# **Supporting Information for:**

# Atropisomerisation in sterically hindered α,β-disubstituted cyclopentenones derived from an intermolecular cobalt(0)-mediated Pauson-Khand reaction<sup>†</sup>

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#### 1.0 X-ray diffraction data and information

**1.1 General details:** Diffraction data were collected at 110 K (unless otherwise specified in the data below) on a Bruker Smart Apex diffractometer with Mo-K<sub> $\alpha$ </sub> radiation ( $\lambda = 0.71073$  Å) using a SMART CCD camera. Diffractometer control, data collection and initial unit cell determination was performed using "SMART".<sup>1</sup> Frame integration and unit-cell refinement was carried out with "SAINT+".<sup>2</sup> Absorption corrections were applied by SADABS.<sup>c</sup> Structures were solved using SHELXS-97 (Sheldrick, 1997),<sup>1</sup> as indicated in the cif files, and refined by full-matrix least squares using SHELXL-97 (Sheldrick, 1997).<sup>2</sup> All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed using a "riding model" and included in the refinement at calculated positions.

The CCDC reference numbers for compounds 6 and  $7\beta$  are 780325 and 780326, respectively.

#### **1.1.1 References**

- "SMART" control software Bruker SMART Apex X-ray Diffractometer.
  v5.625, Bruker-AXS GMBH, Karlsruhe, Germany.
- 2 "SAINT+" integration software for Bruker SMART detectors. v6.45,
  Bruker-AXS GMBH, Karlsruhe, Germany.
- 3 "SADABS" program for absorption correction. v2.10. G. M. Sheldrick, Bruker AXS Inc., Madison, Wisconsin, USA, 2007.
- 4 "SHELXS-97" program for structure solution. G. M. Sheldrick, University of Göttingen, Göttingen, Germany, 1997.
- 5 "SHELXL-97" program for the Refinement of Crystal Structures. G. M. Sheldrick, University of Göttingen, Göttingen, Germany, 1997.

Supplementary Material (ESI) for Organic and Biomolecular Chemistry This journal is The Royal Society of Chemistry 2010

### 1.2 X-ray structures of 6 and $7\beta$



**Figure S1**. X-ray crystal structure of **6** (determined at 110 K). Thermal ellipsoids are shown at 50% probability.



**Figure S2**. X-ray crystal structure of the major regioisomeric product  $7\beta$  (determined at 298 K). Thermal ellipsoids are shown at 30% probability.

# Table S1 Key X-ray -data for 6 and 7β.

Compound reference	ijf0629m	ijf0810a
Chemical formula	$C_{23}H_{10}Co_2O_8$	$C_{25}H_{20}O_3$
Formula Mass	532.17	368.41
Crystal system	Triclinic	Monoclinic
<i>a</i> /Å	8.6456(6)	13.6217(8)
<i>b</i> /Å	8.9910(6)	12.1491(7)
c/Å	14.7003(10)	12.2859(7)
$\alpha/^{\circ}$	80.2050(10)	90.00
$\beta/^{\circ}$	74.6770(10)	111.6790(10)
$\gamma/^{\circ}$	73.2410(10)	90.00
Unit cell volume/Å <sup>3</sup>	1049.79(12)	1889.40(19)
Temperature/K	110(2)	298(2)
Space group	<i>P</i> 1	<i>P2(1)/c</i>
No. of formula units per unit cell, $Z$	2	4
No. of reflections measured	10916	19047
No. of independent reflections	5160	4702
R <sub>int</sub>	0.0226	0.0258
Final $R_1$ values $(I > 2\sigma(I))$	0.0290	0.0464
Final $wR(F^2)$ values $(I > 2\sigma(I))$	0.0709	0.1106
Final $R_1$ values (all data)	0.0346	0.0692
Final $wR(F^2)$ values (all data)	0.0737	0.1213
Final $wR(F^2)$ values (all data)	0.0737	0.1213

