824000 |
| 1  | -2.095082000 | -3.756579000 | -2.921032000 |
| 1  | -1.387075000 | -2.211778000 | -2.399774000 |
| 6  | 1.685920000  | -1.920080000 | 2.987482000  |
| 1  | 2.460361000  | -2.676384000 | 2.936927000  |
| 6  | 0.096368000  | -0.586412000 | 4.201904000  |
| 1  | -0.409801000 | -0.301296000 | 5.116479000  |
| 6  | 1.067833000  | -1.585819000 | 4.191200000  |
| 1  | 1.346406000  | -2.093773000 | 5.108013000  |
| 6  | 0.713402000  | 2.030727000  | -4.370488000 |
| 1  | 0.903968000  | 2.337513000  | -5.393094000 |
| 6  | -7.403235000 | -0.490057000 | 0.192104000  |
| 1  | -7.367786000 | -0.730240000 | -0.875267000 |
| 1  | -8.411868000 | -0.129832000 | 0.418779000  |
| 1  | -7.244223000 | -1.412337000 | 0.759830000  |
| 6  | -6.528672000 | 0.896436000  | 2.075802000  |
| 1  | -6.298646000 | 0.008634000  | 2.673014000  |
| 1  | -7.555834000 | 1.205743000  | 2.300048000  |
| 1  | -5.856751000 | 1.699505000  | 2.392113000  |
| 6  | -4.312433000 | -3.736856000 | -1.362590000 |
| 1  | -4.853603000 | -3.911476000 | -0.426967000 |
| 1  | -4.046387000 | -4.713235000 | -1.780290000 |
| 1  | -4.989847000 | -3.246421000 | -2.069216000 |
| 17 | 5.682165000  | -1.451677000 | -0.202253000 |

|   |              |              |              |
|---|--------------|--------------|--------------|
| 8 | 6.095475000  | -0.021335000 | -0.367655000 |
| 8 | 4.604198000  | -1.760012000 | -1.218376000 |
| 8 | 5.067655000  | -1.627730000 | 1.167352000  |
| 8 | 6.831198000  | -2.360982000 | -0.376729000 |
| 1 | -4.063570000 | 2.037805000  | 0.964022000  |

