Supporting Information

# Accuracy of Quantum Chemistry Structures of Chiral Tag Complexes and the Assignment of Absolute Configuration

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Corresponding Figures for Quantum Chemistry Calculations with 6-311++G(d,p)

The numbering used in the figure captions matches the corresponding manuscript figure.

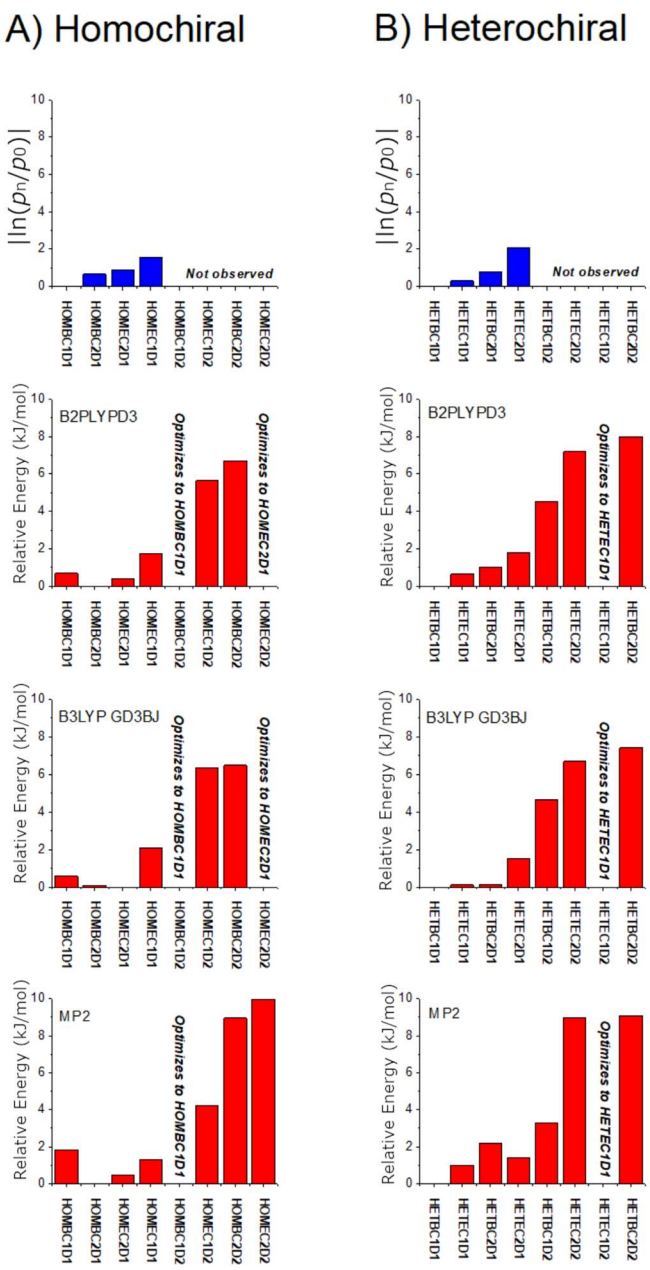



**Fig. 6S**: A graphical representation of the relative isomer energies reported in Table 1 for calculations with the 6-311++G(d,p) basis set is shown. The three quantum chemistry methods re B2PPLYPD3, B3LYP GD3BJ, and MP2. In some cases, the geometry optimization collapsed into the lower energy geometry with different dihedral angle about the O---O axis of the hydrogen bond and these cases are indicated in the figure.

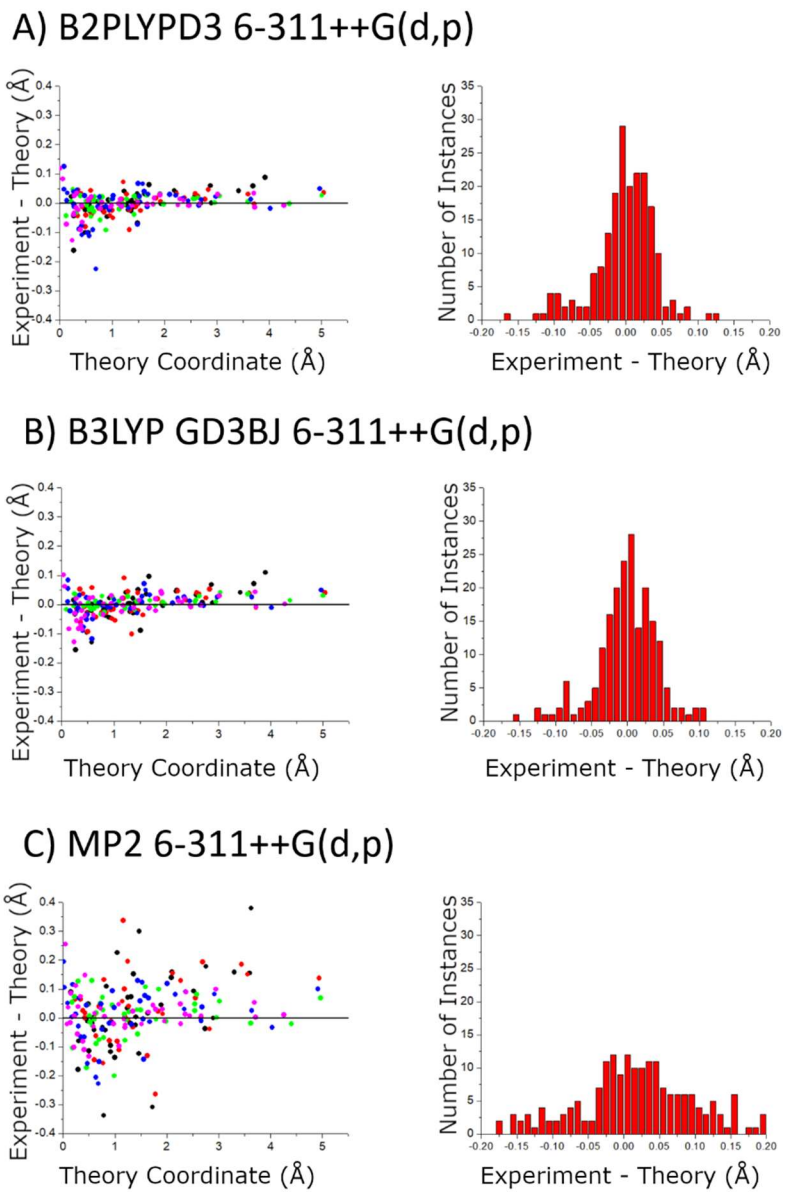



**Fig. 9S**: The accuracy of the quantum chemistry structures is benchmarked using the carbon atom coordinates – in the principal axis system for molecular rotation - obtained from the Kraitchman analysis. The scatter plot shows the difference in the absolute values of these coordinates (coordinate signs are unavailable from the spectroscopic analysis) as a function of the size of the coordinate. The coordinates come from the 5 structures that were measured with $^{13}$C-sensitivity: HOMEC2D1 (black), HOMBC2D1 (blue), HOMBC1D1 (magenta), HETEC1D1 (red), and HETBC1D1 (green).

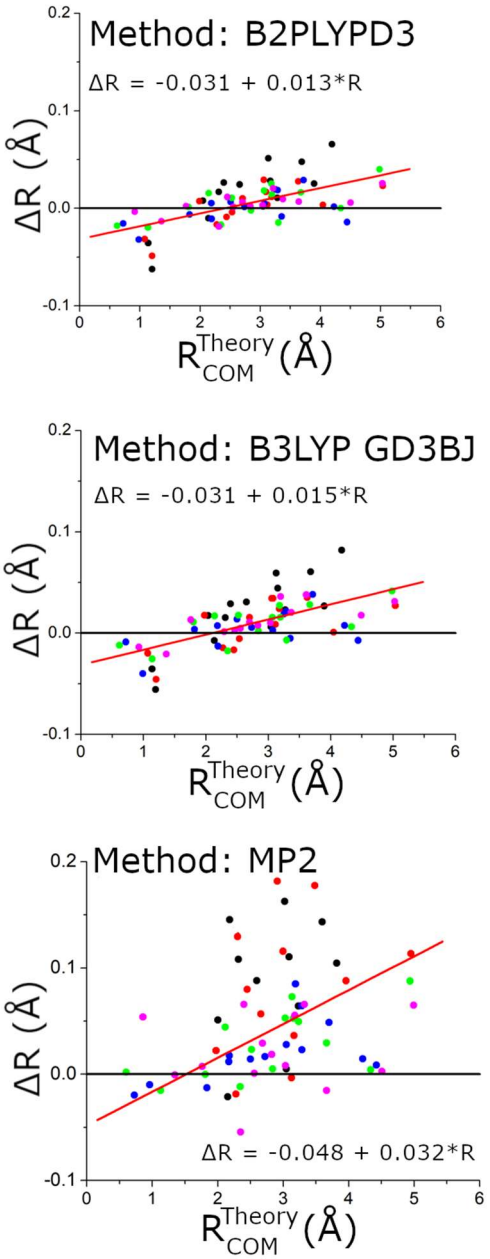



**Fig. 10S**: This figure shows the differences in the experimental and theoretical distance of each carbon atom from the center-of-mass of the chiral tag complex. The red line shows a linear regression analysis for each data set to help quantify the way these errors vary with the center-of-mass distance. The linear fit formulas are shown as insets in each figure. The coordinates come from the 5 structures that were measured with $^{13}$C-sensitivity: HOMEC2D1 (black), HOMBC2D1 (blue), HOMBC1D1 (magenta), HETEC1D1 (red), and HETBC1D1 (green).

