**Supplementary Information**

# Synthesis and Study of *C*-Substituted Methylthio Derivatives of Cobalt Bis(Dicarbollide)

**Marina Yu. Stogniy,[a] Olga N. Kazheva,[b] Denis M. Chudak,[c] Gennady V. Shilov,[b] Oleg A. Filippov,[a] Igor B. Sivaev,[a] Andrey V. Kravchenko,[c] Vladimir A. Starodub,[d] Lev I. Buravov,[b] Vladimir I. Bregadze,[a] Oleg A. Dyachenko[b]**

[a] *A. N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences*
*28 Vavilov Str, Moscow, 119991, Russia*
[b] *Institute of Problems of Chemical Physics, Russian Academy of Sciences,*
*1 Semenov Av., Chernogolovka, Moscow Region, 142432, Russia*
[c] *V. N. Karazin Kharkiv National University*
*4 Svoboda Sq., Kharkiv, 61077, Ukraine*
[d] *Institute of Chemistry, Jan Kochanowski University*
*15G Świętokrzyska Str., Kielce, 25-406, Poland*

**Figure S1.** Bond critical points in the rotamers of *rac*-[1,1′-$(MeS)_2$-3,3′-$Co(1,2\text{-}C_2B_9H_{10})_2]^-$ (a – *cisoid1*, b – *cisoid2*, c – *gauche1*, d – *gauche2*, e – *transoid*) and *meso*-[1,2′-$(MeS)_2$-3,3′-$Co(1,2\text{-}C_2B_9H_{10})_2]^-$ (f – *cisoid*, g – *gauche*, h – *transoid*) isomers.

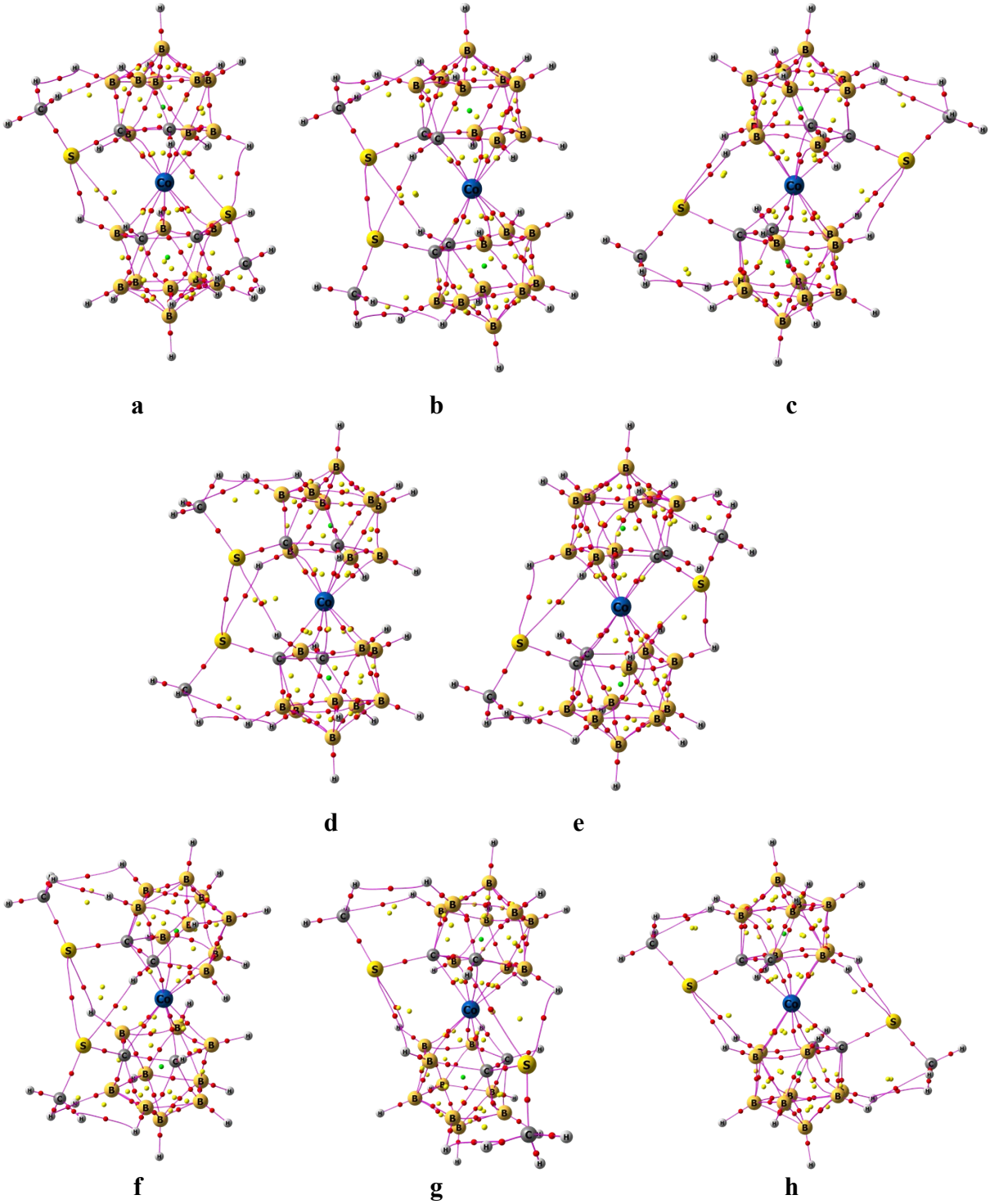

Table S1. Characteristics of (3,-1) bond critical points associated with the intramolecular interactions of SMe group in [1,1′-$(MeS)_2$-,3′-Co(1,2-$C_2B_9H_{10})_2]^-$ and [1,2′-$(MeS)_2$-,3′-Co(1,2-$C_2B_9H_{10})_2]^-$ (interatomic distance r in Å, electron density at BCP $\rho_c$ in a.u., energies in kcal·$mol^{-1}$)

| | | rac-isomer | | | | | meso-isomer | | |
|---|---|---|---|---|---|---|---|---|---|
| | | cisoid1 | gauche1 | transoid | gauche2 | cisoid2 | cisoid | gauche | transoid |
| | $\Delta E$ | 0.0 | 4.9 | 3.4 | 3.7 | 2.1 | 3.4 | 1.2 | 4.9 |
| | $\Delta G^{298}$ | 0.0 | 5.1 | 3.6 | 4.1 | 2.1 | 3.3 | 1.6 | 5.2 |
| | r | 2.693 | | | | 2.664 | 2.656 | 2.797 | |
| CH···S | $\rho_c$ | 0.012 | | | | 0.012 | 0.012 | 0.010 | |
| | $E_{BCP}$ | -2.1 | | | | -2.1 | -2.1 | -1.7 | |
| | r | 2.693 | | | | 2.666 | | | |
| CH···S | $\rho_c$ | 0.012 | | | | 0.012 | | | |
| | $E_{BCP}$ | -2.1 | | | | -2.1 | | | |
| | r | 2.777 | 2.693 | 2.739 | 2.612 | | 2.727 | 2.644 | 2.667 |
| BH···S | $\rho_c$ | 0.011 | 0.013 | 0.012 | 0.014 | | 0.012 | 0.014 | 0.014 |
| | $E_{BCP}$ | -1.8 | -2.2 | -1.9 | -2.3 | | -1.9 | -2.3 | -2.2 |
| | r | 2.777 | 2.693 | 2.739 | 2.613 | | | 2.708 | 2.665 |
| BH···S | $\rho_c$ | 0.011 | 0.013 | 0.012 | 0.014 | | | 0.013 | 0.014 |
| | $E_{BCP}$ | -1.8 | -2.2 | -1.9 | -2.3 | | | -2.0 | -2.3 |
| | r | | 2.835 | 2.898 | | | | 2.966 | 2.855 |
| BH···S | $\rho_c$ | | 0.011 | 0.010 | | | | 0.009 | 0.011 |
| | $E_{BCP}$ | | -1.8 | -1.6 | | | | -1.4 | -1.8 |
| | r | | 2.835 | 2.898 | | | | | 2.854 |
| BH···S | $\rho_c$ | | 0.011 | 0.010 | | | | | 0.011 |
| | $E_{BCP}$ | | -1.8 | -1.6 | | | | | -1.8 |
| | r | | | | 3.464 | 3.187 | 3.276 | | |
| S···S | $\rho_c$ | | | | 0.011 | 0.015 | 0.013 | | |
| | $E_{BCP}$ | | | | -1.6 | -2.2 | -1.9 | | |
| | r | 2.234 | 2.203 | 2.207 | 2.297 | 2.369 | 2.307 | 2.271 | 2.209 |
| BH···$HC^{Me}$ | $\rho_c$ | 0.010 | 0.010 | 0.010 | 0.008 | 0.007 | 0.008 | 0.010 | 0.010 |
| | $E_{BCP}$ | -1.7 | -1.8 | -1.7 | -1.5 | -1.2 | -1.3 | -1.6 | -1.7 |
| | r | 2.279 | 2.255 | 2.252 | 2.299 | 2.243 | 2.210 | 2.378 | 2.242 |
| BH···$HC^{Me}$ | $\rho_c$ | 0.008 | 0.010 | 0.010 | 0.009 | 0.010 | 0.011 | 0.007 | 0.010 |
| | $E_{BCP}$ | -1.4 | -1.7 | -1.6 | -1.5 | -1.8 | -1.9 | -1.2 | -1.7 |
| | r | 2.234 | 2.204 | 2.206 | 2.297 | 2.383 | 2.173 | 2.193 | 2.208 |
| BH···$HC^{Me}$ | $\rho_c$ | 0.010 | 0.010 | 0.010 | 0.008 | 0.007 | 0.010 | 0.010 | 0.010 |
| | $E_{BCP}$ | -1.7 | -1.8 | -1.7 | -1.5 | -1.2 | -1.9 | -1.8 | -1.7 |
| | r | 2.279 | 2.256 | 2.252 | 2.299 | 2.242 | 2.238 | 2.268 | 2.241 |
| BH···$HC^{Me}$ | $\rho_c$ | 0.008 | 0.010 | 0.010 | 0.009 | 0.010 | 0.010 | 0.009 | 0.010 |
| | $E_{BCP}$ | -1.4 | -1.7 | -1.6 | -1.5 | -1.8 | -1.7 | -1.6 | -1.7 |
| $\Sigma E_{BCP}$(Me) | | -6.2 | -6.8 | -6.7 | -6.0 | -5.9 | -6.7 | -6.2 | -6.9 |
| $\Sigma E_{BCP}$(S) | | -7.7 | -7.9 | -7.0 | -6.2 | -6.4 | -5.9 | -7.5 | -8.1 |