# 2.0 Cartesian coordinates of the optimized geometries

### 2.1 Raw data

$ \begin{array}{c} \mathbf{E} & -1190, 0622892 \ a. u. \\ \mathbf{C} & 0. 1367300 \\ \mathbf{C} & -1. 36677500 \\ -1. 36767700 \\ 4. 30371700 \\ -1. 18535200 \\ \mathbf{C} & -1. 36677500 \\ -1. 36767700 \\ 4. 30371700 \\ -1. 18535200 \\ \mathbf{C} & 0. 172720 \\ 3. 50720200 \\ -1. 6757700 \\ -1. 18532200 \\ -1. 0004800 \\ -1. 512200 \\ -1. 50010500 \\ 0. 22831100 \\ \mathbf{C} & -0. 11622300 \\ 2. 25170300 \\ -0. 11623500 \\ 2. 25160000 \\ 1. 18529700 \\ 0. 0. 73058000 \\ \mathbf{C} & 2. 55160000 \\ 1. 18529700 \\ 0. 0. 73058000 \\ \mathbf{C} & 2. 55160000 \\ 1. 18529700 \\ 0. 0. 7143500 \\ \mathbf{C} & 2. 55160000 \\ 1. 18529700 \\ 0. 0. 4735300 \\ 0. 0. 4735300 \\ 0. 0. 4735300 \\ 0. 0. 4735300 \\ 0. 0. 4735300 \\ 0. 0. 4735300 \\ 0. 0. 4735300 \\ 0. 0. 4735300 \\ 0. 0. 4735300 \\ 0. 0. 4735300 \\ 0. 0. 4735300 \\ 0. 0. 4735300 \\ 0. 0. 4735300 \\ 0. 0. 4735300 \\ 0. 0. 4735300 \\ 0. 0. 4735300 \\ 0. 0. 4735300 \\ 0. 0. 4735300 \\ 0. 0. 47353200 \\ 0. 0. 47353200 \\ 0. 0. 47353200 \\ 0. 0. 47353200 \\ 0. 0. 47353200 \\ 0. 0. 48351100 \\ 0. 0. 0.4885200 \\ 0. 0. 483500 \\ 0. 0. 483500 \\ 0. 0. 483500 \\ 0. 0. 483500 \\ 0. 0. 480500 \\ 0. 0. 480500 \\ 0. 0. 480500 \\ 0. 0. 480500 \\ 0. 0. 480500 \\ 0. 0. 480500 \\ 0. 0. 33012100 \\ 0. 0. 3012100 \\ 0. 0. 3012100 \\ 0. 0. 3012100 \\ 0. 0. 3012100 \\ 0. 0. 3012100 \\ 0. 0. 3012100 \\ 0. 0. 3012100 \\ 0. 0. 3004000 \\ 01. 5676300 \\ 0. 0. 1674300 \\ 0. 0. 4851200 \\ 0. 0. 3301300 \\ 0. 0. 3004000 \\ 01. 806700 \\ 0. 0. 3052200 \\ 0. 1. 8128000 \\ 0. 1. 8128000 \\ 0. 1. 813800 \\ 0. 0. 180400 \\ 0. 2. 2882300 \\ 0. 1. 44003800 \\ 0. 1. 4602300 \\ 0. 1. 450300 \\ 0. 1. 450300 \\ 0. 1. 450300 \\ 0. 1. 450300 \\ 0. 1. 450300 \\ 0. 1. 450300 \\ 0. 1. 4503000 \\ 0. 1. 450300 \\ 0. 1. 4503000 \\ 0. 1. 450300 \\ 0. 1. 4$	7 <b>β</b>	A			С	-1.01653600	4.82514900	-0.81092800
C      -1. 86877300      3.07658800      -1. 85857800      C      0. 07501700      3.67829200      0.18763200        C      -1. 187679700      3.0071700      -1. 18335200      C      0.341100      2.4723300      -0.19435100        C      -0.1237300      -0.370300      -0.3765800      C      0.573700      1.18308900      0.24333500        C      -0.99498300      2.26170300      -0.3765800      C      2.55160000      1.18308900      0.53333600        C      0.80180800      1.18529700      0.07143500      C      0.56331100      -0.0494700      0.4335300        C      2.85450900      0.16529400      0.97327100      C      -0.8865700      -0.38852600      0.14658300      -1.89511700      2.39171700        C      -0.8364500      -0.93345200      -0.3412000      C      -1.86680300      -1.20271800      -0.33194100        C      -1.8972100      -2.41123300      -1.7533400      -0.23749700      -2.3717700      -2.3918400      -2.3717700        C      -2.8925000      -1.67860300      -0.33194100      -2.31022101      -3.3194100	E =	 = -1190.0622892	2 a. 11.		С	0.19648900	4.86154600	-0.11454800