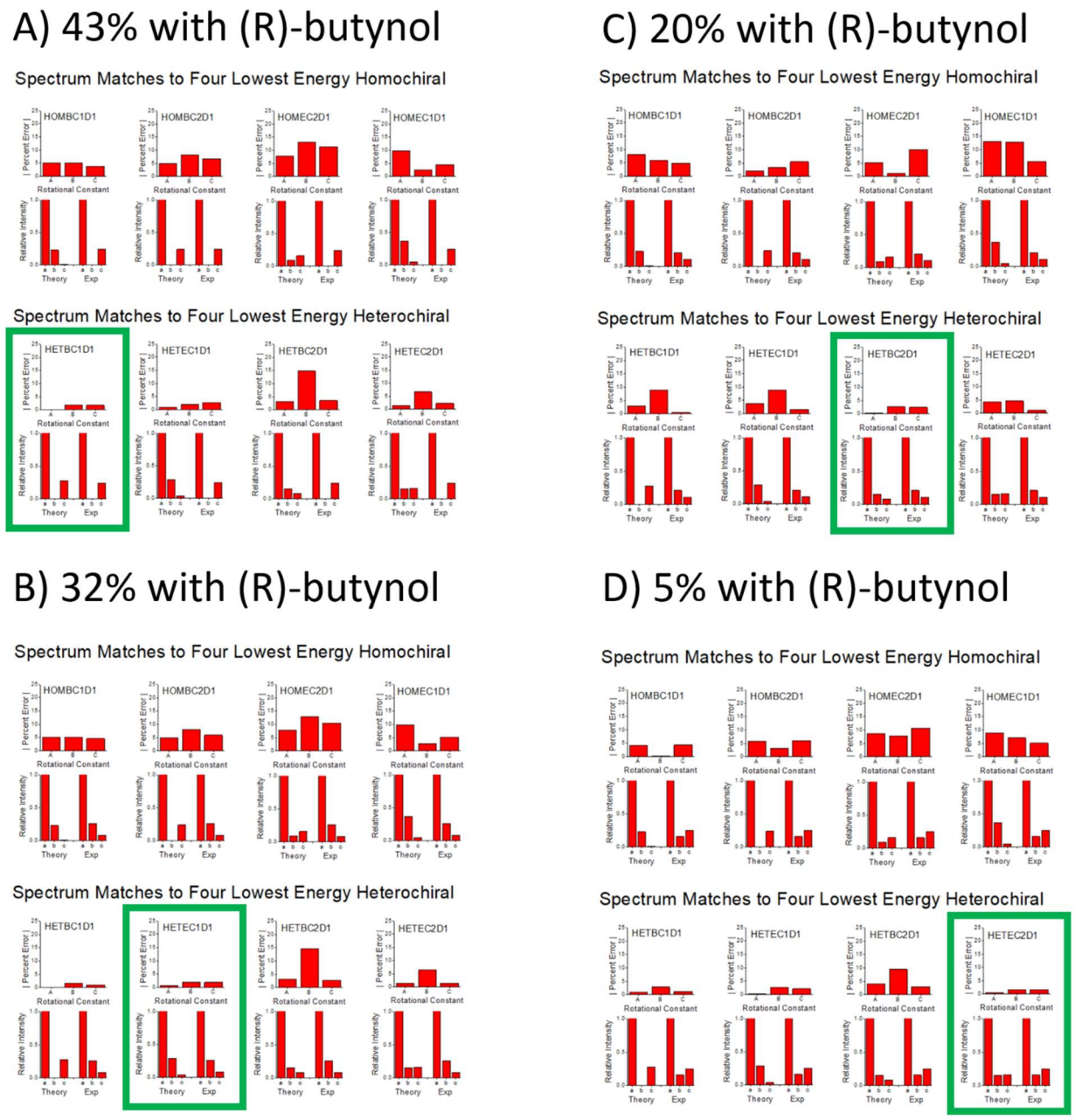



**Fig. 12S**: This figure illustrates the way that the spectral assignments guided by quantum chemistry are used to establish the absolute configuration of verbenone. Panel (A) shows the comparison between the experimental spectrum parameters for the highest abundance species observed when (R)-butynol is used as the tag and the lowest energy isomers of homochiral and heterochiral complexes identified in the quantum chemistry analysis using B3LYP GD3BJ def2TZVP. This comparison uses the percent error for the rotational constants and a comparison of the relative spectral intensities to the square of the dipole moment components. The best match for the spectrum is to the heterochiral complex, HETBC1D1 – outlined in green. Since the spectrum matches a heterochiral geometry and the tag is known to be (R)-butynol, the absolute configuration is established as (S)-verbenone. The confidence in this determination is increased by the fact that the other three spectra observed in the (R)-butynol tag measurement also have exclusive matches to theoretical homochiral geometries.

Substitution Structures and Experimental Carbon Atom Positions

Carbon Atom Positions for HOMBC1D1

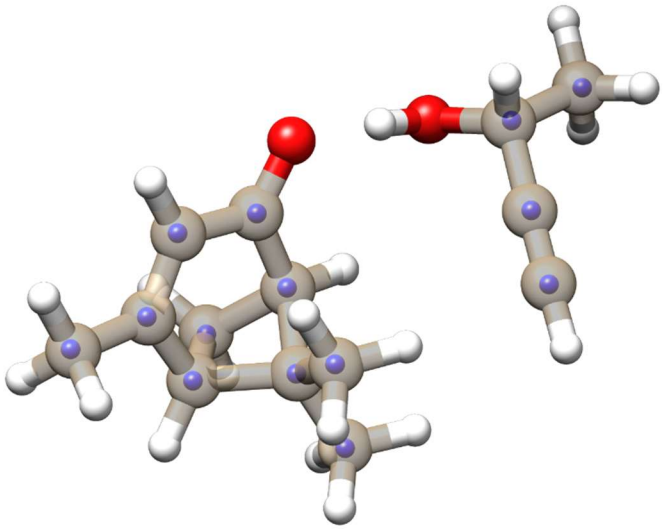


**Table S1**: Atomic coordinates in the principal axis system calculated using Kraitchman's equations. The carbon atom labels correspond to the atom labeling in the quantum chemistry structures reported below.

| Carbon | a(Å) | Error(Å) | b(Å) | Error(Å) | c(Å) | Error(Å) |
|---|---|---|---|---|---|---|
| C2 | 1.293 | 0.006 | 1.212 | 0.007 | 0.0749*i | 0.106 |
| C3 | 2.588 | 0.003 | 0.521 | 0.013 | 0.623 | 0.011 |
| C4 | 0.516 | 0.014 | 0.157*i | 0.047 | 0.769 | 0.010 |
| C5 | 1.702 | 0.005 | 0.112*i | 0.069 | 1.788 | 0.004 |
| C6 | 2.964 | 0.003 | 0.659 | 0.011 | 0.227 | 0.033 |
| C7 | 1.116 | 0.007 | 1.382 | 0.005 | 1.452 | 0.005 |
| C8 | 0.997 | 0.007 | 2.564 | 0.003 | 0.716 | 0.010 |
| C9 | 0.598 | 0.011 | 1.201 | 0.006 | 0.079 | 0.084 |
| C10 | 1.978 | 0.003 | 1.528 | 0.004 | 0.544 | 0.012 |
| C11 | 4.384 | 0.002 | 0.801 | 0.009 | 0.685 | 0.010 |
| C26 | 3.600 | 0.002 | 0.510 | 0.016 | 0.296 | 0.027 |
| C27 | 5.033 | 0.001 | 0.418 | 0.018 | 0.284 | 0.026 |
| C30 | 3.076 | 0.002 | 0.831 | 0.009 | 0.551 | 0.013 |
| C31 | 2.660 | 0.003 | 1.944 | 0.004 | 0.790 | 0.009 |

Carbon Atom Positions for HOMBC2D1

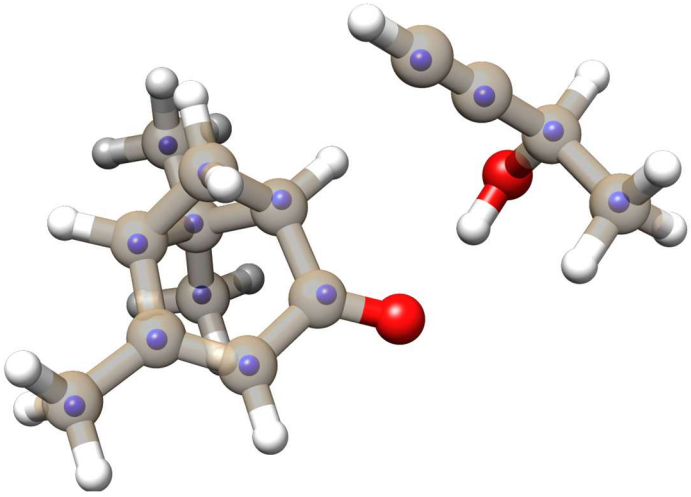


**Table S2**: Atomic coordinates in the principal axis system calculated using Kraitchman's equations. The carbon atom labels correspond to the atom labeling in the quantum chemistry structures reported below.

| Carbon | a(Å) | Error(Å) | b(Å) | Error(Å) | c(Å) | Error(Å) |
|---|---|---|---|---|---|---|
| C2 | 1.821 | 0.014 | 1.179 | 0.022 | 0.329 | 0.080 |
| C3 | 2.370 | 0.010 | 0.227 | 0.106 | 0.805 | 0.030 |
| C4 | 0.306 | 0.079 | 0.624 | 0.039 | 0.138 | 0.175 |
| C5 | 0.957 | 0.029 | 0.410 | 0.066 | 1.494 | 0.019 |
| C6 | 2.449 | 0.012 | 1.176 | 0.025 | 0.356 | 0.084 |
| C7 | 2.311 | 0.012 | 0.981 | 0.028 | 1.778 | 0.016 |
| C8 | 1.949 | 0.016 | 2.672 | 0.012 | 0.122 | 0.283 |
| C9 | 0.110 | 0.251 | 0.761 | 0.036 | 0.557 | 0.050 |
| C10 | 1.371 | 0.018 | 1.671 | 0.015 | 0.296 | 0.085 |
| C11 | 3.713 | 0.006 | 1.945 | 0.012 | 0.571 | 0.042 |
| C26 | 3.743 | 0.006 | 0.223 | 0.110 | 0.053 | 0.463 |
| C27 | 4.272 | 0.006 | 1.123 | 0.025 | 0.364 | 0.078 |
| C30 | 3.049 | 0.008 | 0.240 | 0.107 | 1.166 | 0.022 |
| C31 | 2.462 | 0.012 | 0.300 | 0.094 | 2.250 | 0.013 |

Carbon Atom Positions for HOMEC2D1

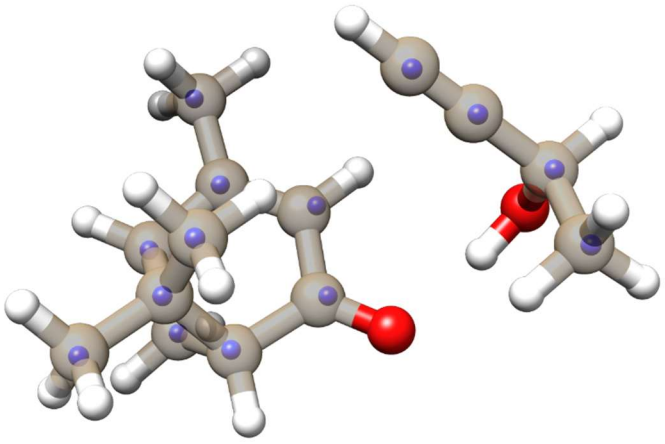


**Table S3**: Atomic coordinates in the principal axis system calculated using Kraitchman's equations. The carbon atom labels correspond to the atom labeling in the quantum chemistry structures reported below.

| Carbon | a(Å) | Error(Å) | b(Å) | Error(Å) | c(Å) | Error(Å) |
|---|---|---|---|---|---|---|
| C2 | 2.231 | 0.014 | 0.547 | 0.056 | 0.773 | 0.040 |
| C3 | 2.612 | 0.010 | 0.559 | 0.049 | 0.245 | 0.112 |
| C4 | 1.657 | 0.016 | 1.283 | 0.021 | 0.386 | 0.072 |
| C5 | 2.699 | 0.011 | 0.538 | 0.053 | 1.319 | 0.022 |
| C6 | 1.385 | 0.020 | 1.406 | 0.019 | 0.572 | 0.049 |
| C7 | 1.272 | 0.027 | 0.221 | 0.150 | 1.937 | 0.018 |
| C8 | 3.459 | 0.007 | 1.277 | 0.020 | 1.337 | 0.020 |
| C9 | 0.110 | 0.265 | 0.727 | 0.040 | 0.821 | 0.036 |
| C10 | 0.0675*i | 0.430 | 0.748 | 0.039 | 0.863 | 0.034 |
| C11 | 1.511 | 0.016 | 2.895 | 0.008 | 0.463 | 0.058 |
| C26 | 3.750 | 0.007 | 0.212*i | 0.121 | 0.183*i | 0.140 |
| C27 | 4.007 | 0.007 | 1.377 | 0.021 | 0.445 | 0.068 |
| C30 | 2.937 | 0.009 | 0.799 | 0.032 | 0.943 | 0.027 |
| C31 | 2.257 | 0.014 | 1.417 | 0.021 | 1.768 | 0.018 |

Carbon Atom Positions for HETBC1D1

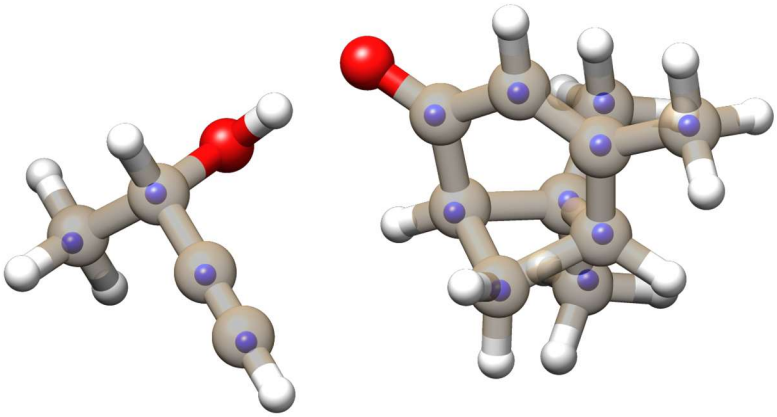


**Table S4**: Atomic coordinates in the principal axis system calculated using Kraitchman's equations. The carbon atom labels correspond to the atom labeling in the quantum chemistry structures reported below.