Table S2. Key geometrical characteristics of [1,1′-$(MeS)_2$-,3′-Co(1,2-$C_2B_9H_{10})_2]^-$ obtained by X-Ray and DFT.

| | Xray (A) | Xray (B) | DFT |
|---|---|---|---|
| C1(S)-Co | 2.099 | 2.096 | 2.116 |
| C2-Co | 2.082 | 2.078 | 2.083 |
| B1Co | 2.099 | 2.088 | 2.111 |
| B2Co | 2.119 | 2.118 | 2.142 |
| B3Co | 2.104 | 2.105 | 2.116 |
| C(S)-B10-B10'-C'(S) | 94.3 | 95.7 | 97.6 |
| B8-B10-B10'-B8' | 33.2 | 35.1 | 33.8 |
| Co-C-S-C(Me) | 166.6 | 169.1 | 169.0 |

Table S3. Selected bond lengths (Å) and angles (°) in X-ray structure of (BEDT-TTF)[1,1′-$(MeS)_2$-,3′-Co(1,2-$C_2B_9H_{10})_2$]

| | | | |
|---|---|---|---|
| Co(1)-C(2) | 2.082(2) | C(4)-C(5) | 1.511(4) |
| Co(1)-C(1) | 2.098(2) | C(6)-C(7) | 1.360(3) |
| Co(1)-B(4) | 2.099(2) | C(8)-C(9) | 1.397(3) |
| Co(1)-B(7) | 2.104(2) | C(10)-C(11) | 1.362(3) |
| Co(1)-B(8) | 2.119(2) | C(12)-C(13) | 1.500(4) |
| Co(2)-C(1') | 2.078(2) | C(1)-C(2) | 1.631(3) |
| Co(2)-B(4') | 2.088(2) | C(1)-B(5) | 1.696(3) |
| Co(2)-C(2') | 2.096(2) | C(1)-B(6) | 1.735(3) |
| Co(2)-B(7') | 2.105(2) | C(1)-B(4) | 1.736(3) |
| Co(2)-B(8') | 2.118(2) | C(2)-B(7) | 1.706(3) |
| S(1)-C(3) | 1.795(2) | C(2)-B(11) | 1.713(3) |
| S(1)-C(1) | 1.796(2) | C(2)-B(6) | 1.713(3) |
| S(1')-C(2') | 1.797(2) | B(4)-B(9) | 1.775(3) |
| S(1')-C(3') | 1.803(2) | B(4)-B(5) | 1.789(3) |
| S(2)-C(6) | 1.741(2) | B(4)-B(8) | 1.811(3) |
| S(2)-C(4) | 1.799(2) | B(5)-B(6) | 1.771(3) |
| S(3)-C(7) | 1.741(2) | B(5)-B(9) | 1.775(4) |
| S(3)-C(5) | 1.809(3) | B(5)-B(10) | 1.787(3) |
| S(4)-C(8) | 1.721(2) | B(6)-B(11) | 1.757(3) |
| S(4)-C(6) | 1.740(2) | B(6)-B(10) | 1.763(3) |
| S(5)-C(8) | 1.717(2) | B(7)-B(12) | 1.778(3) |
| S(5)-C(7) | 1.735(2) | B(7)-B(11) | 1.783(3) |
| S(6)-C(9) | 1.719(2) | B(7)-B(8) | 1.791(3) |
| S(6)-C(10) | 1.736(2) | B(8)-B(12) | 1.788(3) |
| S(7)-C(9) | 1.720(2) | B(8)-B(9) | 1.788(3) |
| S(7)-C(11) | 1.732(2) | B(9)-B(10) | 1.775(4) |
| S(8)-C(10) | 1.735(2) | B(9)-B(12) | 1.776(4) |
| S(8)-C(12) | 1.826(2) | B(10)-B(11) | 1.778(3) |
| S(9)-C(11) | 1.738(2) | B(10)-B(12) | 1.785(4) |
| S(9)-C(13) | 1.840(3) | B(11)-B(12) | 1.766(4) |

| | | | |
|---|---|---|---|
| C(1')-C(2') | 1.637(3) | B(6')-B(11') | 1.754(3) |
| C(1')-B(7') | 1.705(3) | B(6')-B(10') | 1.760(3) |
| C(1')-B(11') | 1.710(3) | B(7')-B(12') | 1.773(3) |
| C(1')-B(6') | 1.722(3) | B(7')-B(11') | 1.784(3) |
| C(2')-B(5') | 1.707(3) | B(7')-B(8') | 1.786(3) |
| C(2')-B(4') | 1.720(3) | B(8')-B(9') | 1.787(3) |
| C(2')-B(6') | 1.737(3) | B(8')-B(12') | 1.792(3) |
| B(4')-B(9') | 1.776(3) | B(9')-B(10') | 1.780(4) |
| B(4')-B(5') | 1.793(3) | B(9')-B(12') | 1.781(3) |
| B(4')-B(8') | 1.800(3) | B(10')-B(11') | 1.771(3) |
| B(5')-B(9') | 1.771(4) | B(10')-B(12') | 1.778(4) |
| B(5')-B(10') | 1.772(3) | B(11')-B(12') | 1.755(3) |
| B(5')-B(6') | 1.773(3) | | |

| | | | |
|---|---|---|---|
| C(3)-S(1)-C(1) | 105.6(1) | C(6)-C(7)-S(3) | 129.1(2) |
| C(2')-S(1')-C(3') | 105.8(1) | S(5)-C(7)-S(3) | 114.3(1) |
| C(6)-S(2)-C(4) | 100.3(1) | C(9)-C(8)-S(5) | 121.2(1) |
| C(7)-S(3)-C(5) | 101.2(1) | C(9)-C(8)-S(4) | 122.6 (1) |
| C(8)-S(4)-C(6) | 95.1(1) | S(5)-C(8)-S(4) | 116.0(1) |
| C(8)-S(5)-C(7) | 95.58(9) | C(8)-C(9)-S(6) | 122.4(1) |
| C(9)-S(6)-C(10) | 95.2(1) | C(8)-C(9)-S(7) | 121.3(1) |
| C(9)-S(7)-C(11) | 95.2(1) | S(6)-C(9)-S(7) | 116.1(1) |
| C(10)-S(8)-C(12) | 94.2(1) | C(11)-C(10)-S(8) | 122.7(2) |
| C(11)-S(9)-C(13) | 103.0(1) | C(11)-C(10)-S(6) | 116.5(2) |
| C(5)-C(4)-S(2) | 114.2(2) | S(8)-C(10)-S(6) | 120.2(1) |
| C(4)-C(5)-S(3) | 113.5(2) | C(10)-C(11)-S(7) | 116.7(2) |
| C(7)-C(6)-S(4) | 116.7(2) | C(10)-C(11)-S(9) | 124.9(2) |
| C(7)-C(6)-S(2) | 128.2(2) | S(7)-C(11)-S(9) | 118.2(1) |
| S(4)-C(6)-S(2) | 114.9(1) | C(13)-C(12)-S(8) | 113.5(2) |
| C(6)-C(7)-S(5) | 116.4(2) | C(12)-C(13)-S(9) | 116.3(2) |

Table S4. XYZ coordinates of optimized rotamers and rotation transition states for [1,1′-$(MeS)_2$-,3′-Co(1,2-$C_2B_9H_{10})_2$]

TS(*cisoid1-cisoid2*), E=-2871.46318003

| | | | |
|---|---|---|---|
| 6 | -1.409025000 | 0.448449000 | -1.147070000 |
| 5 | -1.109708000 | -1.112557000 | -1.752063000 |
| 5 | -3.051314000 | 0.792039000 | -0.733751000 |
| 5 | -2.647035000 | -0.237195000 | -2.112241000 |
| 6 | -1.791584000 | 0.472467000 | 0.445178000 |
| 1 | -0.921660000 | 1.346635000 | -1.547589000 |
| 5 | -1.407933000 | -2.216075000 | -0.353945000 |
| 5 | -3.326374000 | -0.258073000 | 0.676277000 |
| 5 | -2.697700000 | -1.933562000 | -1.587863000 |
| 5 | -1.784587000 | -1.140964000 | 1.056009000 |
| 5 | -3.889330000 | -0.758147000 | -0.943293000 |
| 1 | -1.654241000 | -1.324639000 | 2.235740000 |
| 1 | -3.445200000 | 1.924158000 | -0.842830000 |
| 1 | -0.439137000 | -1.261808000 | -2.737518000 |
| 1 | -2.815483000 | 0.209206000 | -3.219759000 |
| 5 | -3.114477000 | -1.945001000 | 0.155022000 |
| 1 | -3.024066000 | -2.816703000 | -2.345692000 |
| 1 | -1.006975000 | -3.343868000 | -0.262662000 |
| 1 | -4.021448000 | 0.111811000 | 1.586570000 |
| 1 | -5.066474000 | -0.772243000 | -1.216736000 |
| 1 | -3.750610000 | -2.828260000 | 0.681591000 |
| 6 | 1.409033000 | 0.448457000 | 1.147092000 |
| 5 | 1.109772000 | -1.112572000 | 1.752082000 |
| 5 | 3.051311000 | 0.792050000 | 0.733708000 |
| 5 | 2.647101000 | -0.237195000 | 2.112208000 |
| 6 | 1.791517000 | 0.472504000 | -0.445179000 |
| 1 | 0.921676000 | 1.346635000 | 1.547646000 |
| 5 | 1.407958000 | -2.216070000 | 0.353961000 |
| 5 | 3.326315000 | -0.258055000 | -0.676333000 |
| 5 | 2.697762000 | -1.933556000 | 1.587821000 |
| 5 | 1.784529000 | -1.140966000 | -1.056020000 |
| 5 | 3.889347000 | -0.758130000 | 0.943208000 |
| 1 | 1.654154000 | -1.324656000 | -2.235743000 |
| 1 | 3.445202000 | 1.924173000 | 0.842744000 |
| 1 | 0.439224000 | -1.261850000 | 2.737551000 |
| 1 | 2.815594000 | 0.209205000 | 3.219720000 |
| 5 | 3.114463000 | -1.944985000 | -0.155081000 |
| 1 | 3.024165000 | -2.816699000 | 2.345632000 |
| 1 | 1.006984000 | -3.343859000 | 0.262700000 |
| 1 | 4.021372000 | 0.111817000 | -1.586636000 |
| 1 | 5.066504000 | -0.772215000 | 1.216598000 |
| 1 | 3.750589000 | -2.828227000 | -0.681687000 |
| 27 | 0.000012000 | -0.617286000 | 0.000030000 |
| 16 | -1.376568000 | 1.979040000 | 1.408562000 |
| 6 | -2.974321000 | 2.609066000 | 2.045754000 |
| 1 | -3.704539000 | 2.758271000 | 1.226877000 |
| 1 | -3.394916000 | 1.943319000 | 2.822678000 |

| | | | |
|---|---|---|---|
| 1 | -2.715915000 | 3.589546000 | 2.495170000 |
| 16 | 1.376551000 | 1.979178000 | -1.408437000 |
| 6 | 2.974281000 | 2.609002000 | -2.045864000 |
| 1 | 2.715947000 | 3.589617000 | -2.495031000 |
| 1 | 3.704703000 | 2.757921000 | -1.227116000 |
| 1 | 3.394591000 | 1.943337000 | -2.823012000 |