**HS-4-trans** ( $E_{\text{total}} = -3636.95633307$  a.u.,  $E_{\text{ZPE}} = -3636.300697$  a.u.)

|    |              |              |              |
|----|--------------|--------------|--------------|
| 26 | -0.050042000 | 0.264182000  | 0.293512000  |
| 8  | -1.675309000 | 1.139171000  | 0.964431000  |
| 8  | -1.361362000 | -0.896772000 | -0.592579000 |
| 7  | 1.212382000  | 1.645535000  | 1.379771000  |
| 7  | 0.340850000  | 1.426295000  | -1.524717000 |
| 7  | 1.952381000  | -0.435200000 | -0.375892000 |
| 7  | 0.493838000  | -1.278623000 | 1.763450000  |
| 6  | -2.616803000 | -0.556503000 | -0.360517000 |
| 6  | -5.194394000 | 0.401146000  | 0.291815000  |
| 6  | -3.748199000 | -1.224950000 | -0.895678000 |
| 6  | -2.790232000 | 0.580184000  | 0.504074000  |
| 6  | -5.002844000 | -0.717730000 | -0.548636000 |
| 1  | -5.878620000 | -1.210438000 | -0.947831000 |
| 6  | -4.070604000 | 1.043582000  | 0.816522000  |
| 6  | 2.532157000  | 1.484007000  | 1.192127000  |
| 6  | 1.388398000  | 1.019474000  | -2.268660000 |
| 6  | 1.560137000  | -2.036800000 | 1.437689000  |
| 6  | -6.594930000 | 0.931927000  | 0.637152000  |
| 6  | 0.770803000  | 2.620922000  | 2.200315000  |
| 1  | -0.307697000 | 2.689148000  | 2.295593000  |
| 6  | -3.581850000 | -2.447674000 | -1.808849000 |
| 6  | 2.006639000  | -0.294796000 | -1.856637000 |
| 1  | 1.403493000  | -1.103008000 | -2.284951000 |
| 1  | 3.036182000  | -0.389488000 | -2.218106000 |
| 6  | 3.468771000  | 2.304090000  | 1.831597000  |
| 1  | 4.525714000  | 2.137026000  | 1.651300000  |
| 6  | 3.019759000  | 0.394589000  | 0.269066000  |
| 1  | 3.644641000  | 0.840531000  | -0.509463000 |
| 1  | 3.698644000  | -0.261151000 | 0.820857000  |
| 6  | -0.309646000 | 2.551804000  | -1.861711000 |
| 1  | -1.144736000 | 2.822379000  | -1.224227000 |
| 6  | -0.070010000 | -1.424166000 | 2.973762000  |
| 1  | -0.926806000 | -0.790093000 | 3.176273000  |
| 6  | 2.084585000  | -1.859749000 | 0.033329000  |
| 1  | 3.124179000  | -2.193344000 | -0.054693000 |
| 1  | 1.459936000  | -2.455229000 | -0.641764000 |
| 6  | 3.013578000  | 3.306695000  | 2.677641000  |
| 1  | 3.720619000  | 3.954965000  | 3.184461000  |
| 6  | 1.638283000  | 3.471577000  | 2.867500000  |
| 1  | 1.246595000  | 4.244153000  | 3.518575000  |
| 6  | -6.728183000 | 2.387989000  | 0.133423000  |
| 1  | -5.977218000 | 3.039342000  | 0.589366000  |
| 1  | -7.718754000 | 2.784516000  | 0.383236000  |
| 1  | -6.602769000 | 2.435363000  | -0.952782000 |
| 6  | -2.833462000 | -3.567092000 | -1.047346000 |
| 1  | -1.850144000 | -3.225669000 | -0.719904000 |
| 1  | -2.703820000 | -4.438948000 | -1.698840000 |
| 1  | -3.404708000 | -3.881668000 | -0.167756000 |
| 6  | 1.833302000  | 1.750398000  | -3.368848000 |
| 1  | 2.697433000  | 1.408114000  | -3.926884000 |
| 6  | 0.062650000  | 3.323499000  | -2.956096000 |
| 1  | -0.489562000 | 4.224256000  | -3.196462000 |

|    |              |              |              |
|----|--------------|--------------|--------------|
| 6  | -2.777386000 | -2.054021000 | -3.070010000 |
| 1  | -3.304549000 | -1.278856000 | -3.635836000 |
| 1  | -2.655502000 | -2.927616000 | -3.720611000 |
| 1  | -1.789430000 | -1.677303000 | -2.800695000 |
| 6  | 2.110318000  | -2.951831000 | 2.333452000  |
| 1  | 2.986421000  | -3.522410000 | 2.046924000  |
| 6  | 0.410036000  | -2.328857000 | 3.913535000  |
| 1  | -0.075632000 | -2.415827000 | 4.878237000  |
| 6  | 1.523989000  | -3.101288000 | 3.587806000  |
| 1  | 1.935239000  | -3.805155000 | 4.303327000  |
| 6  | 1.157048000  | 2.917122000  | -3.718115000 |
| 1  | 1.484748000  | 3.504245000  | -4.569282000 |
| 6  | -7.720267000 | 0.100683000  | -0.003063000 |
| 1  | -7.659362000 | 0.108606000  | -1.095878000 |
| 1  | -8.689259000 | 0.524996000  | 0.278799000  |
| 1  | -7.700224000 | -0.939415000 | 0.337556000  |
| 6  | -6.793282000 | 0.907793000  | 2.169950000  |
| 1  | -6.715855000 | -0.113935000 | 2.554308000  |
| 1  | -7.783548000 | 1.299423000  | 2.428372000  |
| 1  | -6.044159000 | 1.519186000  | 2.680701000  |
| 6  | -4.935043000 | -3.014942000 | -2.272064000 |
| 1  | -5.548959000 | -3.346172000 | -1.428245000 |
| 1  | -4.757363000 | -3.882891000 | -2.915144000 |
| 1  | -5.506827000 | -2.282995000 | -2.851778000 |
| 17 | 6.042678000  | -0.719106000 | -0.765054000 |
| 8  | 6.149732000  | 0.418452000  | 0.208624000  |
| 8  | 5.229568000  | -0.258617000 | -1.952100000 |
| 8  | 5.295139000  | -1.850388000 | -0.099062000 |
| 8  | 7.378504000  | -1.171009000 | -1.200204000 |
| 1  | -4.159044000 | 1.906173000  | 1.469542000  |