| Carbon | a(Å) | Error(Å) | b(Å) | Error(Å) | c(Å) | Error(Å) |
|---|---|---|---|---|---|---|
| C2 | 1.717 | 0.023 | 1.303 | 0.030 | 0.128 | 0.312 |
| C3 | 2.371 | 0.016 | 0.261 | 0.141 | 0.874 | 0.043 |
| C4 | 0.284 | 0.158 | 0.502 | 0.089 | 0.180 | 0.251 |
| C5 | 0.928 | 0.040 | 0.206 | 0.175 | 1.540 | 0.024 |
| C6 | 2.652 | 0.013 | 1.022 | 0.035 | 0.141 | 0.258 |
| C7 | 2.245 | 0.016 | 1.414 | 0.025 | 1.567 | 0.024 |
| C8 | 1.651 | 0.019 | 2.716 | 0.012 | 0.452 | 0.079 |
| C9 | 0.339 | 0.105 | 0.781 | 0.045 | 0.718 | 0.050 |
| C10 | 1.660 | 0.023 | 1.544 | 0.024 | 0.544 | 0.072 |
| C11 | 4.001 | 0.009 | 1.657 | 0.022 | 0.301 | 0.126 |
| C26 | 3.664 | 0.011 | 0.376 | 0.104 | 0.267 | 0.147 |
| C27 | 5.015 | 0.007 | 0.314 | 0.121 | 0.129*i | 0.293 |
| C30 | 3.003 | 0.013 | 0.428 | 0.094 | 1.046 | 0.039 |
| C31 | 2.461 | 0.016 | 0.465 | 0.079 | 2.127 | 0.019 |

Carbon Atom Positions for HETEC1D1

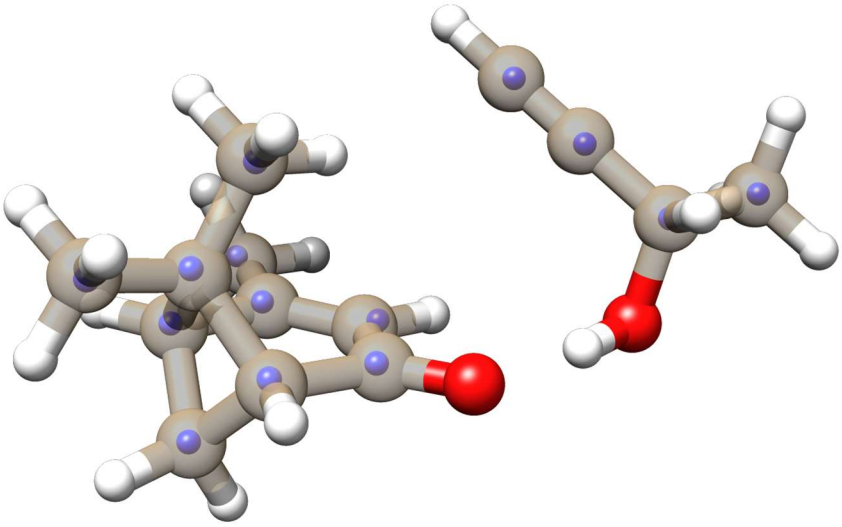


**Table S5**: Atomic coordinates in the principal axis system calculated using Kraitchman's equations. The carbon atom labels correspond to the atom labeling in the quantum chemistry structures reported below.

| Carbon | a(Å) | Error(Å) | b(Å) | Error(Å) | c(Å) | Error(Å) |
|---|---|---|---|---|---|---|
| C2 | 2.398 | 0.019 | 0.10878*i | 0.423 | 0.817 | 0.057 |
| C3 | 2.624 | 0.005 | 0.573 | 0.022 | 0.407 | 0.031 |
| C4 | 1.856 | 0.023 | 1.314 | 0.033 | 0.256*i | 0.176 |
| C5 | 2.787 | 0.018 | 0.736 | 0.068 | 1.202 | 0.043 |
| C6 | 1.307 | 0.037 | 1.202 | 0.040 | 0.915 | 0.054 |
| C7 | 1.443 | 0.040 | 0.301 | 0.179 | 1.934 | 0.030 |
| C8 | 3.708 | 0.016 | 0.635 | 0.088 | 1.496 | 0.039 |
| C9 | 0.442 | 0.105 | 0.965 | 0.048 | 0.460 | 0.103 |
| C10 | 0.0832*i | 0.633 | 0.400 | 0.129 | 0.972 | 0.054 |
| C11 | 1.284 | 0.038 | 2.659 | 0.018 | 1.239 | 0.045 |
| C26 | 3.627 | 0.015 | 0.421 | 0.130 | 0.278 | 0.197 |
| C27 | 5.076 | 0.009 | 0.260*i | 0.182 | 0.231*i | 0.204 |
| C30 | 2.884 | 0.016 | 0.615 | 0.072 | 0.920 | 0.050 |
| C31 | 2.267 | 0.021 | 1.520 | 0.030 | 1.496 | 0.033 |

Summaries of Rotational Spectroscopy Fits

**Table S6:** Verbenone-butynol homochiral final fits with rms errors.

| PARAMETER | HOMBC1D1 | HOMBC2D1 | HOMEC2D1 | HOMEC1D1 |
|---|---|---|---|---|
| ***A*/MHz** | 948.88846(16) | 859.16530(29) | 836.94277(32) | 986.19310(21) |
| ***B*/MHz** | 295.400123(72) | 306.202160(88) | 314.414180(85) | 276.808690(79) |
| ***C*/MHz** | 260.857248(70) | 291.24858(10) | 299.497080(87) | 261.963460(79) |
| $D_J$/kHz | 0.01751(20) | 0.02624(36) | 0.06229(29) | 0.03479(22) |
| $D_{JK}$/kHz | 0.10790(92) | 0.0618(14) | -0.1389(12) | 0.0631(15) |
| $D_K$/kHz | - | - | 0.228(17) | - |
| $d_1$/kHz | -0.00164(11) | - | -0.00800(24) | 0.00122(13) |
| $d_2$/kHz | -0.000359(57) | 0.000860(76) | - | - |
| **N** | 254 | 106 | 162 | 151 |
| **RMS/kHz** | 6.00 | 5.00 | 4.88 | 5.29 |

**Table S7:** Verbenone-butynol heterochiral final fits with rms errors.

| PARAMETER | HETBC1D1 | HETEC1D1 | HETBC2D1 | HETEC2D1 |
|---|---|---|---|---|
| ***A*/MHz** | 905.34973(27) | 905.85816(20) | 879.94543(19) | 913.47713(32) |
| ***B*/MHz** | 286.528600(82) | 286.904050(86) | 320.343510(84) | 300.393330(78) |
| ***C*/MHz** | 276.457860(86) | 278.454670(84) | 279.561300(89) | 278.019490(84) |
| $D_J$/kHz | 0.02377(23) | 0.03298(27) | 0.02770(27) | 0.04308(28) |
| $D_{JK}$/kHz | 0.1258(13) | 0.0317(14) | 0.0535(13) | -0.0178(33) |
| $D_K$/kHz | - | - | - | - |
| $d_1$/kHz | -0.00185(19) | -0.00361(14) | -0.00425(14) | - |
| $d_2$/kHz | - | - | | |
| **N** | 137 | 170 | 183 | 121 |
| **RMS/kHz** | 4.92 | 6.08 | 5.79 | 4.78 |

**Table S8:** Table of $^{13}C$ fits for the HOMBC1D1 homochiral complex.

| Parameter | C2 | C3 | C4 | C5 | C6 |
|---|---|---|---|---|---|
| *A* /MHz | 946.296(10) | 947.723(12) | 947.882(14) | 943.269(12) | 948.032(13) |
| *B* /MHz | 295.11250(10) | 294.18281(14) | 295.25240(15) | 294.35335(12) | 293.88388(13) |
| *C* /MHz | 260.435460(94) | 259.92289(13) | 260.82475(15) | 260.46929(12) | 259.62358(12) |
| N | 46 | 54 | 48 | 52 | 58 |
| RMS /kHz | 4.7 | 6.8 | 7.0 | 5.9 | 6.5 |
| Parameter | C7 | C8 | C9 | C10 | C11 |
| *A* /MHz | 941.795(11) | 936.458(12) | 946.319(11) | 944.2470(74) | 946.946(11) |
| *B* /MHz | 294.82544(10) | 295.14209(13) | 295.33734(11) | 294.675140(79) | 292.04191(11) |
| *C* /MHz | 260.43088(10) | 259.84180(12) | 260.61547(10) | 260.019250(72) | 258.21243(11) |
| N | 57 | 53 | 56 | 57 | 62 |
| RMS /kHz | 5.4 | 6.4 | 6.0 | 4.1 | 6.3 |
| Parameter | C26 | C27 | C30 | C31 | |
| *A* /MHz | 948.276(15) | 948.444(14) | 947.136(12) | 941.160(12) | |
| *B* /MHz | 293.16654(14) | 291.08171(14) | 293.72479(12) | 294.07634(12) | |
| *C* /MHz | 259.09127(13) | 257.47190(13) | 259.49867(12) | 259.40375(11) | |
| N | 48 | 56 | 57 | 57 | |
| RMS /kHz | 6.9 | 7.2 | 6.1 | 6.2 | |

*Notes:*

*(1) The distortion constants are fixed to the values in the fit of the parent compound with all $^{12}C$ nuclei.*

*(2) The carbon atom labels match the atom number in the quantum chemistry summaries.*

**Table S9:** Table of $^{13}C$ fits for the HOMBC2D11homochiral complex.

| Parameter | C2 | C3 | C4 | C5 | C6 |
|---|---|---|---|---|---|
| *A* /MHz | 856.995(46) | 858.159(31) | 858.571(33) | 855.684(43) | 856.982(57) |
| *B* /MHz | 305.56852(20) | 305.04561(14) | 306.18133(15) | 305.62051(20) | 305.07073(24) |
| *C* /MHz | 290.46135(21) | 290.30079(14) | 291.16768(16) | 291.06581(18) | 290.01615(23) |
| N | 37 | 36 | 34 | 31 | 31 |
| RMS /kHz | 7.1 | 5.1 | 5.4 | 6.1 | 7.7 |
| Parameter | C7 | C8 | C9 | C10 | C11 |
| *A* /MHz | 853.227(61) | 848.890(60) | 857.871(41) | 854.999(50) | 853.296(39) |
| *B* /MHz | 304.64050(28) | 305.49244(27) | 306.14275(19) | 305.83777(25) | 303.60302(19) |
| *C* /MHz | 290.18728(27) | 289.42596(24) | 291.14926(17) | 290.46695(25) | 288.33006(19) |
| N | 32 | 25 | 33 | 34 | 35 |
| RMS /kHz | 8.8 | 7.6 | 6.0 | 8.5 | 6.7 |
| Parameter | C26 | C27 | C30 | C31 | |
| *A* /MHz | 859.090(29) | 857.174(64) | 857.128(50) | 851.758(50) | |
| *B* /MHz | 303.62764(13) | 302.83015(29) | 304.24078(22) | 304.15558(23) | |
| *C* /MHz | 288.91081(13) | 288.01350(29) | 289.68718(22) | 290.21589(23) | |
| N | 34 | 29 | 29 | 30 | |
| RMS /kHz | 5.1 | 9.2 | 8.0 | 6.7 | |

*Notes:*

*(1) The distortion constants are fixed to the values in the fit of the parent compound with all $^{12}C$ nuclei.*

*(2) The carbon atom labels match the atom number in the quantum chemistry summaries.*

**Table S10:** Table of $^{13}C$ fits for the HOMEC2D1homochiral complex.

| Parameter | C2 | C3 | C4 | C5 | C6 |
|---|---|---|---|---|---|
| *A* /MHz | 835.716(50) | 836.431(44) | 834.473(50) | 834.162(63) | 833.779(52) |
| *B* /MHz | 313.32932(25) | 313.07475(22) | 313.84953(25) | 312.66160(29) | 313.97707(26) |
| *C* /MHz | 298.56399(24) | 298.23729(21) | 298.71996(23) | 298.15727(27) | 298.80681(27) |
| N | 25 | 31 | 28 | 29 | 32 |
| RMS /kHz | 6.7 | 6.7 | 7.7 | 9.2 | 7.9 |
| Parameter | C7 | C8 | C9 | C10 | C11 |
| *A* /MHz | 831.728(42) | 832.294(35) | 835.289(63) | 835.148(44) | 825.248(44) |
| *B* /MHz | 313.36871(20) | 311.75342(17) | 314.28091(31) | 314.27050(22) | 313.92729(24) |
| *C* /MHz | 299.20037(18) | 297.09632(17) | 299.40047(29) | 299.39782(20) | 297.61543(24) |
| N | 27 | 31 | 26 | 28 | 32 |
| RMS /kHz | 5.1 | 5.8 | 8.9 | 6.4 | 7.9 |
| Parameter | C26 | C27 | C30 | C31 | |
| *A* /MHz | 837.052(42) | 834.101(63) | 834.857(48) | 829.939(65) | |
| *B* /MHz | 311.69732(19) | 311.26522(31) | 312.56659(23) | 312.82969(32) | |
| *C* /MHz | 297.03286(20) | 296.34664(31) | 297.86139(24) | 298.22675(35) | |
| N | 35 | 30 | 27 | 27 | |
| RMS /kHz | 6.9 | 9.4 | 7.7 | 8.6 | |