*cisoid1*, E=-2871.47212676

| | | | |
|---|---|---|---|
| 6 | 1.366348000 | 0.967946000 | -0.740253000 |
| 5 | 0.906506000 | 1.908803000 | 0.613035000 |
| 5 | 3.054651000 | 0.627368000 | -0.853589000 |
| 5 | 2.468460000 | 2.176934000 | -0.238037000 |
| 6 | 1.867881000 | -0.543619000 | -0.334432000 |
| 1 | 0.910907000 | 1.075137000 | -1.734661000 |
| 5 | 1.200355000 | 0.861512000 | 2.049240000 |
| 5 | 3.336488000 | -0.453372000 | 0.534639000 |
| 5 | 2.420485000 | 2.098070000 | 1.540299000 |
| 5 | 1.764075000 | -0.735426000 | 1.395705000 |
| 5 | 3.743907000 | 1.283401000 | 0.646331000 |
| 1 | 1.684546000 | -1.839186000 | 1.865954000 |
| 1 | 3.550067000 | 0.510545000 | -1.941377000 |
| 1 | 0.120516000 | 2.810553000 | 0.484880000 |
| 1 | 2.607676000 | 3.149075000 | -0.938264000 |
| 5 | 2.952700000 | 0.454348000 | 2.025535000 |
| 1 | 2.624797000 | 3.081390000 | 2.212675000 |
| 1 | 0.678578000 | 1.015773000 | 3.123614000 |
| 1 | 4.118840000 | -1.366229000 | 0.438468000 |
| 1 | 4.893969000 | 1.654859000 | 0.661654000 |
| 1 | 3.557578000 | 0.221807000 | 3.046282000 |
| 6 | -1.366304000 | -0.968064000 | -0.740180000 |
| 5 | -0.906522000 | -1.908762000 | 0.613275000 |
| 5 | -3.054612000 | -0.627483000 | -0.853572000 |
| 5 | -2.468435000 | -2.176976000 | -0.237824000 |
| 6 | -1.867860000 | 0.543518000 | -0.334577000 |
| 1 | -0.910904000 | -1.075406000 | -1.734591000 |
| 5 | -1.200419000 | -0.861252000 | 2.049326000 |
| 5 | -3.336509000 | 0.453419000 | 0.534521000 |
| 5 | -2.420530000 | -2.097893000 | 1.540506000 |
| 5 | -1.764125000 | 0.735589000 | 1.395553000 |
| 5 | -3.743926000 | -1.283336000 | 0.646404000 |
| 1 | -1.684599000 | 1.839423000 | 1.865623000 |
| 1 | -3.550025000 | -0.510863000 | -1.941390000 |
| 1 | -0.120511000 | -2.810518000 | 0.485270000 |
| 1 | -2.607643000 | -3.149198000 | -0.937940000 |
| 5 | -2.952762000 | -0.454108000 | 2.025537000 |
| 1 | -2.624850000 | -3.081147000 | 2.212977000 |
| 1 | -0.678666000 | -1.015362000 | 3.123735000 |
| 1 | -4.118821000 | 1.366295000 | 0.438135000 |
| 1 | -4.893982000 | -1.654813000 | 0.661693000 |
| 1 | -3.557654000 | -0.221441000 | 3.046245000 |
| 27 | -0.000010000 | 0.000011000 | 0.498439000 |
| 16 | 1.626689000 | -1.944832000 | -1.491812000 |
| 6 | 3.209011000 | -2.125428000 | -2.403992000 |

| | | | |
|---|---|---|---|
| 1 | 3.351630000 | -1.342099000 | -3.172985000 |
| 1 | 4.067067000 | -2.139565000 | -1.704559000 |
| 1 | 3.122983000 | -3.116445000 | -2.894809000 |
| 16 | -1.626638000 | 1.944729000 | -1.491953000 |
| 6 | -3.208956000 | 2.125201000 | -2.404201000 |
| 1 | -3.123215000 | 3.116266000 | -2.894961000 |
| 1 | -3.351529000 | 1.341859000 | -3.173191000 |
| 1 | -4.066957000 | 2.139143000 | -1.704689000 |

TS(*cisoid1-gauche1)*, E= -2871.44867422

| | | | |
|---|---|---|---|
| 6 | 1.429509000 | 0.783067000 | -1.094651000 |
| 5 | 0.640569000 | 1.977674000 | -0.189722000 |
| 5 | 3.151405000 | 0.793442000 | -0.929672000 |
| 5 | 2.240704000 | 2.298292000 | -0.922880000 |
| 6 | 2.095863000 | -0.390290000 | -0.168518000 |
| 1 | 1.136872000 | 0.487151000 | -2.111908000 |
| 5 | 0.848520000 | 1.525570000 | 1.536538000 |
| 5 | 3.367338000 | 0.274933000 | 0.763372000 |
| 5 | 1.922677000 | 2.763191000 | 0.766964000 |
| 5 | 1.736090000 | -0.047714000 | 1.500724000 |
| 5 | 3.480620000 | 2.001305000 | 0.327094000 |
| 1 | 1.780301000 | -0.941348000 | 2.300311000 |
| 1 | 3.818573000 | 0.441589000 | -1.865429000 |
| 1 | -0.208784000 | 2.641864000 | -0.710639000 |
| 1 | 2.317647000 | 3.014603000 | -1.890469000 |
| 5 | 2.620744000 | 1.495593000 | 1.818500000 |
| 1 | 1.842794000 | 3.926175000 | 1.086110000 |
| 1 | 0.160081000 | 1.907467000 | 2.446374000 |
| 1 | 4.286877000 | -0.433156000 | 1.078189000 |
| 1 | 4.545459000 | 2.572922000 | 0.331616000 |
| 1 | 3.087165000 | 1.710532000 | 2.913165000 |
| 6 | -1.429547000 | -0.783021000 | -1.094653000 |
| 5 | -0.640608000 | -1.977669000 | -0.189815000 |
| 5 | -3.151442000 | -0.793348000 | -0.929608000 |
| 5 | -2.240775000 | -2.298225000 | -0.922924000 |
| 6 | -2.095854000 | 0.390321000 | -0.168441000 |
| 1 | -1.136947000 | -0.487060000 | -2.111908000 |
| 5 | -0.848487000 | -1.525640000 | 1.536488000 |
| 5 | -3.367304000 | -0.274916000 | 0.763472000 |
| 5 | -1.922700000 | -2.763202000 | 0.766892000 |
| 5 | -1.736022000 | 0.047664000 | 1.500791000 |
| 5 | -3.480639000 | -2.001263000 | 0.327116000 |
| 1 | -1.780193000 | 0.941250000 | 2.300433000 |
| 1 | -3.818643000 | -0.441413000 | -1.865315000 |
| 1 | 0.208762000 | -2.641893000 | -0.710656000 |
| 1 | -2.317776000 | -3.014492000 | -1.890541000 |
| 5 | -2.620699000 | -1.495642000 | 1.818520000 |
| 1 | -1.842824000 | -3.926202000 | 1.085980000 |
| 1 | -0.160002000 | -1.907583000 | 2.446271000 |
| 1 | -4.286822000 | 0.433170000 | 1.078356000 |
| 1 | -4.545492000 | -2.572856000 | 0.331648000 |
| 1 | -3.087090000 | -1.710621000 | 2.913190000 |
| 27 | -0.000002000 | 0.000001000 | 0.259374000 |

| | | | |
|---|---|---|---|
| 16 | 2.418660000 | -2.062911000 | -0.879511000 |
| 6 | 4.248745000 | -2.218620000 | -0.963496000 |
| 1 | 4.724471000 | -1.385443000 | -1.515929000 |
| 1 | 4.699023000 | -2.320253000 | 0.041881000 |
| 1 | 4.391548000 | -3.163723000 | -1.527533000 |
| 16 | -2.418643000 | 2.062932000 | -0.879469000 |
| 6 | -4.248739000 | 2.218506000 | -0.963567000 |
| 1 | -4.391612000 | 3.163470000 | -1.527818000 |
| 1 | -4.724355000 | 1.385159000 | -1.515843000 |
| 1 | -4.699072000 | 2.320311000 | 0.041767000 |