*Notes:*

*(1) The distortion constants are fixed to the values in the fit of the parent compound with all $^{12}C$ nuclei.*

*(2) The carbon atom labels match the atom number in the quantum chemistry summaries.*

**Table S11:** Table of $^{13}C$ fits for the heterochiral HETBC1D1 verbenone-butynol complex.

| Parameter | C2 | C3 | C4 | C5 | C6 |
|---|---|---|---|---|---|
| *A* /MHz | 902.590(55) | 904.010(59) | 904.895(70) | 901.462(46) | 903.640(50) |
| *B* /MHz | 286.04805(15) | 285.49607(15) | 286.51024(20) | 286.00532(11) | 285.38785(13) |
| *C* /MHz | 275.75824(14) | 275.60018(14) | 276.40761(17) | 276.32084(11) | 275.24318(13) |
| N | 43 | 40 | 38 | 42 | 43 |
| RMS /kHz | 5.2 | 5.7 | 5.8 | 4.6 | 5.2 |
| Parameter | C7 | C8 | C9 | C10 | C11 |
| *A* /MHz | 898.222(78) | 893.263(47) | 903.536(58) | 901.040(67) | 900.844(48) |
| *B* /MHz | 285.32821(20) | 286.05487(13) | 286.42707(15) | 286.03524(18) | 283.93548(12) |
| *C* /MHz | 275.38554(19) | 274.93725(13) | 276.34767(15) | 275.68207(17) | 273.65388(12) |
| N | 47 | 44 | 37 | 46 | 42 |
| RMS /kHz | 8.2 | 5.5 | 5.9 | 6.7 | 5.0 |
| Parameter | C26 | C27 | C30 | C31 | |
| *A* /MHz | 905.017(47) | 905.222(59) | 903.309(64) | 897.776(90) | |
| *B* /MHz | 284.35501(11) | 282.50683(14) | 284.89730(16) | 284.82405(22) | |
| *C* /MHz | 274.42350(11) | 272.69541(14) | 275.07327(16) | 275.50767(22) | |
| N | 43 | 43 | 40 | 44 | |
| RMS /kHz | 4.5 | 5.9 | 5.9 | 8.7 | |

*Notes:*

*(1) The distortion constants are fixed to the values in the fit of the parent compound with all $^{12}C$ nuclei.*

*(2) The carbon atom labels match the atom number in the quantum chemistry summaries.*

**Table S12:** Table of $^{13}C$ fits for the heterochiral HETEC1D1 verbenone-butynol complex.

| Parameter | C2 | C3 | C4 | C5 | C6 |
|---|---|---|---|---|---|
| *A* /MHz | 904.809(82) | 905.061(81) | 903.181(85) | 902.67(11) | 902.189(69) |
| *B* /MHz | 285.86382(16) | 285.76098(16) | 286.35415(19) | 285.41496(22) | 286.49413(13) |
| *C* /MHz | 277.57777(17) | 277.35289(16) | 277.66473(20) | 277.18344(22) | 277.96902(14) |
| N | 41 | 43 | 42 | 39 | 35 |
| RMS /kHz | 6.6 | 6.6 | 7.2 | 8.5 | 5.3 |
| Parameter | C7 | C8 | C9 | C10 | C11 |
| *A* /MHz | 899.70(11) | 901.64(10) | 904.018(99) | 904.07(11) | 892.137(93) |
| *B* /MHz | 285.96118(19) | 284.32898(20) | 286.83839(20) | 286.75206(22) | 286.41495(21) |
| *C* /MHz | 278.12010(19) | 276.29695(18) | 278.28170(20) | 278.43074(22) | 277.09667(22) |
| N | 42 | 38 | 40 | 39 | 32 |
| RMS /kHz | 7.5 | 6.8 | 7.9 | 8.0 | 7.1 |
| Parameter | C26 | C27 | C30 | C31 | |
| *A* /MHz | 905.450(89) | 906.056(81) | 903.90(10) | 898.58(10) | |
| *B* /MHz | 284.76732(19) | 282.78158(16) | 285.42142(22) | 285.72250(20) | |
| *C* /MHz | 276.42654(18) | 274.57184(16) | 277.12648(23) | 277.30180(21) | |
| N | 34 | 47 | 40 | 41 | |
| RMS /kHz | 6.1 | 6.4 | 8.4 | 8.2 | |

*Notes:*

*(1) The distortion constants are fixed to the values in the fit of the parent compound with all $^{12}C$ nuclei.*

*(2) The carbon atom labels match the atom number in the quantum chemistry summaries.*

Quantum Chemistry Summaries for B3LYP GD3BJ def2TZVP

*Note: The quantum chemistry calculations used (R)-verbenone for the analyte. The homochiral complexes, therefore, have (R)-butynol as the tag.*

Species: HOMEC2D1

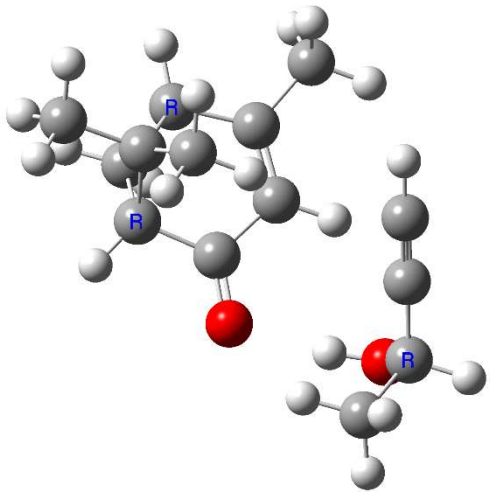
E = -696.2099142 H

Principal axis orientation:

| Center Number | Atomic Number | Coordinates (Angstroms) a | b | c |
|---|---|---|---|---|
| 1 | 8 | 0.704889 | 1.455353 | 0.999076 |
| 2 | 6 | -2.186603 | 0.553252 | -0.800462 |
| 3 | 6 | -2.572842 | -0.575379 | 0.232549 |
| 4 | 6 | -1.631706 | 1.306893 | 0.467033 |
| 5 | 6 | -2.698138 | 0.545205 | 1.302202 |
| 6 | 6 | -1.355339 | -1.392726 | 0.585275 |
| 7 | 6 | -1.229159 | 0.236514 | -1.939771 |
| 8 | 6 | -3.418999 | 1.242265 | -1.382373 |
| 9 | 6 | -0.274348 | 0.739765 | 0.828921 |
| 10 | 6 | -0.238565 | -0.723330 | 0.918168 |
| 11 | 6 | -1.442534 | -2.877969 | 0.521409 |
| 12 | 1 | -3.441425 | -1.194501 | 0.007214 |
| 13 | 1 | -1.606942 | 2.395091 | 0.465416 |
| 14 | 1 | -3.663210 | 1.043449 | 1.299959 |
| 15 | 1 | -2.429897 | 0.273913 | 2.321219 |
| 16 | 1 | -1.714739 | -0.418658 | -2.667721 |
| 17 | 1 | -0.956329 | 1.157392 | -2.459816 |
| 18 | 1 | -0.308640 | -0.240188 | -1.613460 |
| 19 | 1 | -3.896294 | 0.591162 | -2.118607 |
| 20 | 1 | -4.166494 | 1.502658 | -0.635180 |
| 21 | 1 | -3.126503 | 2.160823 | -1.895517 |
| 22 | 1 | 0.693502 | -1.208298 | 1.172754 |
| 23 | 1 | -1.704986 | -3.194971 | -0.493180 |
| 24 | 1 | -2.238056 | -3.247209 | 1.175613 |
| 25 | 1 | -0.503478 | -3.351505 | 0.803351 |
| 26 | 6 | 3.674656 | -0.020109 | 0.009342 |
| 27 | 6 | 3.923259 | 1.375042 | -0.567724 |
| 28 | 1 | 4.636558 | -0.523570 | 0.143219 |
| 29 | 8 | 3.096615 | 0.033632 | 1.301526 |
| 30 | 6 | 2.876487 | -0.840126 | -0.917627 |
| 31 | 6 | 2.223857 | -1.502830 | -1.676983 |
| 32 | 1 | 1.650678 | -2.094593 | -2.346699 |
| 33 | 1 | 2.976973 | 1.901654 | -0.697031 |
| 34 | 1 | 4.422846 | 1.311947 | -1.535559 |
| 35 | 1 | 4.549065 | 1.941129 | 0.122443 |
| 36 | 1 | 2.289149 | 0.585251 | 1.254370 |

Rotational constants (MHZ):
835.0281289 324.0043891 307.7471816

Dipole moment (Debye):
-4.7435838 -1.4083122 -1.8847956 Tot= 5.2950340



Species: HOMBC2D1

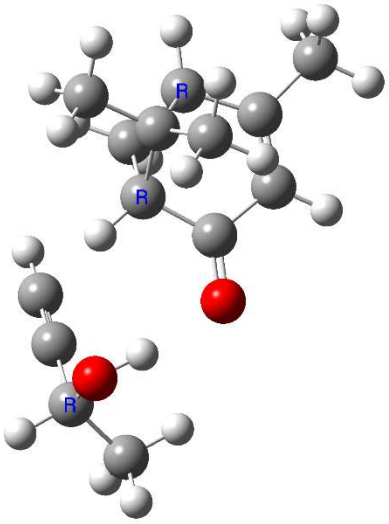
E = -696.2097177 H

Principal axis orientation:

| Center Number | Atomic Number | Coordinates (Angstroms) a | b | c |
|---|---|---|---|---|
| 1 | 8 | -0.732521 | -1.156906 | 1.181833 |
| 2 | 6 | 1.801123 | 1.179705 | 0.377044 |
| 3 | 6 | 2.346486 | 0.284392 | -0.802750 |
| 4 | 6 | 0.394311 | 0.596772 | -0.032551 |
| 5 | 6 | 0.953261 | 0.449597 | -1.474162 |
| 6 | 6 | 2.452711 | -1.151466 | -0.356622 |
| 7 | 6 | 2.305938 | 0.949450 | 1.793873 |
| 8 | 6 | 1.908282 | 2.669695 | 0.061804 |
| 9 | 6 | 0.244505 | -0.797793 | 0.537284 |
| 10 | 6 | 1.387947 | -1.678618 | 0.272374 |
| 11 | 6 | 3.717419 | -1.892944 | -0.618863 |
| 12 | 1 | 3.237549 | 0.625075 | -1.330533 |
| 13 | 1 | -0.494803 | 1.195424 | 0.144492 |
| 14 | 1 | 0.850946 | 1.363973 | -2.050520 |
| 15 | 1 | 0.594177 | -0.393680 | -2.059408 |
| 16 | 1 | 3.339518 | 1.291956 | 1.887891 |
| 17 | 1 | 1.702877 | 1.526512 | 2.498065 |
| 18 | 1 | 2.265973 | -0.093070 | 2.100322 |
| 19 | 1 | 2.947037 | 2.996816 | 0.151373 |
| 20 | 1 | 1.562228 | 2.925094 | -0.937635 |
| 21 | 1 | 1.316160 | 3.245340 | 0.775963 |
| 22 | 1 | 1.352619 | -2.697119 | 0.636360 |
| 23 | 1 | 4.554959 | -1.394918 | -0.120097 |
| 24 | 1 | 3.949519 | -1.891511 | -1.688008 |
| 25 | 1 | 3.666550 | -2.923690 | -0.270610 |
| 26 | 6 | -3.698018 | 0.256317 | 0.143713 |
| 27 | 6 | -4.276611 | -1.138593 | 0.391036 |
| 28 | 1 | -4.516323 | 0.982050 | 0.133029 |
| 29 | 8 | -2.844083 | 0.670263 | 1.195849 |
| 30 | 6 | -3.031382 | 0.324558 | -1.167360 |
| 31 | 6 | -2.489822 | 0.367068 | -2.238136 |
| 32 | 1 | -2.014454 | 0.410778 | -3.186466 |
| 33 | 1 | -3.474820 | -1.877524 | 0.416393 |
| 34 | 1 | -4.979561 | -1.413560 | -0.396805 |
| 35 | 1 | -4.793000 | -1.145930 | 1.351078 |
| 36 | 1 | -2.123481 | 0.012650 | 1.279287 |

Rotational constants (MHZ):
861.4463588 309.8432008 294.9079653

Dipole moment (Debye):
4.7266656 -0.2215616 -2.3324785 Tot= 5.2755012



Species: HOMBC1D1

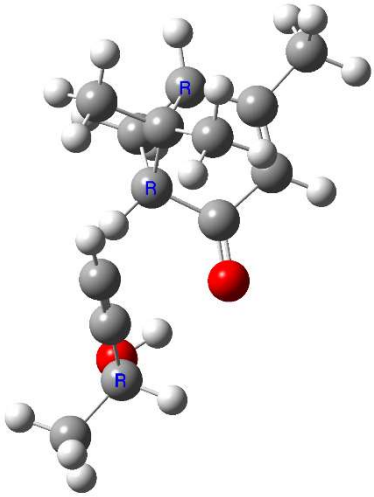
E = -696.2096729 H

Principal axis orientation:

| Center Number | Atomic Number | Coordinates (Angstroms) a | b | c |
|---|---|---|---|---|
| 1 | 8 | 0.350976 | 1.896649 | 0.414113 |
| 2 | 6 | -1.260477 | -1.215442 | -0.071773 |
| 3 | 6 | -2.566618 | -0.528133 | -0.634017 |
| 4 | 6 | -0.511164 | -0.018610 | -0.772238 |
| 5 | 6 | -1.687186 | 0.029619 | -1.788851 |
| 6 | 6 | -2.950831 | 0.641826 | 0.234947 |
| 7 | 6 | -1.097217 | -1.406577 | 1.429138 |
| 8 | 6 | -0.965794 | -2.544376 | -0.762495 |
| 9 | 6 | -0.616000 | 1.214064 | 0.100434 |
| 10 | 6 | -1.977511 | 1.510598 | 0.558745 |
| 11 | 6 | -4.362269 | 0.759893 | 0.694644 |
| 12 | 1 | -3.416641 | -1.167488 | -0.873787 |
| 13 | 1 | 0.507003 | -0.172549 | -1.120183 |
| 14 | 1 | -1.552971 | -0.668710 | -2.609402 |
| 15 | 1 | -1.966073 | 1.004924 | -2.182894 |
| 16 | 1 | -1.747923 | -2.211702 | 1.779492 |
| 17 | 1 | -0.066377 | -1.685644 | 1.651879 |
| 18 | 1 | -1.327863 | -0.512669 | 2.003574 |
| 19 | 1 | -1.642291 | -3.317282 | -0.389995 |
| 20 | 1 | -1.070917 | -2.502223 | -1.844726 |
| 21 | 1 | 0.056022 | -2.856621 | -0.540693 |
| 22 | 1 | -2.136881 | 2.383918 | 1.177603 |
| 23 | 1 | -4.638070 | -0.118506 | 1.286787 |
| 24 | 1 | -5.044318 | 0.782660 | -0.160435 |
| 25 | 1 | -4.523034 | 1.652533 | 1.297624 |
| 26 | 6 | 3.557209 | 0.513764 | 0.256949 |
| 27 | 6 | 4.988558 | 0.434708 | -0.263883 |
| 28 | 1 | 3.552543 | 1.095853 | 1.187921 |
| 29 | 8 | 2.772093 | 1.165847 | -0.724626 |
| 30 | 6 | 3.041767 | -0.828557 | 0.576615 |
| 31 | 6 | 2.645475 | -1.932010 | 0.836530 |
| 32 | 1 | 2.307719 | -2.911660 | 1.067641 |
| 33 | 1 | 5.009515 | -0.126274 | -1.198334 |
| 34 | 1 | 5.637723 | -0.059535 | 0.459091 |
| 35 | 1 | 5.357138 | 1.443173 | -0.450830 |
| 36 | 1 | 1.934522 | 1.460629 | -0.312453 |

Rotational constants (MHZ):
951.4193940 301.2209677 265.9370931

Dipole moment (Debye):
-4.7263056 -2.2453126 0.4504829 Tot= 5.2518881

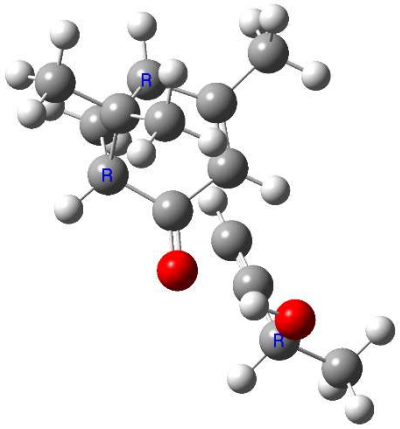


Species: HOMEC1D1

E = -696.2091326 H

Principal axis orientation:

| Center Number | Atomic Number | Coordinates (Angstroms) a | b | c |
|---|---|---|---|---|
| 1 | 8 | 0.512084 | 1.714888 | 0.035104 |
| 2 | 6 | -2.810078 | 0.499774 | -0.056843 |
| 3 | 6 | -2.349347 | -0.970913 | 0.280113 |
| 4 | 6 | -1.599348 | 0.923739 | 0.856168 |
| 5 | 6 | -1.797062 | -0.414422 | 1.623458 |
| 6 | 6 | -1.157879 | -1.350339 | -0.563566 |
| 7 | 6 | -2.835730 | 0.967198 | -1.504748 |
| 8 | 6 | -4.154257 | 0.840078 | 0.582978 |
| 9 | 6 | -0.306988 | 0.805877 | 0.075218 |
| 10 | 6 | -0.143435 | -0.471861 | -0.627090 |
| 11 | 6 | -1.169362 | -2.658811 | -1.274670 |
| 12 | 1 | -3.112126 | -1.749517 | 0.301352 |
| 13 | 1 | -1.643688 | 1.873368 | 1.386193 |
| 14 | 1 | -2.545970 | -0.340907 | 2.406718 |
| 15 | 1 | -0.902663 | -0.894179 | 2.015604 |
| 16 | 1 | -3.664009 | 0.494888 | -2.038670 |
| 17 | 1 | -2.994025 | 2.047231 | -1.542209 |
| 18 | 1 | -1.917678 | 0.746546 | -2.043564 |
| 19 | 1 | -4.962402 | 0.348814 | 0.035874 |
| 20 | 1 | -4.227090 | 0.537792 | 1.625997 |
| 21 | 1 | -4.330180 | 1.916858 | 0.534346 |
| 22 | 1 | 0.765973 | -0.647183 | -1.185029 |
| 23 | 1 | -2.013054 | -2.703230 | -1.970790 |
| 24 | 1 | -1.310114 | -3.480438 | -0.565758 |
| 25 | 1 | -0.247765 | -2.827005 | -1.829741 |
| 26 | 6 | 3.727426 | 0.531240 | 0.095140 |
| 27 | 6 | 5.090790 | 0.079425 | -0.415763 |
| 28 | 1 | 3.867337 | 1.404248 | 0.746943 |
| 29 | 8 | 2.941631 | 0.889380 | -1.029292 |
| 30 | 6 | 3.085217 | -0.519128 | 0.901216 |
| 31 | 6 | 2.554462 | -1.378163 | 1.550618 |
| 32 | 1 | 2.087875 | -2.140306 | 2.123876 |
| 33 | 1 | 4.972631 | -0.785762 | -1.068284 |
| 34 | 1 | 5.744677 | -0.190334 | 0.413638 |
| 35 | 1 | 5.546005 | 0.889751 | -0.985064 |
| 36 | 1 | 2.100230 | 1.273059 | -0.707860 |



Rotational constants (MHZ):
994.3639047 279.3250565 263.8725244

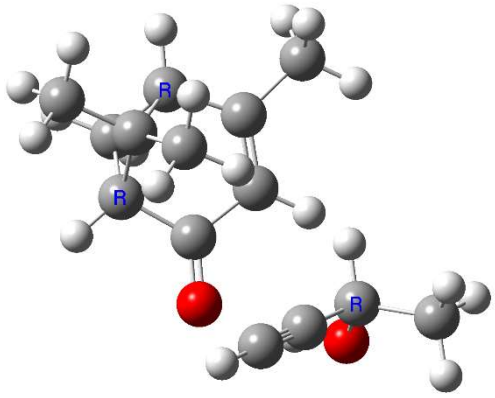
Dipole moment (Debye):
-4.3517532 -2.6491482 1.0088218 Tot= 5.1935983

Species: HOMEC1D2

E = -696.2075383 H

Principal axis orientation:

| Center Number | Atomic Number | Coordinates (Angstroms) a | b | c |
|---|---|---|---|---|
| 1 | 8 | -0.475136 | 0.367612 | -1.914590 |
| 2 | 6 | 2.001263 | 0.921844 | 0.511894 |
| 3 | 6 | 2.576125 | -0.543452 | 0.388712 |
| 4 | 6 | 1.721404 | 0.774586 | -1.033464 |
| 5 | 6 | 2.924815 | -0.205662 | -1.088564 |
| 6 | 6 | 1.449107 | -1.545097 | 0.359187 |
| 7 | 6 | 0.832341 | 1.196327 | 1.446102 |
| 8 | 6 | 3.097139 | 1.945994 | 0.797176 |
| 9 | 6 | 0.453092 | -0.029659 | -1.225450 |
| 10 | 6 | 0.426174 | -1.293234 | -0.475510 |
| 11 | 6 | 1.519777 | -2.732390 | 1.255388 |
| 12 | 1 | 3.376001 | -0.834274 | 1.069875 |
| 13 | 1 | 1.708313 | 1.669035 | -1.653310 |
| 14 | 1 | 3.875312 | 0.306935 | -1.202598 |
| 15 | 1 | 2.865412 | -1.026583 | -1.800470 |
| 16 | 1 | 1.164483 | 1.155365 | 2.486356 |
| 17 | 1 | 0.435742 | 2.196568 | 1.263432 |
| 18 | 1 | 0.009797 | 0.496911 | 1.326474 |
| 19 | 1 | 3.415885 | 1.869898 | 1.839391 |
| 20 | 1 | 3.978353 | 1.825545 | 0.170104 |
| 21 | 1 | 2.712677 | 2.956343 | 0.642656 |
| 22 | 1 | -0.434906 | -1.940405 | -0.579794 |
| 23 | 1 | 1.566034 | -2.411154 | 2.300850 |
| 24 | 1 | 2.433469 | -3.303762 | 1.066753 |
| 25 | 1 | 0.660472 | -3.389392 | 1.129353 |
| 26 | 6 | -2.962827 | -0.331980 | 0.302924 |
| 27 | 6 | -4.217589 | -0.935193 | 0.924023 |
| 28 | 1 | -2.090949 | -0.680360 | 0.877651 |
| 29 | 8 | -2.877324 | -0.799569 | -1.032372 |
| 30 | 6 | -2.972389 | 1.134201 | 0.380878 |
| 31 | 6 | -2.969270 | 2.332412 | 0.446877 |
| 32 | 1 | -2.972110 | 3.393474 | 0.489327 |
| 33 | 1 | -5.098313 | -0.597189 | 0.378688 |
| 34 | 1 | -4.311135 | -0.638507 | 1.968780 |
| 35 | 1 | -4.161575 | -2.022252 | 0.862229 |
| 36 | 1 | -2.115525 | -0.370922 | -1.468815 |




Rotational constants (MHZ):
791.2267841 334.1116894 300.6792071

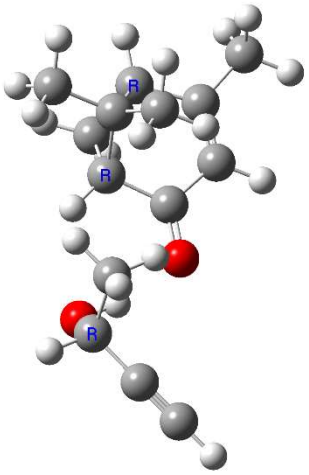
Dipole moment (Debye):
5.1326205 -0.6096326 3.2213596 Tot= 6.0903696