*gauche1*, E= -2871.46433153

| | | | |
|---|---|---|---|
| 6 | 1.528586000 | -0.513765000 | 1.292860000 |
| 5 | 0.558437000 | -1.834411000 | 0.873988000 |
| 5 | 3.191961000 | -0.685281000 | 0.891911000 |
| 5 | 2.243469000 | -2.074433000 | 1.430877000 |
| 6 | 2.082127000 | 0.328462000 | -0.024866000 |
| 1 | 1.401158000 | 0.075160000 | 2.210921000 |
| 5 | 0.540951000 | -1.869298000 | -0.938449000 |
| 5 | 3.178883000 | -0.662026000 | -0.892987000 |
| 5 | 1.649737000 | -2.944553000 | -0.004816000 |
| 5 | 1.476157000 | -0.430167000 | -1.477508000 |
| 5 | 3.289428000 | -2.212347000 | -0.008014000 |
| 1 | 1.402364000 | 0.210361000 | -2.493609000 |
| 1 | 4.008376000 | -0.133895000 | 1.582022000 |
| 1 | -0.272391000 | -2.217714000 | 1.661022000 |
| 1 | 2.454673000 | -2.506088000 | 2.537463000 |
| 5 | 2.240273000 | -2.065732000 | -1.454133000 |
| 1 | 1.484161000 | -4.141852000 | 0.017812000 |
| 1 | -0.327577000 | -2.369813000 | -1.605789000 |
| 1 | 4.079091000 | -0.144165000 | -1.499168000 |
| 1 | 4.319784000 | -2.843910000 | 0.004839000 |
| 1 | 2.530493000 | -2.610918000 | -2.493861000 |
| 6 | -1.528634000 | 0.513714000 | 1.292753000 |
| 5 | -0.558732000 | 1.834624000 | 0.874149000 |
| 5 | -3.191979000 | 0.684984000 | 0.891817000 |
| 5 | -2.243818000 | 2.074294000 | 1.430890000 |
| 6 | -2.081965000 | -0.328527000 | -0.024978000 |
| 1 | -1.401086000 | -0.075168000 | 2.210822000 |
| 5 | -0.541101000 | 1.869567000 | -0.938350000 |
| 5 | -3.178778000 | 0.661834000 | -0.893101000 |
| 5 | -1.650176000 | 2.944610000 | -0.004689000 |
| 5 | -1.475980000 | 0.430282000 | -1.477532000 |
| 5 | -3.289721000 | 2.212132000 | -0.008054000 |
| 1 | -1.401988000 | -0.209990000 | -2.493775000 |
| 1 | -4.008271000 | 0.133290000 | 1.581834000 |
| 1 | 0.272059000 | 2.218121000 | 1.661123000 |
| 1 | -2.455202000 | 2.505677000 | 2.537550000 |
| 5 | -2.240439000 | 2.065786000 | -1.454103000 |
| 1 | -1.484814000 | 4.141938000 | 0.018030000 |
| 1 | 0.327396000 | 2.370371000 | -1.605556000 |
| 1 | -4.078797000 | 0.143869000 | -1.499441000 |
| 1 | -4.320325000 | 2.843294000 | 0.004717000 |

| | | | |
|---|---|---|---|
| 1 | -2.530760000 | 2.610934000 | -2.493822000 |
| 27 | 0.000152000 | 0.000253000 | -0.029923000 |
| 16 | 2.516516000 | 2.103071000 | 0.176656000 |
| 6 | 4.306320000 | 2.203463000 | -0.207434000 |
| 1 | 4.904848000 | 1.491774000 | 0.394493000 |
| 1 | 4.509027000 | 2.059368000 | -1.285876000 |
| 1 | 4.573644000 | 3.241463000 | 0.080100000 |
| 16 | -2.516342000 | -2.103188000 | 0.176557000 |
| 6 | -4.306194000 | -2.203794000 | -0.207346000 |
| 1 | -4.573400000 | -3.241744000 | 0.080483000 |
| 1 | -4.904638000 | -1.492017000 | 0.394549000 |
| 1 | -4.509017000 | -2.059943000 | -1.285790000 |

TS(*gauche1-trans*), E= -2871.45074441

| | | | |
|---|---|---|---|
| 6 | 1.723306000 | -0.077390000 | 1.323797000 |
| 5 | 0.810870000 | -1.508519000 | 1.434214000 |
| 5 | 3.339158000 | -0.299439000 | 0.777800000 |
| 5 | 2.562330000 | -1.502770000 | 1.810936000 |
| 6 | 2.076964000 | 0.363655000 | -0.245398000 |
| 1 | 1.666587000 | 0.742439000 | 2.048966000 |
| 5 | 0.610661000 | -2.044749000 | -0.259966000 |
| 5 | 3.136380000 | -0.806469000 | -0.922600000 |
| 5 | 1.887807000 | -2.776248000 | 0.773996000 |
| 5 | 1.362491000 | -0.792645000 | -1.306453000 |
| 5 | 3.453999000 | -2.018018000 | 0.351002000 |
| 1 | 1.106533000 | -0.482064000 | -2.440676000 |
| 1 | 4.182751000 | 0.449605000 | 1.192262000 |
| 1 | 0.105091000 | -1.711371000 | 2.393938000 |
| 1 | 2.928975000 | -1.574816000 | 2.957809000 |
| 5 | 2.237889000 | -2.332636000 | -0.928928000 |
| 1 | 1.805498000 | -3.921462000 | 1.152285000 |
| 1 | -0.248180000 | -2.786672000 | -0.646785000 |
| 1 | 3.925083000 | -0.459835000 | -1.760993000 |
| 1 | 4.524149000 | -2.575624000 | 0.416175000 |
| 1 | 2.425472000 | -3.149955000 | -1.800245000 |
| 6 | -1.723323000 | 0.077369000 | 1.323783000 |
| 5 | -0.810880000 | 1.508484000 | 1.434240000 |
| 5 | -3.339170000 | 0.299438000 | 0.777771000 |
| 5 | -2.562348000 | 1.502744000 | 1.810939000 |
| 6 | -2.076959000 | -0.363654000 | -0.245413000 |
| 1 | -1.666617000 | -0.742474000 | 2.048935000 |
| 5 | -0.610641000 | 2.044746000 | -0.259921000 |
| 5 | -3.136356000 | 0.806490000 | -0.922618000 |
| 5 | -1.887799000 | 2.776233000 | 0.774032000 |
| 5 | -1.362462000 | 0.792664000 | -1.306445000 |
| 5 | -3.453991000 | 2.018022000 | 0.350999000 |
| 1 | -1.106497000 | 0.482099000 | -2.440672000 |
| 1 | -4.182775000 | -0.449615000 | 1.192196000 |
| 1 | -0.105113000 | 1.711312000 | 2.393977000 |
| 1 | -2.929003000 | 1.574771000 | 2.957810000 |
| 5 | -2.237857000 | 2.332652000 | -0.928905000 |
| 1 | -1.805484000 | 3.921442000 | 1.152335000 |
| 1 | 0.248210000 | 2.786667000 | -0.646719000 |

| | | | |
|---|---|---|---|
| 1 | -3.925045000 | 0.459879000 | -1.761032000 |
| 1 | -4.524138000 | 2.575634000 | 0.416165000 |
| 1 | -2.425423000 | 3.149985000 | -1.800213000 |
| 27 | 0.000004000 | -0.000009000 | 0.156895000 |
| 16 | 2.469859000 | 2.117490000 | -0.654923000 |
| 6 | 4.251958000 | 2.126459000 | -1.110580000 |
| 1 | 4.894673000 | 1.671252000 | -0.332227000 |
| 1 | 4.432951000 | 1.643802000 | -2.089570000 |
| 1 | 4.480847000 | 3.209855000 | -1.187267000 |
| 16 | -2.469876000 | -2.117485000 | -0.654934000 |
| 6 | -4.251981000 | -2.126412000 | -1.110578000 |
| 1 | -4.480918000 | -3.209802000 | -1.187207000 |
| 1 | -4.894667000 | -1.671138000 | -0.332239000 |
| 1 | -4.432964000 | -1.643797000 | -2.089591000 |

*trans*, E= -2871.46665226

| | | | |
|---|---|---|---|
| 6 | -1.795377000 | 0.465564000 | -1.270798000 |
| 5 | -1.131478000 | -0.976245000 | -1.914106000 |
| 5 | -3.343849000 | 0.272663000 | -0.540797000 |
| 5 | -2.891455000 | -0.649161000 | -1.983736000 |
| 6 | -1.881993000 | 0.449404000 | 0.406103000 |
| 1 | -1.704524000 | 1.452724000 | -1.740377000 |
| 5 | -0.807350000 | -2.014144000 | -0.495823000 |
| 5 | -3.020343000 | -0.742435000 | 0.891238000 |
| 5 | -2.305480000 | -2.249516000 | -1.461979000 |
| 5 | -1.245017000 | -1.053735000 | 0.966990000 |
| 5 | -3.671345000 | -1.472809000 | -0.602024000 |
| 1 | -0.784713000 | -1.097926000 | 2.077840000 |
| 1 | -4.107090000 | 1.201853000 | -0.573594000 |
| 1 | -0.577286000 | -0.985825000 | -2.982991000 |
| 1 | -3.405184000 | -0.340285000 | -3.030319000 |
| 5 | -2.373094000 | -2.300779000 | 0.327131000 |
| 1 | -2.457370000 | -3.224729000 | -2.160181000 |
| 1 | 0.025425000 | -2.889587000 | -0.519304000 |
| 1 | -3.642329000 | -0.570009000 | 1.906171000 |
| 1 | -4.814706000 | -1.860901000 | -0.654024000 |
| 1 | -2.591269000 | -3.309810000 | 0.957288000 |
| 6 | 1.795381000 | -0.465450000 | -1.270886000 |
| 5 | 1.131438000 | 0.976417000 | -1.914025000 |
| 5 | 3.343907000 | -0.272603000 | -0.540955000 |
| 5 | 2.891416000 | 0.649364000 | -1.983768000 |
| 6 | 1.882061000 | -0.449474000 | 0.405959000 |
| 1 | 1.704517000 | -1.452555000 | -1.740577000 |
| 5 | 0.807348000 | 2.014170000 | -0.495630000 |
| 5 | 3.020412000 | 0.742323000 | 0.891206000 |
| 5 | 2.305441000 | 2.249659000 | -1.461816000 |
| 5 | 1.245082000 | 1.053589000 | 0.967052000 |
| 5 | 3.671350000 | 1.472879000 | -0.601999000 |
| 1 | 0.784842000 | 1.097636000 | 2.077933000 |
| 1 | 4.107143000 | -1.201791000 | -0.573884000 |
| 1 | 0.577229000 | 0.986089000 | -2.982901000 |
| 1 | 3.405084000 | 0.340614000 | -3.030418000 |
| 5 | 2.373120000 | 2.300723000 | 0.327299000 |

| | | | |
|---|---|---|---|
| 1 | 2.457292000 | 3.224947000 | -2.159921000 |
| 1 | -0.025425000 | 2.889618000 | -0.518986000 |
| 1 | 3.642421000 | 0.569800000 | 1.906107000 |
| 1 | 4.814704000 | 1.860996000 | -0.653997000 |
| 1 | 2.591309000 | 3.309684000 | 0.957564000 |
| 27 | -0.000006000 | 0.000005000 | -0.405413000 |
| 16 | -1.854475000 | 2.032705000 | 1.330384000 |
| 6 | -3.478172000 | 2.118043000 | 2.180253000 |
| 1 | -4.323822000 | 1.986002000 | 1.477130000 |
| 1 | -3.553196000 | 1.390248000 | 3.010794000 |
| 1 | -3.502780000 | 3.148574000 | 2.591071000 |
| 16 | 1.854561000 | -2.032895000 | 1.330060000 |
| 6 | 3.477941000 | -2.118023000 | 2.180556000 |
| 1 | 3.502776000 | -3.148747000 | 2.590874000 |
| 1 | 4.323832000 | -1.985306000 | 1.477851000 |
| 1 | 3.552340000 | -1.390616000 | 3.011491000 |