Species: HOMBC2D2

E = -696.2073940 H

Principal axis orientation:

| Center Number | Atomic Number | Coordinates (Angstroms) a | b | c |
|---|---|---|---|---|
| 1 | 8 | -0.673171 | -1.458005 | -0.372081 |
| 2 | 6 | 1.599623 | 1.179496 | 0.276887 |
| 3 | 6 | 2.815533 | 0.364235 | -0.311200 |
| 4 | 6 | 0.758929 | 0.430613 | -0.827074 |
| 5 | 6 | 2.062589 | 0.362256 | -1.671568 |
| 6 | 6 | 2.791792 | -1.050661 | 0.210599 |
| 7 | 6 | 1.221704 | 1.006276 | 1.740877 |
| 8 | 6 | 1.713629 | 2.673610 | -0.016619 |
| 9 | 6 | 0.451543 | -0.977283 | -0.355684 |
| 10 | 6 | 1.621345 | -1.708120 | 0.146705 |
| 11 | 6 | 4.043630 | -1.626912 | 0.775300 |
| 12 | 1 | 3.806654 | 0.814686 | -0.252056 |
| 13 | 1 | -0.128922 | 0.914016 | -1.227276 |
| 14 | 1 | 2.223408 | 1.261094 | -2.259025 |
| 15 | 1 | 2.202566 | -0.514065 | -2.301176 |
| 16 | 1 | 1.980866 | 1.462695 | 2.381016 |
| 17 | 1 | 0.275365 | 1.511068 | 1.942215 |
| 18 | 1 | 1.113333 | -0.034246 | 2.036946 |
| 19 | 1 | 2.463791 | 3.126564 | 0.635973 |
| 20 | 1 | 1.991234 | 2.892472 | -1.045766 |
| 21 | 1 | 0.760101 | 3.166768 | 0.182905 |
| 22 | 1 | 1.486698 | -2.724875 | 0.491860 |
| 23 | 1 | 4.381231 | -1.027956 | 1.627091 |
| 24 | 1 | 4.849659 | -1.594697 | 0.036241 |
| 25 | 1 | 3.907536 | -2.656292 | 1.103953 |
| 26 | 6 | -3.504591 | 0.673666 | -0.166232 |
| 27 | 6 | -2.733330 | 1.197564 | 1.049033 |
| 28 | 1 | -4.145657 | 1.474350 | -0.546114 |
| 29 | 8 | -2.639899 | 0.348496 | -1.241484 |
| 30 | 6 | -4.366935 | -0.455028 | 0.208338 |
| 31 | 6 | -5.053484 | -1.385135 | 0.530290 |
| 32 | 1 | -5.659041 | -2.213960 | 0.802488 |
| 33 | 1 | -2.087938 | 0.414949 | 1.448918 |
| 34 | 1 | -3.417381 | 1.516766 | 1.836646 |
| 35 | 1 | -2.118958 | 2.046104 | 0.745124 |
| 36 | 1 | -2.048605 | -0.377868 | -0.959231 |



Rotational constants (MHZ):
940.3243769 280.6439125 253.7784984

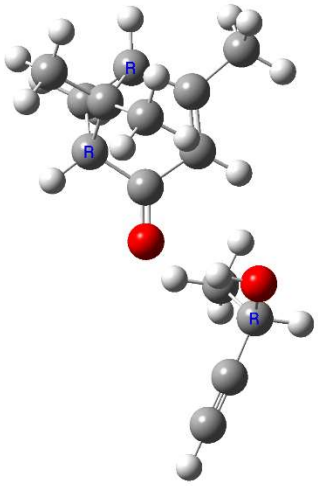
Dipole moment (Debye):
5.6468519 1.2487348 1.7525350 Tot= 6.0429838

Species: HOMEC2D2

E = -696.2068612 H

Principal axis orientation:

| Center Number | Atomic Number | Coordinates (Angstroms) a | b | c |
|---|---|---|---|---|
| 1 | 8 | -0.715705 | 1.129065 | 0.060362 |
| 2 | 6 | 2.795725 | 0.794895 | 0.249853 |
| 3 | 6 | 2.774486 | -0.597779 | -0.492592 |
| 4 | 6 | 1.568828 | 1.134020 | -0.678923 |
| 5 | 6 | 2.170880 | 0.146230 | -1.717174 |
| 6 | 6 | 1.686321 | -1.473670 | 0.075071 |
| 7 | 6 | 2.609083 | 0.847639 | 1.759419 |
| 8 | 6 | 4.030754 | 1.617029 | -0.111674 |
| 9 | 6 | 0.316975 | 0.495631 | -0.112297 |
| 10 | 6 | 0.467863 | -0.925666 | 0.224375 |
| 11 | 6 | 2.018166 | -2.876746 | 0.448426 |
| 12 | 1 | 3.720949 | -1.126579 | -0.606371 |
| 13 | 1 | 1.382587 | 2.171656 | -0.949771 |
| 14 | 1 | 2.916803 | 0.614288 | -2.352459 |
| 15 | 1 | 1.471193 | -0.418180 | -2.330408 |
| 16 | 1 | 3.500694 | 0.466333 | 2.263312 |
| 17 | 1 | 2.469370 | 1.882672 | 2.078698 |
| 18 | 1 | 1.753539 | 0.274850 | 2.108866 |
| 19 | 1 | 4.909136 | 1.213027 | 0.397058 |
| 20 | 1 | 4.243357 | 1.634586 | -1.178813 |
| 21 | 1 | 3.902946 | 2.649393 | 0.220484 |
| 22 | 1 | -0.385287 | -1.458437 | 0.623256 |
| 23 | 1 | 2.802087 | -2.887721 | 1.212382 |
| 24 | 1 | 2.418869 | -3.419293 | -0.413161 |
| 25 | 1 | 1.150187 | -3.412003 | 0.830325 |
| 26 | 6 | -3.799716 | -0.666818 | 0.108365 |
| 27 | 6 | -3.306774 | -0.976179 | -1.308064 |
| 28 | 1 | -4.413362 | -1.502069 | 0.457866 |
| 29 | 8 | -2.728839 | -0.580065 | 1.034761 |
| 30 | 6 | -4.635337 | 0.541515 | 0.122049 |
| 31 | 6 | -5.305093 | 1.537312 | 0.118319 |
| 32 | 1 | -5.893300 | 2.421419 | 0.127093 |
| 33 | 1 | -2.687739 | -0.157386 | -1.676429 |
| 34 | 1 | -4.147066 | -1.108723 | -1.991041 |
| 35 | 1 | -2.712437 | -1.890513 | -1.291832 |
| 36 | 1 | -2.124983 | 0.133198 | 0.746218 |



Rotational constants (MHZ):
985.7115923 247.8701446 227.1354582

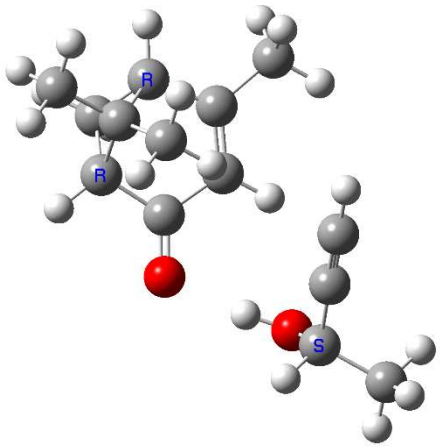
Dipole moment (Debye):
5.3494585 -1.5676351 -1.7046530 Tot= 5.8292391

Species: HETEC1D1

E = -696.20981700

Principal axis orientation:

| Center Number | Atomic Number | Coordinates (Angstroms) a | b | c |
|---|---|---|---|---|
| 1 | 8 | 0.491394 | 1.844407 | 0.353210 |
| 2 | 6 | -2.381899 | 0.184333 | -0.843558 |
| 3 | 6 | -2.576583 | -0.609938 | 0.506064 |
| 4 | 6 | -1.838786 | 1.331148 | 0.091003 |
| 5 | 6 | -2.762234 | 0.765780 | 1.205964 |
| 6 | 6 | -1.256672 | -1.171017 | 0.972433 |
| 7 | 6 | -1.465563 | -0.377804 | -1.920772 |
| 8 | 6 | -3.715622 | 0.555847 | -1.487700 |
| 9 | 6 | -0.408030 | 1.023121 | 0.481532 |
| 10 | 6 | -0.203243 | -0.336872 | 0.990628 |
| 11 | 6 | -1.183503 | -2.606635 | 1.361402 |
| 12 | 1 | -3.382535 | -1.342656 | 0.552106 |
| 13 | 1 | -1.935749 | 2.365975 | -0.232298 |
| 14 | 1 | -3.775166 | 1.152487 | 1.144423 |
| 15 | 1 | -2.405221 | 0.839634 | 2.231174 |
| 16 | 1 | -1.919839 | -1.262043 | -2.375294 |
| 17 | 1 | -1.326692 | 0.362470 | -2.711690 |
| 18 | 1 | -0.480868 | -0.652013 | -1.551298 |
| 19 | 1 | -4.157992 | -0.323226 | -1.962359 |
| 20 | 1 | -4.442633 | 0.954208 | -0.782444 |
| 21 | 1 | -3.559179 | 1.306466 | -2.265328 |
| 22 | 1 | 0.789973 | -0.636798 | 1.294373 |
| 23 | 1 | -1.469894 | -3.239894 | 0.515454 |
| 24 | 1 | -1.893059 | -2.825792 | 2.164989 |
| 25 | 1 | -0.183091 | -2.888518 | 1.685942 |
| 26 | 6 | 3.589822 | 0.428116 | -0.287548 |
| 27 | 6 | 5.026873 | 0.003428 | -0.005977 |
| 28 | 1 | 3.603777 | 1.285883 | -0.973247 |
| 29 | 8 | 2.999546 | 0.803465 | 0.944574 |
| 30 | 6 | 2.840178 | -0.651710 | -0.950643 |
| 31 | 6 | 2.233680 | -1.539486 | -1.485218 |
| 32 | 1 | 1.700451 | -2.325593 | -1.959538 |
| 33 | 1 | 5.033503 | -0.842851 | 0.681147 |
| 34 | 1 | 5.532491 | -0.286137 | -0.927300 |
| 35 | 1 | 5.561849 | 0.834100 | 0.454024 |
| 36 | 1 | 2.142970 | 1.241223 | 0.761214 |




Rotational constants (MHZ):
912.0501881 292.3047201 283.7846838

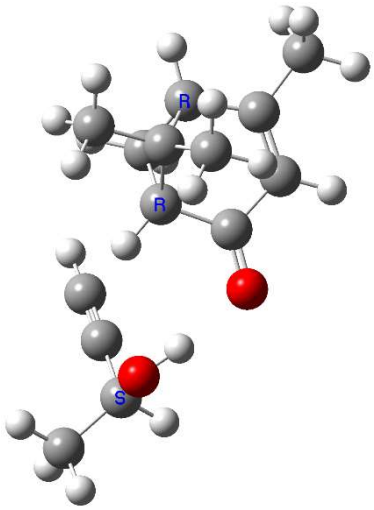
Dipole moment (Debye):
-4.4974074 -2.4397263 -0.8796834 Tot= 5.1916067

Species: HETBC1D1

E = -696.2097061 H

Principal axis orientation:

| Center Number | Atomic Number | Coordinates (Angstroms) a | b | c |
|---|---|---|---|---|
| 1 | 8 | -0.494091 | -1.117686 | 1.464483 |
| 2 | 6 | 1.684671 | 1.317099 | 0.101128 |
| 3 | 6 | 2.340877 | 0.274465 | -0.885331 |
| 4 | 6 | 0.369587 | 0.477267 | -0.126560 |
| 5 | 6 | 0.933415 | 0.105597 | -1.525470 |
| 6 | 6 | 2.649028 | -1.007269 | -0.153935 |
| 7 | 6 | 2.227394 | 1.461859 | 1.515242 |
| 8 | 6 | 1.580556 | 2.707842 | -0.520175 |
| 9 | 6 | 0.419167 | -0.772633 | 0.725782 |
| 10 | 6 | 1.672723 | -1.526752 | 0.610278 |
| 11 | 6 | 4.002103 | -1.611609 | -0.302430 |
| 12 | 1 | 3.171928 | 0.612408 | -1.504919 |
| 13 | 1 | -0.592578 | 0.975290 | -0.046091 |
| 14 | 1 | 0.701485 | 0.855410 | -2.275664 |
| 15 | 1 | 0.690970 | -0.882625 | -1.909369 |
| 16 | 1 | 3.202064 | 1.955901 | 1.497872 |
| 17 | 1 | 1.553277 | 2.085206 | 2.106486 |
| 18 | 1 | 2.339351 | 0.511749 | 2.032182 |
| 19 | 1 | 2.563421 | 3.185043 | -0.534936 |
| 20 | 1 | 1.198085 | 2.699419 | -1.538879 |
| 21 | 1 | 0.916614 | 3.334339 | 0.078817 |
| 22 | 1 | 1.781891 | -2.440260 | 1.180081 |
| 23 | 1 | 4.767174 | -0.910559 | 0.045968 |
| 24 | 1 | 4.221381 | -1.809804 | -1.355799 |
| 25 | 1 | 4.097934 | -2.540418 | 0.258247 |
| 26 | 6 | -3.636426 | -0.336189 | 0.270194 |
| 27 | 6 | -4.955232 | 0.417663 | 0.139934 |
| 28 | 1 | -3.843009 | -1.343057 | 0.657614 |
| 29 | 8 | -2.820529 | 0.375369 | 1.184411 |
| 30 | 6 | -2.987027 | -0.497504 | -1.041136 |
| 31 | 6 | -2.464181 | -0.625750 | -2.114368 |
| 32 | 1 | -2.004511 | -0.739711 | -3.064579 |
| 33 | 1 | -4.769889 | 1.422641 | -0.239485 |
| 34 | 1 | -5.630167 | -0.098701 | -0.542777 |
| 35 | 1 | -5.422768 | 0.492796 | 1.121593 |
| 36 | 1 | -2.019662 | -0.157210 | 1.367800 |




Rotational constants (MHZ):
905.4867080 291.8294272 281.2872239

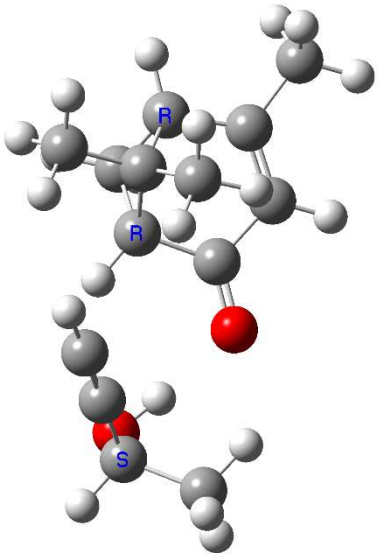
Dipole moment (Debye):
4.6132424 0.1079323 -2.4503227 Tot= 5.2247236

Species: HETBC2D1

E = -696.2097133 H

Principal axis orientation:

| Center Number | Atomic Number | Coordinates (Angstroms) a | b | c |
|---|---|---|---|---|
| 1 | 8 | -0.536491 | -1.841885 | -0.009707 |
| 2 | 6 | 1.232409 | 1.218028 | 0.057825 |
| 3 | 6 | 2.565918 | 0.539955 | -0.448974 |
| 4 | 6 | 0.520718 | 0.152003 | -0.860660 |
| 5 | 6 | 1.796846 | 0.168980 | -1.748133 |
| 6 | 6 | 2.810956 | -0.743884 | 0.301671 |
| 7 | 6 | 0.916988 | 1.233988 | 1.546379 |
| 8 | 6 | 1.059576 | 2.633242 | -0.487550 |
| 9 | 6 | 0.484802 | -1.179150 | -0.140155 |
| 10 | 6 | 1.777685 | -1.596501 | 0.412871 |
| 11 | 6 | 4.159469 | -0.986219 | 0.884975 |
| 12 | 1 | 3.459620 | 1.160643 | -0.518363 |
| 13 | 1 | -0.448056 | 0.397006 | -1.288765 |
| 14 | 1 | 1.777761 | 0.967055 | -2.484037 |
| 15 | 1 | 2.081542 | -0.764068 | -2.230353 |
| 16 | 1 | 1.549176 | 1.964380 | 2.057443 |
| 17 | 1 | -0.123357 | 1.525185 | 1.696812 |
| 18 | 1 | 1.061897 | 0.269097 | 2.026520 |
| 19 | 1 | 1.715033 | 3.323332 | 0.049053 |
| 20 | 1 | 1.282308 | 2.719581 | -1.549311 |
| 21 | 1 | 0.030012 | 2.962326 | -0.337805 |
| 22 | 1 | 1.837844 | -2.544484 | 0.931302 |
| 23 | 1 | 4.403313 | -0.198892 | 1.605306 |
| 24 | 1 | 4.927758 | -0.942003 | 0.107339 |
| 25 | 1 | 4.221037 | -1.950847 | 1.386936 |
| 26 | 6 | -3.659627 | -0.254919 | -0.214343 |
| 27 | 6 | -3.928823 | -1.229438 | 0.934271 |
| 28 | 1 | -4.607008 | -0.024760 | -0.710930 |
| 29 | 8 | -2.838442 | -0.825940 | -1.215959 |
| 30 | 6 | -3.116364 | 1.018063 | 0.290363 |
| 31 | 6 | -2.693749 | 2.059796 | 0.712733 |
| 32 | 1 | -2.333954 | 2.987493 | 1.083027 |
| 33 | 1 | -2.995259 | -1.484931 | 1.436955 |
| 34 | 1 | -4.609801 | -0.790759 | 1.664942 |
| 35 | 1 | -4.372107 | -2.141163 | 0.533338 |
| 36 | 1 | -2.050895 | -1.218541 | -0.786809 |




Rotational constants (MHZ):
876.6152824 328.7519000 286.2211556

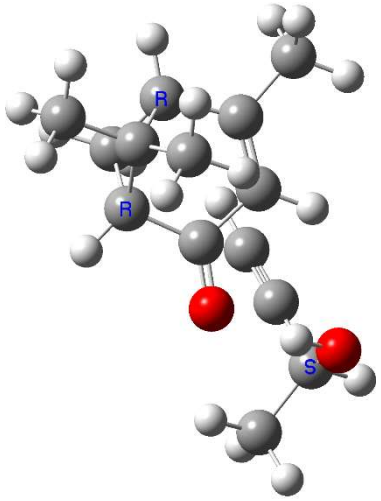
Dipole moment (Debye):
4.8232488 1.8380192 1.3295888 Tot= 5.3300891

Species: HETEC2D1

E = -696.2092252 H

Principal axis orientation:

| Center Number | Atomic Number | Coordinates (Angstroms) a | b | c |
|---|---|---|---|---|
| 1 | 8 | 0.742670 | 1.490991 | -0.430505 |
| 2 | 6 | -2.666818 | 0.655988 | 0.001752 |
| 3 | 6 | -2.315659 | -0.803527 | 0.485905 |
| 4 | 6 | -1.319508 | 1.050561 | 0.715891 |
| 5 | 6 | -1.554742 | -0.150267 | 1.674790 |
| 6 | 6 | -1.274635 | -1.419231 | -0.415724 |
| 7 | 6 | -2.819971 | 0.939540 | -1.485408 |
| 8 | 6 | -3.884092 | 1.223570 | 0.728594 |
| 9 | 6 | -0.148892 | 0.691630 | -0.175761 |
| 10 | 6 | -0.194568 | -0.675088 | -0.706336 |
| 11 | 6 | -1.494380 | -2.800989 | -0.925681 |
| 12 | 1 | -3.143320 | -1.482032 | 0.693453 |
| 13 | 1 | -1.206726 | 2.057881 | 1.112633 |
| 14 | 1 | -2.193791 | 0.104349 | 2.515116 |
| 15 | 1 | -0.670955 | -0.674947 | 2.031062 |
| 16 | 1 | -3.748521 | 0.500898 | -1.858998 |
| 17 | 1 | -2.875026 | 2.017377 | -1.652976 |
| 18 | 1 | -1.999287 | 0.551586 | -2.083586 |
| 19 | 1 | -4.796215 | 0.756090 | 0.350188 |
| 20 | 1 | -3.855256 | 1.073010 | 1.806093 |
| 21 | 1 | -3.962447 | 2.297073 | 0.543949 |
| 22 | 1 | 0.624404 | -1.023063 | -1.320709 |
| 23 | 1 | -2.414144 | -2.844117 | -1.517716 |
| 24 | 1 | -1.629207 | -3.499609 | -0.094252 |
| 25 | 1 | -0.664317 | -3.143552 | -1.541559 |
| 26 | 6 | 3.785396 | 0.018406 | -0.227367 |
| 27 | 6 | 4.218712 | 1.334006 | 0.423336 |
| 28 | 1 | 4.676587 | -0.528302 | -0.548550 |
| 29 | 8 | 3.032997 | 0.235033 | -1.409552 |
| 30 | 6 | 3.065780 | -0.832494 | 0.734025 |
| 31 | 6 | 2.469405 | -1.513415 | 1.522728 |
| 32 | 1 | 1.947563 | -2.125883 | 2.215297 |
| 33 | 1 | 3.342593 | 1.899238 | 0.743172 |
| 34 | 1 | 4.850803 | 1.148263 | 1.293090 |
| 35 | 1 | 4.774563 | 1.925972 | -0.304012 |
| 36 | 1 | 2.242643 | 0.759673 | -1.168569 |




Rotational constants (MHZ):
918.1223955 305.5393775 282.5830183

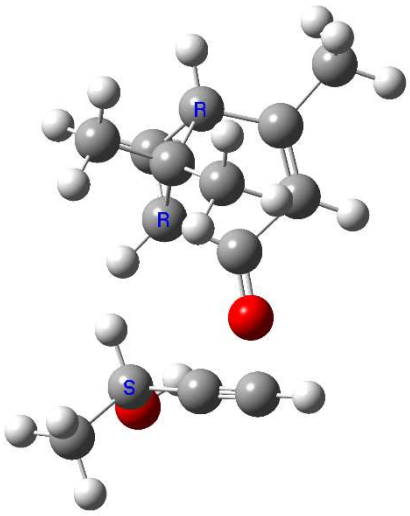
Dipole moment (Debye):
-4.5908709 -1.8023876 1.8179615 Tot= 5.2563943

Species: HETBC1D2

E = -696.2080071 H

Principal axis orientation:

| Center Number | Atomic Number | Coordinates (Angstroms) a | b | c |
|---|---|---|---|---|
| 1 | 8 | -0.330232 | -1.716799 | -1.026642 |
| 2 | 6 | 1.067352 | 1.168517 | 0.442955 |
| 3 | 6 | 2.519006 | 0.822368 | -0.073819 |
| 4 | 6 | 0.597206 | 0.505770 | -0.908750 |
| 5 | 6 | 1.956770 | 0.945392 | -1.517696 |
| 6 | 6 | 2.821523 | -0.636918 | 0.157940 |
| 7 | 6 | 0.582794 | 0.580878 | 1.760076 |
| 8 | 6 | 0.808014 | 2.672887 | 0.461071 |
| 9 | 6 | 0.624666 | -1.002668 | -0.757886 |
| 10 | 6 | 1.888625 | -1.525137 | -0.225535 |
| 11 | 6 | 4.112188 | -1.007054 | 0.802118 |
| 12 | 1 | 3.337030 | 1.473115 | 0.235732 |
| 13 | 1 | -0.333036 | 0.835844 | -1.366037 |
| 14 | 1 | 1.934139 | 1.965437 | -1.889497 |
| 15 | 1 | 2.399888 | 0.293928 | -2.268186 |
| 16 | 1 | 1.101792 | 1.057542 | 2.595516 |
| 17 | 1 | -0.485420 | 0.764385 | 1.885283 |
| 18 | 1 | 0.736917 | -0.492500 | 1.833260 |
| 19 | 1 | 1.344402 | 3.133121 | 1.294207 |
| 20 | 1 | 1.114242 | 3.178125 | -0.452843 |
| 21 | 1 | -0.256522 | 2.866043 | 0.609036 |
| 22 | 1 | 1.995905 | -2.595039 | -0.104466 |
| 23 | 1 | 4.176820 | -0.559911 | 1.799191 |
| 24 | 1 | 4.955241 | -0.608944 | 0.229605 |
| 25 | 1 | 4.227859 | -2.086036 | 0.895067 |
| 26 | 6 | -3.015648 | 0.301344 | -0.143203 |
| 27 | 6 | -4.368002 | 0.995467 | -0.260300 |
| 28 | 1 | -2.248555 | 1.072716 | 0.029253 |
| 29 | 8 | -2.765820 | -0.363090 | -1.368109 |
| 30 | 6 | -2.972370 | -0.610053 | 1.007032 |
| 31 | 6 | -2.921369 | -1.350592 | 1.949985 |
| 32 | 1 | -2.879665 | -2.018746 | 2.774345 |
| 33 | 1 | -5.150522 | 0.253949 | -0.418557 |
| 34 | 1 | -4.591322 | 1.560878 | 0.644608 |
| 35 | 1 | -4.348840 | 1.674037 | -1.113340 |
| 36 | 1 | -1.958003 | -0.907688 | -1.282599 |