TS(*trans- gauche2*) , E= -2871.45564369

| | | | |
|---|---|---|---|
| 6 | 1.813851000 | -1.056775000 | 0.866488000 |
| 5 | 1.368960000 | -2.140831000 | -0.382627000 |
| 5 | 3.346187000 | -0.284112000 | 0.628114000 |
| 5 | 3.078871000 | -1.949463000 | 0.115768000 |
| 6 | 1.813413000 | 0.524225000 | 0.393973000 |
| 1 | 1.626509000 | -1.245495000 | 1.930574000 |
| 5 | 1.077723000 | -1.092136000 | -1.814844000 |
| 5 | 3.055474000 | 0.775407000 | -0.774933000 |
| 5 | 2.652209000 | -1.948980000 | -1.619116000 |
| 5 | 1.328977000 | 0.590577000 | -1.256015000 |
| 5 | 3.871330000 | -0.795538000 | -0.990765000 |
| 1 | 0.859677000 | 1.616371000 | -1.663647000 |
| 1 | 3.996371000 | -0.003347000 | 1.599591000 |
| 1 | 0.984345000 | -3.244854000 | -0.124453000 |
| 1 | 3.599732000 | -2.832655000 | 0.750166000 |
| 5 | 2.628837000 | -0.249823000 | -2.164651000 |
| 1 | 2.958429000 | -2.878667000 | -2.328626000 |
| 1 | 0.361595000 | -1.396661000 | -2.744020000 |
| 1 | 3.576686000 | 1.857879000 | -0.839074000 |
| 1 | 5.053224000 | -0.859258000 | -1.234889000 |
| 1 | 2.919708000 | 0.102437000 | -3.284521000 |
| 6 | -1.813852000 | -1.056834000 | -0.866491000 |
| 5 | -1.368976000 | -2.140841000 | 0.382677000 |
| 5 | -3.346192000 | -0.284170000 | -0.628150000 |
| 5 | -3.078877000 | -1.949499000 | -0.115743000 |
| 6 | -1.813411000 | 0.524211000 | -0.394021000 |
| 1 | -1.626492000 | -1.245578000 | -1.930570000 |
| 5 | -1.077762000 | -1.092100000 | 1.814855000 |
| 5 | -3.055497000 | 0.775406000 | 0.774859000 |
| 5 | -2.652237000 | -1.948950000 | 1.619143000 |
| 5 | -1.329000000 | 0.590593000 | 1.255972000 |
| 5 | -3.871352000 | -0.795536000 | 0.990738000 |
| 1 | -0.859736000 | 1.616405000 | 1.663602000 |
| 1 | -3.996370000 | -0.003449000 | -1.599638000 |
| 1 | -0.984356000 | -3.244863000 | 0.124507000 |

| | | | |
|---|---|---|---|
| 1 | -3.599729000 | -2.832712000 | -0.750119000 |
| 5 | -2.628877000 | -0.249777000 | 2.164616000 |
| 1 | -2.958462000 | -2.878614000 | 2.328681000 |
| 1 | -0.361668000 | -1.396611000 | 2.744059000 |
| 1 | -3.576713000 | 1.857879000 | 0.838952000 |
| 1 | -5.053247000 | -0.859255000 | 1.234853000 |
| 1 | -2.919757000 | 0.102520000 | 3.284472000 |
| 27 | -0.000030000 | -0.550964000 | -0.000005000 |
| 16 | 1.558808000 | 1.851189000 | 1.639020000 |
| 6 | 3.157778000 | 2.751919000 | 1.721575000 |
| 1 | 4.011310000 | 2.077736000 | 1.928945000 |
| 1 | 3.348139000 | 3.340949000 | 0.804374000 |
| 1 | 3.018309000 | 3.441814000 | 2.579414000 |
| 16 | -1.558788000 | 1.851169000 | -1.639070000 |
| 6 | -3.157596000 | 2.752195000 | -1.721386000 |
| 1 | -3.018059000 | 3.442163000 | -2.579154000 |
| 1 | -4.011284000 | 2.078216000 | -1.928762000 |
| 1 | -3.347760000 | 3.341158000 | -0.804100000 |

*gauche2* , E= -2871.46626604

| | | | |
|---|---|---|---|
| 6 | 1.703318000 | -0.798049000 | 1.153391000 |
| 5 | 1.394745000 | -2.198608000 | 0.206802000 |
| 5 | 3.230227000 | -0.038783000 | 0.853987000 |
| 5 | 3.049332000 | -1.796337000 | 0.785262000 |
| 6 | 1.706262000 | 0.595033000 | 0.278714000 |
| 1 | 1.417541000 | -0.707840000 | 2.208897000 |
| 5 | 1.241669000 | -1.575073000 | -1.488465000 |
| 5 | 3.050191000 | 0.601451000 | -0.798640000 |
| 5 | 2.794325000 | -2.274934000 | -0.917525000 |
| 5 | 1.387665000 | 0.207697000 | -1.381861000 |
| 5 | 3.920958000 | -0.936564000 | -0.512871000 |
| 1 | 0.900329000 | 1.034902000 | -2.110456000 |
| 1 | 3.771389000 | 0.535733000 | 1.761882000 |
| 1 | 0.981104000 | -3.201421000 | 0.723458000 |
| 1 | 3.528307000 | -2.452207000 | 1.676226000 |
| 5 | 2.796033000 | -0.772932000 | -1.897968000 |
| 1 | 3.199319000 | -3.337235000 | -1.328053000 |
| 1 | 0.635299000 | -2.140735000 | -2.369050000 |
| 1 | 3.559893000 | 1.648917000 | -1.098847000 |
| 1 | 5.122143000 | -1.009051000 | -0.626050000 |
| 1 | 3.196855000 | -0.718756000 | -3.037849000 |
| 6 | -1.703187000 | -0.798061000 | -1.153383000 |
| 5 | -1.394669000 | -2.198622000 | -0.206718000 |
| 5 | -3.230151000 | -0.038842000 | -0.854127000 |
| 5 | -3.049203000 | -1.796380000 | -0.785349000 |
| 6 | -1.706242000 | 0.595018000 | -0.278737000 |
| 1 | -1.417292000 | -0.707904000 | -2.208859000 |
| 5 | -1.241777000 | -1.575020000 | 1.488546000 |
| 5 | -3.050291000 | 0.601433000 | 0.798502000 |
| 5 | -2.794351000 | -2.274919000 | 0.917484000 |
| 5 | -1.387783000 | 0.207745000 | 1.381883000 |
| 5 | -3.920981000 | -0.936620000 | 0.512694000 |
| 1 | -0.900560000 | 1.034993000 | 2.110510000 |

| | | | |
|---|---|---|---|
| 1 | -3.771232000 | 0.535674000 | -1.762069000 |
| 1 | -0.980979000 | -3.201490000 | -0.723220000 |
| 1 | -3.528099000 | -2.452278000 | -1.676335000 |
| 5 | -2.796194000 | -0.772903000 | 1.897885000 |
| 1 | -3.199346000 | -3.337244000 | 1.327953000 |
| 1 | -0.635465000 | -2.140668000 | 2.369187000 |
| 1 | -3.560027000 | 1.648902000 | 1.098631000 |
| 1 | -5.122177000 | -1.009121000 | 0.625743000 |
| 1 | -3.197143000 | -0.718692000 | 3.037719000 |
| 27 | 0.000010000 | -0.640627000 | 0.000107000 |
| 16 | 1.273976000 | 2.139114000 | 1.173523000 |
| 6 | 2.713290000 | 3.241411000 | 0.906045000 |
| 1 | 3.664273000 | 2.763430000 | 1.213561000 |
| 1 | 2.779387000 | 3.588786000 | -0.142937000 |
| 1 | 2.506986000 | 4.108064000 | 1.567519000 |
| 16 | -1.273971000 | 2.139139000 | -1.173516000 |
| 6 | -2.713273000 | 3.241442000 | -0.906037000 |
| 1 | -2.506926000 | 4.108151000 | -1.567428000 |
| 1 | -3.664246000 | 2.763505000 | -1.213651000 |
| 1 | -2.779430000 | 3.588750000 | 0.142963000 |