Rotational constants (MHZ):
875.5976020 318.5905253 301.2785076

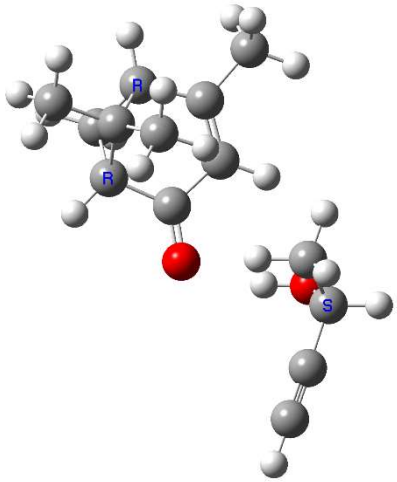
Dipole moment (Debye):
5.2417076 2.4668537 2.1995135 Tot= 6.1966705

Species: HETEC2D2

E = -696.2072347 H

Principal axis orientation:

| Center Number | Atomic Number | Coordinates (Angstroms) a | b | c |
|---|---|---|---|---|
| 1 | 8 | -0.729825 | 0.713942 | -1.243159 |
| 2 | 6 | 2.295860 | 0.936916 | 0.552097 |
| 3 | 6 | 2.850479 | -0.407076 | -0.063701 |
| 4 | 6 | 1.605442 | 1.113753 | -0.853780 |
| 5 | 6 | 2.772621 | 0.282384 | -1.454967 |
| 6 | 6 | 1.782084 | -1.470856 | -0.035330 |
| 7 | 6 | 1.422264 | 0.888575 | 1.797279 |
| 8 | 6 | 3.402290 | 1.964897 | 0.777145 |
| 9 | 6 | 0.355213 | 0.259567 | -0.906779 |
| 10 | 6 | 0.562652 | -1.132970 | -0.489034 |
| 11 | 6 | 2.125167 | -2.816184 | 0.503711 |
| 12 | 1 | 3.813142 | -0.771467 | 0.295362 |
| 13 | 1 | 1.400266 | 2.118735 | -1.217966 |
| 14 | 1 | 3.641420 | 0.890962 | -1.687053 |
| 15 | 1 | 2.540182 | -0.360220 | -2.301710 |
| 16 | 1 | 2.028250 | 0.647069 | 2.673902 |
| 17 | 1 | 0.969383 | 1.867231 | 1.970471 |
| 18 | 1 | 0.620116 | 0.158431 | 1.730145 |
| 19 | 1 | 4.001770 | 1.684304 | 1.646441 |
| 20 | 1 | 4.075369 | 2.069313 | -0.071430 |
| 21 | 1 | 2.965805 | 2.945204 | 0.979790 |
| 22 | 1 | -0.279767 | -1.811552 | -0.506189 |
| 23 | 1 | 2.453441 | -2.732153 | 1.544743 |
| 24 | 1 | 2.963084 | -3.250292 | -0.049988 |
| 25 | 1 | 1.279787 | -3.501096 | 0.457502 |
| 26 | 6 | -3.524915 | -0.649496 | 0.430601 |
| 27 | 6 | -2.633052 | -0.278281 | 1.619521 |
| 28 | 1 | -4.171103 | -1.481977 | 0.723381 |
| 29 | 8 | -2.771296 | -1.134263 | -0.668790 |
| 30 | 6 | -4.386780 | 0.478086 | 0.051366 |
| 31 | 6 | -5.072593 | 1.414469 | -0.253543 |
| 32 | 1 | -5.678886 | 2.238879 | -0.537243 |
| 33 | 1 | -1.983498 | 0.556328 | 1.354674 |
| 34 | 1 | -3.236043 | 0.014156 | 2.480361 |
| 35 | 1 | -2.017450 | -1.136835 | 1.890643 |
| 36 | 1 | -2.169318 | -0.425211 | -0.970824 |




Rotational constants (MHZ):
899.6033428 275.8885747 256.0607364

Dipole moment (Debye):
5.5953517 -0.3086484 2.2102498 Tot= 6.0239878

Species: HETEC1D2

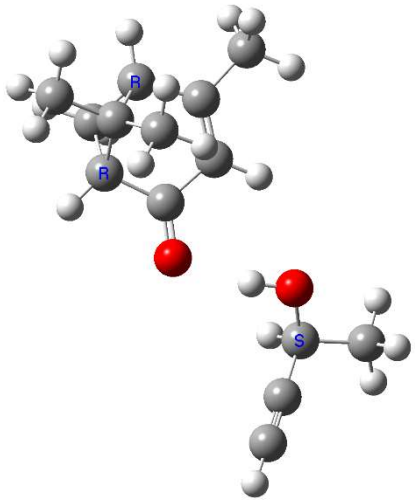
E = -696.2066922 H

Principal axis orientation:

| Center Number | Atomic Number | Coordinates (Angstroms) a | b | c |
|---|---|---|---|---|
| 1 | 8 | 0.588000 | 1.072542 | 0.347038 |
| 2 | 6 | -2.844471 | 0.759730 | -0.400559 |
| 3 | 6 | -2.966525 | -0.609407 | 0.375056 |
| 4 | 6 | -1.784066 | 1.115889 | 0.709608 |
| 5 | 6 | -2.562398 | 0.165534 | 1.661077 |
| 6 | 6 | -1.811063 | -1.512102 | 0.020003 |
| 7 | 6 | -2.409766 | 0.761410 | -1.858765 |
| 8 | 6 | -4.108919 | 1.606569 | -0.273579 |
| 9 | 6 | -0.465353 | 0.450449 | 0.374416 |
| 10 | 6 | -0.577102 | -0.979947 | 0.061175 |
| 11 | 6 | -2.096526 | -2.920645 | -0.370329 |
| 12 | 1 | -3.925823 | -1.126336 | 0.345703 |
| 13 | 1 | -1.631193 | 2.159715 | 0.977472 |
| 14 | 1 | -3.396858 | 0.657199 | 2.152421 |
| 15 | 1 | -1.980550 | -0.386722 | 2.396265 |
| 16 | 1 | -3.214257 | 0.379140 | -2.491885 |
| 17 | 1 | -2.195941 | 1.782989 | -2.180209 |
| 18 | 1 | -1.521635 | 0.162266 | -2.042954 |
| 19 | 1 | -4.899362 | 1.192888 | -0.904251 |
| 20 | 1 | -4.491712 | 1.666228 | 0.743464 |
| 21 | 1 | -3.912329 | 2.624603 | -0.616549 |
| 22 | 1 | 0.322866 | -1.532287 | -0.176401 |
| 23 | 1 | -2.740347 | -2.941848 | -1.255506 |
| 24 | 1 | -2.645267 | -3.436884 | 0.423113 |
| 25 | 1 | -1.185103 | -3.475338 | -0.588282 |
| 26 | 6 | 3.874238 | -0.387225 | 0.303133 |
| 27 | 6 | 4.815502 | -1.544721 | -0.009724 |
| 28 | 1 | 3.644033 | -0.401830 | 1.377754 |
| 29 | 8 | 2.685787 | -0.584421 | -0.446447 |
| 30 | 6 | 4.500238 | 0.908451 | 0.006333 |
| 31 | 6 | 5.010093 | 1.968081 | -0.233682 |
| 32 | 1 | 5.451879 | 2.908872 | -0.451431 |
| 33 | 1 | 5.051001 | -1.550602 | -1.073940 |
| 34 | 1 | 5.742287 | -1.452000 | 0.556469 |
| 35 | 1 | 4.329032 | -2.485562 | 0.249017 |
| 36 | 1 | 2.036087 | 0.103578 | -0.198597 |

Rotational constants (MHZ):
963.4403124 230.0507018 205.2872003

Dipole moment (Debye):
-5.3004786 -1.4619615 0.8236439 Tot= 5.5597477

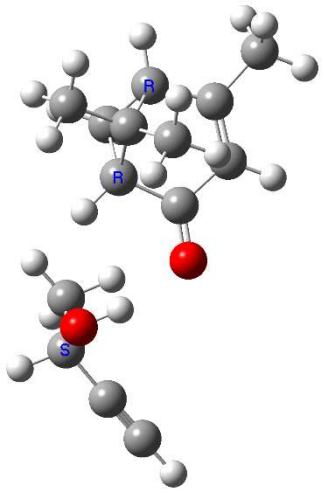


Species: HETBC2D2

E = -696.2069228 H

Principal axis orientation:

| Center Number | Atomic Number | Coordinates (Angstroms) a | b | c |
|---|---|---|---|---|
| 1 | 8 | -0.756681 | -0.906322 | 0.961756 |
| 2 | 6 | 2.087292 | 1.117162 | 0.346669 |
| 3 | 6 | 2.627442 | 0.129836 | -0.760097 |
| 4 | 6 | 0.665565 | 0.680464 | -0.171439 |
| 5 | 6 | 1.325629 | 0.427553 | -1.556807 |
| 6 | 6 | 2.535674 | -1.293838 | -0.272818 |
| 7 | 6 | 2.442769 | 0.881498 | 1.807594 |
| 8 | 6 | 2.390310 | 2.575398 | 0.009350 |
| 9 | 6 | 0.310758 | -0.673893 | 0.411432 |
| 10 | 6 | 1.369968 | -1.680347 | 0.273352 |
| 11 | 6 | 3.729148 | -2.174749 | -0.404826 |
| 12 | 1 | 3.592361 | 0.354015 | -1.215303 |
| 13 | 1 | -0.164770 | 1.376646 | -0.080879 |
| 14 | 1 | 1.381284 | 1.328285 | -2.160573 |
| 15 | 1 | 0.927138 | -0.388639 | -2.156021 |
| 16 | 1 | 3.493155 | 1.125915 | 1.983979 |
| 17 | 1 | 1.841798 | 1.535765 | 2.442705 |
| 18 | 1 | 2.275464 | -0.142041 | 2.133898 |
| 19 | 1 | 3.446803 | 2.787608 | 0.189426 |
| 20 | 1 | 2.170085 | 2.836423 | -1.023916 |
| 21 | 1 | 1.805223 | 3.236329 | 0.651941 |
| 22 | 1 | 1.190645 | -2.675968 | 0.657599 |
| 23 | 1 | 4.571422 | -1.751165 | 0.151466 |
| 24 | 1 | 4.048590 | -2.236127 | -1.449370 |
| 25 | 1 | 3.537131 | -3.181044 | -0.035090 |
| 26 | 6 | -3.578318 | 0.684679 | -0.397169 |
| 27 | 6 | -2.900841 | 0.189065 | -1.678958 |
| 28 | 1 | -4.187931 | 1.559840 | -0.639623 |
| 29 | 8 | -2.636889 | 1.142440 | 0.559793 |
| 30 | 6 | -4.467916 | -0.344866 | 0.156455 |
| 31 | 6 | -5.178161 | -1.202734 | 0.603339 |
| 32 | 1 | -5.803262 | -1.957760 | 1.011902 |
| 33 | 1 | -2.294453 | -0.692127 | -1.467201 |
| 34 | 1 | -3.644220 | -0.077881 | -2.431493 |
| 35 | 1 | -2.259480 | 0.976970 | -2.075856 |
| 36 | 1 | -2.067423 | 0.391057 | 0.819166 |




Rotational constants (MHZ):
933.0884672 268.6752061 246.7262339

Dipole moment (Debye):
5.5482610 -0.5010284 -2.3392286 Tot= 6.0420377