TS(*gauche2-cisoid2*) , E= -2871.43893266

| | | | |
|---|---|---|---|
| 6 | -1.667695000 | -0.337734000 | -1.282559000 |
| 5 | -1.415223000 | -1.977157000 | -0.893336000 |
| 5 | -3.260601000 | 0.255318000 | -0.880199000 |
| 5 | -3.030548000 | -1.394606000 | -1.428384000 |
| 6 | -1.809238000 | 0.634989000 | 0.012454000 |
| 1 | -1.299678000 | 0.133113000 | -2.203676000 |
| 5 | -1.416234000 | -2.027601000 | 0.920675000 |
| 5 | -3.223640000 | 0.259036000 | 0.905800000 |
| 5 | -2.899205000 | -2.451070000 | -0.001199000 |
| 5 | -1.580159000 | -0.303601000 | 1.436857000 |
| 5 | -4.026934000 | -1.064664000 | 0.015495000 |
| 1 | -1.167121000 | 0.238680000 | 2.436775000 |
| 1 | -3.737880000 | 1.115360000 | -1.571804000 |
| 1 | -0.981728000 | -2.731637000 | -1.714293000 |
| 1 | -3.407656000 | -1.690875000 | -2.534508000 |
| 5 | -3.011827000 | -1.404470000 | 1.454632000 |
| 1 | -3.293714000 | -3.593046000 | -0.028611000 |
| 1 | -0.988497000 | -2.917980000 | 1.601115000 |
| 1 | -3.775160000 | 1.130117000 | 1.524307000 |
| 1 | -5.230440000 | -1.174319000 | -0.003578000 |
| 1 | -3.493068000 | -1.775267000 | 2.500192000 |
| 6 | 1.667082000 | -0.338229000 | 1.282533000 |
| 5 | 1.414259000 | -1.977631000 | 0.893069000 |
| 5 | 3.260223000 | 0.254430000 | 0.880582000 |
| 5 | 3.029567000 | -1.395468000 | 1.428588000 |
| 6 | 1.809314000 | 0.634706000 | -0.012480000 |
| 1 | 1.298973000 | 0.132671000 | 2.203583000 |
| 5 | 1.415711000 | -2.027823000 | -0.920943000 |
| 5 | 3.223820000 | 0.258237000 | -0.905446000 |
| 5 | 2.898332000 | -2.451829000 | 0.001266000 |
| 5 | 1.580305000 | -0.303834000 | -1.436889000 |

| | | | |
|---|---|---|---|
| 5 | 4.026452000 | -1.065742000 | -0.014992000 |
| 1 | 1.167580000 | 0.238530000 | -2.436897000 |
| 1 | 3.737589000 | 1.114235000 | 1.572419000 |
| 1 | 0.980645000 | -2.732181000 | 1.713885000 |
| 1 | 3.406331000 | -1.691939000 | 2.534776000 |
| 5 | 3.011636000 | -1.405175000 | -1.454416000 |
| 1 | 3.292534000 | -3.593910000 | 0.028769000 |
| 1 | 0.987618000 | -2.917842000 | -1.601650000 |
| 1 | 3.775768000 | 1.129111000 | -1.523844000 |
| 1 | 5.229920000 | -1.175759000 | 0.004423000 |
| 1 | 3.493033000 | -1.776012000 | -2.499889000 |
| 27 | -0.000149000 | -0.669644000 | -0.000210000 |
| 16 | -1.474714000 | 2.430184000 | -0.213506000 |
| 6 | -3.050323000 | 3.287583000 | 0.185602000 |
| 1 | -3.902553000 | 2.888879000 | -0.398704000 |
| 1 | -3.275336000 | 3.259102000 | 1.268252000 |
| 1 | -2.848514000 | 4.334424000 | -0.122855000 |
| 16 | 1.475723000 | 2.430289000 | 0.213147000 |
| 6 | 3.052091000 | 3.286723000 | -0.185171000 |
| 1 | 2.850772000 | 4.333627000 | 0.123406000 |
| 1 | 3.903828000 | 2.887420000 | 0.399442000 |
| 1 | 3.277590000 | 3.258331000 | -1.267722000 |

*cisoid2*, E= -2871.46874667

| | | | |
|---|---|---|---|
| 6 | 1.402683000 | 0.176045000 | 1.275692000 |
| 5 | 1.168937000 | -1.507769000 | 1.517340000 |
| 5 | 3.017065000 | 0.647110000 | 0.871183000 |
| 5 | 2.694081000 | -0.678370000 | 1.999334000 |
| 6 | 1.728437000 | 0.563055000 | -0.308303000 |
| 1 | 0.895590000 | 0.948775000 | 1.872532000 |
| 5 | 1.426930000 | -2.243780000 | -0.125944000 |
| 5 | 3.266648000 | -0.057585000 | -0.744934000 |
| 5 | 2.755609000 | -2.217347000 | 1.094791000 |
| 5 | 1.723274000 | -0.860945000 | -1.252899000 |
| 5 | 3.896041000 | -0.890811000 | 0.698190000 |
| 1 | 1.492649000 | -0.763015000 | -2.431624000 |
| 1 | 3.400758000 | 1.736065000 | 1.212836000 |
| 1 | 0.546733000 | -1.919026000 | 2.460388000 |
| 1 | 2.917701000 | -0.492315000 | 3.169721000 |
| 5 | 3.103595000 | -1.817939000 | -0.621265000 |
| 1 | 3.136419000 | -3.235558000 | 1.622912000 |
| 1 | 1.031028000 | -3.322231000 | -0.481623000 |
| 1 | 3.927138000 | 0.524800000 | -1.563672000 |
| 1 | 5.082958000 | -0.935570000 | 0.922242000 |
| 1 | 3.735885000 | -2.543579000 | -1.353114000 |
| 6 | -1.403213000 | 0.175340000 | -1.276752000 |
| 5 | -1.169764000 | -1.508996000 | -1.516339000 |
| 5 | -3.017723000 | 0.647130000 | -0.872697000 |
| 5 | -2.695017000 | -0.680047000 | -1.998925000 |
| 6 | -1.728026000 | 0.564854000 | 0.306271000 |
| 1 | -0.896596000 | 0.946828000 | -1.875549000 |
| 5 | -1.427311000 | -2.242753000 | 0.128047000 |
| 5 | -3.266352000 | -0.055181000 | 0.744350000 |

| | | | |
|---|---|---|---|
| 5 | -2.756368000 | -2.217751000 | -1.092229000 |
| 5 | -1.722808000 | -0.857776000 | 1.253102000 |
| 5 | -3.896481000 | -0.890559000 | -0.697174000 |
| 1 | -1.491985000 | -0.758178000 | 2.431677000 |
| 1 | -3.401121000 | 1.735941000 | -1.215119000 |
| 1 | -0.547938000 | -1.921309000 | -2.459181000 |
| 1 | -2.918699000 | -0.495692000 | -3.169570000 |
| 5 | -3.103520000 | -1.815645000 | 0.623441000 |
| 1 | -3.137552000 | -3.236719000 | -1.618614000 |
| 1 | -1.031757000 | -3.320799000 | 0.485322000 |
| 1 | -3.926904000 | 0.527585000 | 1.562650000 |
| 1 | -5.083527000 | -0.935468000 | -0.920516000 |
| 1 | -3.735684000 | -2.539907000 | 1.356763000 |
| 27 | -0.000040000 | -0.646303000 | -0.000217000 |
| 16 | 1.266121000 | 2.212813000 | -0.970882000 |
| 6 | 2.829743000 | 2.939392000 | -1.597928000 |
| 1 | 3.612481000 | 2.943681000 | -0.814665000 |
| 1 | 3.194480000 | 2.423437000 | -2.506027000 |
| 1 | 2.552092000 | 3.984021000 | -1.847677000 |
| 16 | -1.266189000 | 2.217239000 | 0.964154000 |
| 6 | -2.827270000 | 2.935736000 | 1.606540000 |
| 1 | -2.551099000 | 3.980520000 | 1.857396000 |
| 1 | -3.616675000 | 2.939939000 | 0.829971000 |
| 1 | -3.182504000 | 2.415663000 | 2.516049000 |

Table S5. XYZ coordinates of optimized rotamers and rotation transition states for [1,2′-$(MeS)_2$-,3′-Co(1,2-$C_2B_9H_{10})_2$]

TS(*cisoid-cisoid)*, E= -2871.43611280

| | | | |
|---|---|---|---|
| 6 | -1.676961000 | -0.295488000 | -1.290791000 |
| 5 | -1.413813000 | -1.938220000 | -0.950738000 |
| 5 | -3.274262000 | 0.274714000 | -0.890988000 |
| 5 | -3.031853000 | -1.358299000 | -1.482997000 |
| 6 | -1.825463000 | 0.634313000 | 0.028230000 |
| 1 | -1.309217000 | 0.207912000 | -2.196258000 |
| 5 | -1.418163000 | -2.048717000 | 0.862758000 |
| 5 | -3.242724000 | 0.224645000 | 0.893301000 |
| 5 | -2.896331000 | -2.453871000 | -0.088487000 |
| 5 | -1.594755000 | -0.339865000 | 1.433294000 |
| 5 | -4.034653000 | -1.077102000 | -0.035503000 |
| 1 | -1.236427000 | 0.181790000 | 2.457809000 |
| 1 | -3.750988000 | 1.156909000 | -1.555130000 |
| 1 | -0.963396000 | -2.660877000 | -1.793307000 |
| 1 | -3.394005000 | -1.624698000 | -2.602029000 |
| 5 | -3.023253000 | -1.452862000 | 1.396717000 |
| 1 | -3.278788000 | -3.598587000 | -0.149897000 |
| 1 | -0.999182000 | -2.958752000 | 1.518845000 |
| 1 | -3.800739000 | 1.069200000 | 1.541247000 |
| 1 | -5.237544000 | -1.193055000 | -0.054832000 |
| 1 | -3.512578000 | -1.854648000 | 2.426629000 |
| 5 | 1.572302000 | -0.337039000 | 1.477077000 |
| 5 | 1.404815000 | -2.046981000 | 0.910734000 |
| 5 | 3.227843000 | 0.228334000 | 0.972538000 |
| 5 | 3.000866000 | -1.449788000 | 1.473821000 |
| 6 | 1.826937000 | 0.635264000 | 0.081126000 |
| 1 | 1.187305000 | 0.184107000 | 2.491597000 |
| 5 | 1.435691000 | -1.953554000 | -0.901932000 |
| 5 | 3.278287000 | 0.273426000 | -0.812134000 |
| 5 | 2.903401000 | -2.453973000 | -0.009754000 |
| 6 | 1.694341000 | -0.307772000 | -1.245888000 |
| 5 | 4.035064000 | -1.072294000 | 0.059878000 |
| 1 | 1.342402000 | 0.192164000 | -2.159655000 |
| 1 | 3.765247000 | 1.091062000 | 1.620176000 |
| 1 | 0.970023000 | -2.950839000 | 1.565241000 |
| 1 | 3.467304000 | -1.851015000 | 2.514533000 |
| 5 | 3.055231000 | -1.362427000 | -1.406253000 |
| 1 | 3.292127000 | -3.596995000 | -0.064164000 |
| 1 | 1.004626000 | -2.687454000 | -1.744811000 |
| 1 | 3.775349000 | 1.133286000 | -1.485362000 |
| 1 | 5.238283000 | -1.186417000 | 0.055979000 |
| 1 | 3.446994000 | -1.627114000 | -2.515738000 |
| 27 | 0.002828000 | -0.665990000 | 0.018335000 |
| 16 | -1.497220000 | 2.435585000 | -0.136625000 |
| 6 | -3.064585000 | 3.277207000 | 0.317956000 |
| 1 | -3.924964000 | 2.899519000 | -0.268453000 |
| 1 | -3.272568000 | 3.207065000 | 1.402032000 |
| 1 | -2.867504000 | 4.335155000 | 0.046714000 |
| 16 | 1.473250000 | 2.435163000 | 0.025143000 |

| | | | |
|---|---|---|---|
| 6 | 3.091593000 | 3.291562000 | -0.172231000 |
| 1 | 2.850063000 | 4.343528000 | 0.085320000 |
| 1 | 3.842349000 | 2.904338000 | 0.542813000 |
| 1 | 3.479356000 | 3.243025000 | -1.207691000 |

*cisoid*, E= -2871.46674672

| | | | |
|---|---|---|---|
| 6 | -1.415447000 | 0.178588000 | -1.255947000 |
| 5 | -1.140592000 | -1.478128000 | -1.520686000 |
| 5 | -3.036232000 | 0.592073000 | -0.847172000 |
| 5 | -2.687753000 | -0.704590000 | -1.996277000 |
| 6 | -1.743671000 | 0.540399000 | 0.338769000 |
| 1 | -0.938367000 | 0.976569000 | -1.843338000 |
| 5 | -1.363376000 | -2.263544000 | 0.106843000 |
| 5 | -3.254544000 | -0.138253000 | 0.764137000 |
| 5 | -2.693277000 | -2.255720000 | -1.119335000 |
| 5 | -1.689969000 | -0.908954000 | 1.268291000 |
| 5 | -3.870776000 | -0.971105000 | -0.687827000 |
| 1 | -1.479182000 | -0.834597000 | 2.450590000 |
| 1 | -3.459434000 | 1.667022000 | -1.183651000 |
| 1 | -0.460331000 | -1.837158000 | -2.452369000 |
| 1 | -2.920001000 | -0.500655000 | -3.162394000 |
| 5 | -3.043696000 | -1.895719000 | 0.609271000 |
| 1 | -3.041742000 | -3.279896000 | -1.658314000 |
| 1 | -0.938967000 | -3.340702000 | 0.434196000 |
| 1 | -3.931274000 | 0.410566000 | 1.593196000 |
| 1 | -5.058341000 | -1.045154000 | -0.900224000 |
| 1 | -3.654900000 | -2.650739000 | 1.328969000 |
| 5 | 1.348279000 | 0.216121000 | 1.455061000 |
| 5 | 1.211631000 | -1.581601000 | 1.519297000 |
| 5 | 3.026655000 | 0.644329000 | 0.930673000 |
| 5 | 2.747941000 | -0.760244000 | 1.992137000 |
| 6 | 1.726037000 | 0.634112000 | -0.188329000 |
| 1 | 0.821047000 | 1.030553000 | 2.166606000 |
| 5 | 1.441474000 | -2.157282000 | -0.188937000 |
| 5 | 3.274006000 | 0.038612000 | -0.725704000 |
| 5 | 2.801847000 | -2.238686000 | 0.975427000 |
| 6 | 1.765976000 | -0.734461000 | -1.085887000 |
| 5 | 3.925025000 | -0.877387000 | 0.648428000 |
| 1 | 1.500111000 | -0.625925000 | -2.145433000 |
| 1 | 3.498149000 | 1.707367000 | 1.252593000 |
| 1 | 0.628967000 | -2.196921000 | 2.375892000 |
| 1 | 3.110281000 | -0.733150000 | 3.145446000 |
| 5 | 3.110239000 | -1.717130000 | -0.705315000 |
| 1 | 3.209138000 | -3.303553000 | 1.376366000 |
| 1 | 1.066256000 | -3.149325000 | -0.752851000 |
| 1 | 3.849556000 | 0.618112000 | -1.605465000 |
| 1 | 5.121792000 | -0.943720000 | 0.804508000 |
| 1 | 3.628665000 | -2.346999000 | -1.593097000 |
| 27 | 0.010784000 | -0.625474000 | 0.029344000 |
| 16 | -1.355844000 | 2.199670000 | 1.014147000 |
| 6 | -2.980074000 | 2.944845000 | 1.435615000 |
| 1 | -3.682692000 | 2.916950000 | 0.580082000 |
| 1 | -3.436427000 | 2.467485000 | 2.323562000 |

| | | | |
|---|---|---|---|
| 1 | -2.729171000 | 3.999678000 | 1.671009000 |
| 16 | 1.244108000 | 2.218397000 | -0.978532000 |
| 6 | 2.808192000 | 3.055237000 | -1.461097000 |
| 1 | 2.495036000 | 4.097281000 | -1.676813000 |
| 1 | 3.526143000 | 3.057449000 | -0.618430000 |
| 1 | 3.271799000 | 2.611912000 | -2.363073000 |

TS(*cisoid-gauche)*, E= 2871.46012043

| | | | |
|---|---|---|---|
| 6 | -1.395457000 | 0.411938000 | -1.128674000 |
| 5 | -1.068570000 | -1.154825000 | -1.700712000 |
| 5 | -3.044535000 | 0.721350000 | -0.748254000 |
| 5 | -2.604484000 | -0.319207000 | -2.105890000 |
| 6 | -1.800157000 | 0.461076000 | 0.468554000 |
| 1 | -0.925060000 | 1.324743000 | -1.517312000 |
| 5 | -1.362393000 | -2.243093000 | -0.293277000 |
| 5 | -3.316748000 | -0.310169000 | 0.678638000 |
| 5 | -2.634027000 | -2.007105000 | -1.554560000 |
| 5 | -1.759057000 | -1.151341000 | 1.095268000 |
| 5 | -3.852517000 | -0.844987000 | -0.939443000 |
| 1 | -1.628150000 | -1.320263000 | 2.276868000 |
| 1 | -3.465816000 | 1.837075000 | -0.900543000 |
| 1 | -0.337679000 | -1.315580000 | -2.650418000 |
| 1 | -2.772105000 | 0.112609000 | -3.219673000 |
| 5 | -3.069646000 | -1.998707000 | 0.186489000 |
| 1 | -2.929208000 | -2.910128000 | -2.301943000 |
| 1 | -0.947485000 | -3.364107000 | -0.177885000 |
| 1 | -4.035893000 | 0.054587000 | 1.571418000 |
| 1 | -5.027254000 | -0.881209000 | -1.220841000 |
| 1 | -3.695869000 | -2.885861000 | 0.718274000 |
| 5 | 1.355677000 | 0.563795000 | 1.268280000 |
| 5 | 1.170809000 | -1.142788000 | 1.804155000 |
| 5 | 3.060417000 | 0.820512000 | 0.724861000 |
| 5 | 2.711892000 | -0.248245000 | 2.104463000 |
| 6 | 1.786940000 | 0.534660000 | -0.393942000 |
| 1 | 0.871333000 | 1.563771000 | 1.720568000 |
| 5 | 1.443072000 | -2.144354000 | 0.328818000 |
| 5 | 3.347896000 | -0.196946000 | -0.705052000 |
| 5 | 2.769059000 | -1.936669000 | 1.519875000 |
| 6 | 1.828130000 | -1.015225000 | -0.903696000 |
| 5 | 3.933199000 | -0.730236000 | 0.882436000 |
| 1 | 1.613184000 | -1.183064000 | -1.965586000 |
| 1 | 3.543013000 | 1.921038000 | 0.793674000 |
| 1 | 0.546850000 | -1.491303000 | 2.773282000 |
| 1 | 3.028800000 | 0.084852000 | 3.222871000 |
| 5 | 3.140321000 | -1.882657000 | -0.224560000 |
| 1 | 3.135149000 | -2.865192000 | 2.201536000 |
| 1 | 1.079849000 | -3.249709000 | 0.045173000 |
| 1 | 3.941574000 | 0.144736000 | -1.694685000 |
| 1 | 5.122349000 | -0.764863000 | 1.095528000 |
| 1 | 3.661789000 | -2.736442000 | -0.897551000 |
| 27 | 0.016624000 | -0.599277000 | 0.050452000 |
| 16 | -1.498097000 | 1.986913000 | 1.447255000 |
| 6 | -3.164548000 | 2.657965000 | 1.832866000 |

| | | | |
|---|---|---|---|
| 1 | -3.776347000 | 2.818672000 | 0.924134000 |
| 1 | -3.709227000 | 2.019281000 | 2.553831000 |
| 1 | -2.942347000 | 3.637626000 | 2.304225000 |
| 16 | 1.391189000 | 1.826160000 | -1.637386000 |
| 6 | 2.829945000 | 2.958715000 | -1.638092000 |
| 1 | 2.634878000 | 3.639475000 | -2.491661000 |
| 1 | 2.888700000 | 3.544612000 | -0.701599000 |
| 1 | 3.775712000 | 2.409554000 | -1.811570000 |

*gauche*, E= -2871.47016529

| | | | |
|---|---|---|---|
| 6 | -1.309979000 | -1.017950000 | -0.774900000 |
| 5 | -0.836737000 | -1.930045000 | 0.583296000 |
| 5 | -2.999247000 | -0.741437000 | -0.896811000 |
| 5 | -2.371439000 | -2.273081000 | -0.274025000 |
| 6 | -1.866365000 | 0.494831000 | -0.371405000 |
| 1 | -0.833388000 | -1.109411000 | -1.760654000 |
| 5 | -1.179837000 | -0.906964000 | 2.010585000 |
| 5 | -3.332457000 | 0.328606000 | 0.494446000 |
| 5 | -2.344208000 | -2.188597000 | 1.503806000 |
| 5 | -1.780548000 | 0.673439000 | 1.368407000 |
| 5 | -3.683152000 | -1.422212000 | 0.593904000 |
| 1 | -1.745238000 | 1.774789000 | 1.849801000 |
| 1 | -3.489974000 | -0.624776000 | -1.988755000 |
| 1 | 0.007297000 | -2.786796000 | 0.492122000 |
| 1 | -2.469917000 | -3.248416000 | -0.976788000 |
| 5 | -2.935659000 | -0.566529000 | 1.985857000 |
| 1 | -2.505999000 | -3.178673000 | 2.178327000 |
| 1 | -0.618425000 | -1.042816000 | 3.070961000 |
| 1 | -4.161975000 | 1.195477000 | 0.409426000 |
| 1 | -4.823256000 | -1.823253000 | 0.595885000 |
| 1 | -3.562201000 | -0.353046000 | 2.997892000 |
| 5 | 1.274011000 | 1.044453000 | -0.929640000 |
| 5 | 0.841846000 | 2.003715000 | 0.538573000 |
| 5 | 3.046442000 | 0.708864000 | -0.871793000 |
| 5 | 2.419470000 | 2.264969000 | -0.285060000 |
| 6 | 1.883701000 | -0.460340000 | -0.386819000 |
| 1 | 0.826183000 | 1.094780000 | -2.048314000 |
| 5 | 1.145797000 | 0.932983000 | 1.953122000 |
| 5 | 3.358955000 | -0.334275000 | 0.537026000 |
| 5 | 2.347480000 | 2.189252000 | 1.503550000 |
| 6 | 1.799575000 | -0.511721000 | 1.269094000 |
| 5 | 3.704858000 | 1.406505000 | 0.633282000 |
| 1 | 1.695669000 | -1.504684000 | 1.723594000 |
| 1 | 3.658728000 | 0.542239000 | -1.893456000 |
| 1 | 0.034077000 | 2.897884000 | 0.542654000 |
| 1 | 2.649506000 | 3.280271000 | -0.900645000 |
| 5 | 2.910830000 | 0.567985000 | 1.995732000 |
| 1 | 2.527832000 | 3.148537000 | 2.216556000 |
| 1 | 0.647179000 | 0.932104000 | 3.046370000 |
| 1 | 4.098990000 | -1.283565000 | 0.544561000 |
| 1 | 4.851698000 | 1.782280000 | 0.698860000 |
| 1 | 3.417065000 | 0.239971000 | 3.039855000 |
| 27 | -0.002739000 | 0.021829000 | 0.450560000 |

| | | | |
|---|---|---|---|
| 16 | -1.734133000 | 1.852187000 | -1.597343000 |
| 6 | -3.465525000 | 2.333557000 | -1.965645000 |
| 1 | -4.083298000 | 1.466846000 | -2.272391000 |
| 1 | -3.938903000 | 2.860241000 | -1.115067000 |
| 1 | -3.366201000 | 3.033253000 | -2.821132000 |
| 16 | 1.770784000 | -2.034737000 | -1.329012000 |
| 6 | 3.289909000 | -2.071580000 | -2.353657000 |
| 1 | 3.277700000 | -3.083731000 | -2.807869000 |
| 1 | 3.274039000 | -1.307079000 | -3.153536000 |
| 1 | 4.200426000 | -1.959938000 | -1.732987000 |

*TS(gauche-trans)*, E= -2871.45074440

| | | | |
|---|---|---|---|
| 6 | 1.723306000 | -0.077390000 | 1.323797000 |
| 5 | 0.810870000 | -1.508519000 | 1.434214000 |
| 5 | 3.339158000 | -0.299439000 | 0.777800000 |
| 5 | 2.562330000 | -1.502770000 | 1.810936000 |
| 6 | 2.076964000 | 0.363655000 | -0.245397000 |
| 1 | 1.666587000 | 0.742439000 | 2.048966000 |
| 5 | 0.610661000 | -2.044749000 | -0.259966000 |
| 5 | 3.136380000 | -0.806469000 | -0.922600000 |
| 5 | 1.887807000 | -2.776248000 | 0.773996000 |
| 5 | 1.362491000 | -0.792645000 | -1.306453000 |
| 5 | 3.453999000 | -2.018018000 | 0.351002000 |
| 1 | 1.106533000 | -0.482064000 | -2.440676000 |
| 1 | 4.182751000 | 0.449605000 | 1.192262000 |
| 1 | 0.105091000 | -1.711371000 | 2.393938000 |
| 1 | 2.928975000 | -1.574816000 | 2.957809000 |
| 5 | 2.237889000 | -2.332636000 | -0.928928000 |
| 1 | 1.805498000 | -3.921462000 | 1.152285000 |
| 1 | -0.248180000 | -2.786672000 | -0.646785000 |
| 1 | 3.925083000 | -0.459835000 | -1.760993000 |
| 1 | 4.524149000 | -2.575624000 | 0.416175000 |
| 1 | 2.425472000 | -3.149955000 | -1.800245000 |
| 6 | -1.723323000 | 0.077369000 | 1.323783000 |
| 5 | -0.810880000 | 1.508484000 | 1.434240000 |
| 5 | -3.339170000 | 0.299438000 | 0.777771000 |
| 5 | -2.562348000 | 1.502744000 | 1.810939000 |
| 6 | -2.076959000 | -0.363654000 | -0.245413000 |
| 1 | -1.666617000 | -0.742474000 | 2.048935000 |
| 5 | -0.610641000 | 2.044746000 | -0.259921000 |
| 5 | -3.136356000 | 0.806490000 | -0.922618000 |
| 5 | -1.887799000 | 2.776233000 | 0.774032000 |
| 5 | -1.362462000 | 0.792664000 | -1.306445000 |
| 5 | -3.453991000 | 2.018022000 | 0.350999000 |
| 1 | -1.106497000 | 0.482099000 | -2.440672000 |
| 1 | -4.182775000 | -0.449615000 | 1.192196000 |
| 1 | -0.105113000 | 1.711312000 | 2.393977000 |
| 1 | -2.929003000 | 1.574771000 | 2.957810000 |
| 5 | -2.237857000 | 2.332652000 | -0.928905000 |
| 1 | -1.805484000 | 3.921442000 | 1.152335000 |
| 1 | 0.248210000 | 2.786667000 | -0.646719000 |
| 1 | -3.925045000 | 0.459879000 | -1.761032000 |
| 1 | -4.524138000 | 2.575634000 | 0.416165000 |

| | | | |
|---|---|---|---|
| 1 | -2.425423000 | 3.149985000 | -1.800213000 |
| 27 | 0.000004000 | -0.000009000 | 0.156895000 |
| 16 | 2.469859000 | 2.117490000 | -0.654923000 |
| 6 | 4.251958000 | 2.126459000 | -1.110580000 |
| 1 | 4.894673000 | 1.671252000 | -0.332227000 |
| 1 | 4.432951000 | 1.643802000 | -2.089570000 |
| 1 | 4.480847000 | 3.209855000 | -1.187267000 |
| 16 | -2.469876000 | -2.117485000 | -0.654934000 |
| 6 | -4.251981000 | -2.126412000 | -1.110578000 |
| 1 | -4.480918000 | -3.209802000 | -1.187207000 |
| 1 | -4.894667000 | -1.671138000 | -0.332239000 |
| 1 | -4.432964000 | -1.643797000 | -2.089591000 |

*trans*, E= -2871.46435541

| | | | |
|---|---|---|---|
| 6 | -1.502660000 | 0.509432000 | 1.310513000 |
| 5 | -0.539625000 | 1.845225000 | 0.877830000 |
| 5 | -3.172585000 | 0.674399000 | 0.914077000 |
| 5 | -2.221310000 | 2.065611000 | 1.450431000 |
| 6 | -2.078777000 | -0.329722000 | -0.017095000 |
| 1 | -1.370964000 | -0.074484000 | 2.230035000 |
| 5 | -0.558265000 | 1.870445000 | -0.931296000 |
| 5 | -3.190656000 | 0.667641000 | -0.870618000 |
| 5 | -1.651972000 | 2.946707000 | 0.007784000 |
| 5 | -1.497416000 | 0.444663000 | -1.456714000 |
| 5 | -3.289817000 | 2.209858000 | 0.028350000 |
| 1 | -1.387794000 | -0.197472000 | -2.471788000 |
| 1 | -3.979889000 | 0.122076000 | 1.614115000 |
| 1 | 0.302566000 | 2.244222000 | 1.636644000 |
| 1 | -2.426065000 | 2.494725000 | 2.558840000 |
| 5 | -2.262720000 | 2.073597000 | -1.434037000 |
| 1 | -1.491667000 | 4.144616000 | 0.035223000 |
| 1 | 0.298417000 | 2.361654000 | -1.627161000 |
| 1 | -4.099179000 | 0.148445000 | -1.463018000 |
| 1 | -4.320613000 | 2.839473000 | 0.069046000 |
| 1 | -2.558448000 | 2.620871000 | -2.471320000 |
| 5 | 1.497019000 | -0.444331000 | 1.456712000 |
| 5 | 0.558115000 | -1.870439000 | 0.931761000 |
| 5 | 3.190403000 | -0.667256000 | 0.870753000 |
| 5 | 2.262641000 | -2.072898000 | 1.434662000 |
| 6 | 2.078516000 | 0.329614000 | 0.016560000 |
| 1 | 1.387917000 | 0.198527000 | 2.471309000 |
| 5 | 0.540028000 | -1.845341000 | -0.877366000 |
| 5 | 3.173272000 | -0.674961000 | -0.913967000 |
| 5 | 1.652153000 | -2.946719000 | -0.006758000 |
| 6 | 1.503055000 | -0.509704000 | -1.310337000 |
| 5 | 3.289951000 | -2.209802000 | -0.027346000 |
| 1 | 1.371369000 | 0.073572000 | -2.230275000 |
| 1 | 4.098660000 | -0.147778000 | 1.463300000 |
| 1 | -0.298458000 | -2.361316000 | 1.627980000 |
| 1 | 2.558249000 | -2.619650000 | 2.472267000 |
| 5 | 2.221731000 | -2.066218000 | -1.449835000 |
| 1 | 1.491828000 | -4.144629000 | -0.034129000 |
| 1 | -0.302062000 | -2.244797000 | -1.636081000 |

| | | | |
|---|---|---|---|
| 1 | 3.980465000 | -0.122352000 | -1.613868000 |
| 1 | 4.320735000 | -2.839452000 | -0.068057000 |
| 1 | 2.426188000 | -2.496113000 | -2.557983000 |
| 27 | -0.000125000 | -0.000005000 | -0.000076000 |
| 16 | -2.512793000 | -2.107444000 | 0.164156000 |
| 6 | -4.308739000 | -2.199929000 | -0.196764000 |
| 1 | -4.897145000 | -1.495405000 | 0.423184000 |
| 1 | -4.529181000 | -2.043092000 | -1.270032000 |
| 1 | -4.572674000 | -3.240830000 | 0.083553000 |
| 16 | 2.512788000 | 2.107307000 | -0.165663000 |
| 6 | 4.308396000 | 2.200276000 | 0.196788000 |
| 1 | 4.572149000 | 3.241280000 | -0.083335000 |
| 1 | 4.527962000 | 2.043556000 | 1.270248000 |
| 1 | 4.897599000 | 1.495973000 | -0.422646000 |