C −1. 87679700 4. 3371700 −1. 18335200 C 0. 34140100 2. 42723500 −0. 99781800 0 0. 9781800 0 0. 15891600 C −0. 12732300 3. 50010500 0. 25834100 C 1. 05735700 1. 18308900 0. 15891600 C −0. 11623500 2. 25170300 −0. 37058000 C 2. 55160000 1. 10673700 0. 2753544700 0. 72353600 C 2. 55160000 1. 18508900 0. 147583900 0. 05519400 C 0. 54513100 −0. 0494870 0. 84943500 C 2. 2545090 0. 16259490 0. 97143500 C 0. 5455100 −0. 0.14628700 1. 473537900 0. 147583900 0. 65319400 C 0. −1.6665300 −0. 01462870 0. 1.89811800 C 0. 6.86749400 −0. 91365200 0. 0.61230200 C −1. 6465300 −1.1628700 1. 62632300 2. 2.3171700 C −0. 8857600 −0. 39852600 0. 63349100 C −0.27544700 0. −2.5316400 0. 0.5552300 2. 2.3171700 C −0.63646500 −0.9348200 −0.24987600 C −2.8210440 −0.5255230 2. 2.3171700 C −0.63646500 −0.9348200 −0.24987600 C −2.8910400 −0.14628700 1. 26631200 C −1. 16658300 −1.62623300 −1.62633500 0. 6329500 C −2.99008600 −1.45340800 −0.04201800 C −2.99008600 −1.45340800 −0.04201800 C −2.99008600 −1.65660900 0. 36228500 C −3.3013400 −2.3676400 −0.27147500 −2.41275400 −2.54925400 0. 33629500 C −3.30685000 −2.09685700 −2.249275400 −2.249275400 −2.24927660 −0.23766400 −0.21213900 1. 91325100 C −3.30685000 −2.09685700 −0.97430000 C −3.39828600 −2.09685700 −2.249282800 −1.64786400 0. 330122100 C −3.39828300 −2.09685700 −2.249252820 −1.04788400 −2.11267690 0. 7343600 −2.78924600 C 1.84126000 −2.0216300 −1.97328100 −2.9149260 C 1.84126000 −2.92882300 −0.3064700 0. 2.9990860 −1.04738000 −2.78924600 C 1.84126000 −2.288282900 −1.68782000 −2.78924600 C 1.84126000 −2.28782900 −1.68787000 0. 738454700 C 2.9903860 −2.9885700 −2.4884500 −3.3101400 −2.38764000 −2.28828200 −1.68784700 1.29748900 −2.41142600 −2.41142600 0. 38019400 C −2.38924600 −2.78924600 C 1.84126000 −2.28828200 −1.68783000 −2.7899860 0.3409200 −2.48454700 1.28747900 −2.41142600 0.3861400 0.3319100 0. 7433200 −2.78998600 -1.87638000 0.77433200 −2.1885900 1.48788900 1.48653000 1.78248900 1.48653000 1.78248900 0.57648900 −1.83838100 0.0.74133200 −2.18852900 1.48433700 −2.3418400 0.78389	Ē	-1 86677500	3 07658800	-1 85857800	С	0.87501700	3.67829200	0.18763200
$ \begin{array}{c} \mbox{C} & -1.00044800 & 4.51067400 & -0.11419200 \\ \mbox{C} & -0.12373200 & 3.5001500 & 0.23834100 \\ \mbox{C} & -0.12373200 & 2.35107300 & -0.37058000 \\ \mbox{C} & -0.99198300 & 2.06197500 & -1.45736700 \\ \mbox{C} & 2.55160000 & 1.11097900 & 0.24030500 \\ \mbox{C} & 0.99198300 & 2.06197500 & -1.45736700 \\ \mbox{C} & 2.55160000 & 1.11097900 & 0.27333600 \\ \mbox{C} & 2.55169000 & 1.47583900 & 0.59519400 \\ \mbox{C} & 2.55169000 & 1.47583900 & 0.59519400 \\ \mbox{C} & 2.5516000 & 1.475839300 & 0.59519400 \\ \mbox{C} & 2.5516000 & 1.475839300 & 0.59519400 \\ \mbox{C} & 2.5516000 & 1.475839300 & 0.59519400 \\ \mbox{C} & 2.5516000 & 1.4529400 & 0.97327100 \\ \mbox{C} & 0.66346500 & -0.93852600 & 0.6331000 \\ \mbox{C} & -0.66346500 & -0.9385260 & 0.6331400 \\ \mbox{C} & -0.3646500 & -0.6623500 & -1.4605300 & -1.26271800 & 1.20271800 \\ \mbox{C} & -0.36346500 & -0.24987600 & 0.35196400 \\ \mbox{C} & -2.861700 & -2.398238200 & -1.80282900 \\ \mbox{C} & -1.98792100 & -2.41120300 & -1.75338300 \\ \mbox{C} & -2.9905600 & -1.45310800 & -1.20271800 & 1.20251800 \\ \mbox{C} & -2.89256000 & -0.21754300 & 2.37613800 \\ \mbox{C} & -2.89256000 & -1.67866000 \\ \mbox{C} & -3.3983500 & -2.09685700 & -0.97430000 \\ \mbox{C} & -2.89256000 & -1.67866000 \\ \mbox{C} & -3.8086800 & -2.09685700 & -0.97430000 \\ \mbox{C} & -2.80256000 & -1.67861000 & 0.3422500 \\ \mbox{C} & -3.8028600 & -2.26825200 \\ \mbox{C} & -3.8028600 & -2.28528200 \\ \mbox{C} & -3.8028600 & -2.28528200 \\ \mbox{C} & -3.8028600 & -2.27845300 \\ \mbox{C} & -2.8058600 & -0.7754300 & 2.7818800 \\ \mbox{C} & -2.8058600 & -0.7754300 & 2.7818800 \\ \mbox{C} & -2.8058600 & -0.7754300 & 2.7818800 \\ \mbox{C} & -2.8058600 & -0.7874300 \\ \mbox{C} & -2.8028600 & -1.7871000 \\ \mbox{C} & -2.8028600 & -1.7871000 \\ \mbox{C} & -2.8038700 & -1.8758700 \\ \mbox{C} & -2.8038700 & -1.8487700 \\ \mbox{C} & -2.8038700 \\ \mbox{C} & -2.8088700 & -1.8758700 \\ \mbox{C} & -2.8088700 & -0.7781300 \\ \mbox{C} & -2.8089800 & -1.8575800 \\ \mbox{C} & -2.8088700 & -0.7781300 \\ \mbox{C} & -2.8089800 \\ \mbox{C} & -2.85837$	C	-1 87679700	4 30371700	-1 18535200	С	0.34410400	2.42723500	-0.19435100
$ \begin{array}{c} \mbox{C} & -0.12373200 & 3.50010500 & 0.28931100 & C & 1.07735700 & 1.18308900 & 0.18981600 & 0.2403600 & 0.48433300 & 0.45431100 & -0.04048700 & 0.48433300 & 0.45431100 & -0.04048700 & 0.4843300 & 0.45431100 & -0.04048700 & 0.46336100 & 0.0432200 & C & -2.840400 & 0.5552300 & 2.23171700 & -2.810400 & -0.5252300 & 2.23171700 & -2.810400 & -0.5252300 & 2.23171700 & -2.81047700 & -2.4987600 & -1.46531400 & C & -1.6668300 & -1.6624500 & -0.33161600 & -0.6041600 & -0.516600 & 0.3516400 & -2.9990600 & -1.453060 & -0.9133800 & C & -2.9006507 & -1.4330610 & -0.91211800 & -2.5925400 & -2.5925400 & -2.5925400 & -2.5925400 & -2.5925400 & -2.5925400 & -2.5925400 & -2.5925400 & -2.5925400 & -2.5925400 & -2.5925400 & -2.5925400 & -2.39742000 & -2.3982560 & -0.331013400 & -2.35769400 & -2.24875400 & -2.4114260 & 0.390240 & 1.24219820 & -1.6692400 & -1.6694200 & -1.6694200 & -1.6694200 & -1.6694200 & -1.6694200 & -1.6694200 & -1.6694200 & -1.6694200 & -1.6694200 & -1.6694200 & -1.6694200 & -1.6694200 & -1.6694200 & -1.6694200 & -1.6694200 & -2.24114260 & 0.3904900 & -2.24114260 & 0.3904900 & -2.24114260 & 0.3904900 & -2.24114260 & 0.3902400 & -1.24698900 & -2.$	C	-1 00044800	4 51067400	-0 11419200	С	-0.87205200	2.40708800	-0.90781800
C    -0.11623500    2.25170300    -0.37058000    C    2.55160000    1.11097900    0.24305600      C    -0.99498300    2.06197500    -1.45736700    C    2.55160000    -1.06880900    0.83789500      C    2.17690800    1.47583900    0.59519400    C    1.6202500    -1.06880900    0.83789500      C    2.85459900    0.16529400    0.9712100    C    -0.8465700    -0.39852600    0.48435300      C    0.6074900    -0.16581000    0.9123200    C    -2.82106400    -0.52552300    1.06947600    -0.35196400      C    -0.6364500    -0.991363500    -0.29802800    C    -2.9900800    -1.45340800    -2.9525400    -0.45651500    -1.65663900      C    -1.8792100    -2.3175400    2.3642500    C    -2.9008600    -2.9525400    -2.9733000    -2.9733000    -2.9733000    -2.9733000    -2.9733000    -2.9733000    -2.9733000    -2.9743000    -2.9743000    -2.9743000    -2.9743000    -2.9743000    -2.9743000    -2.9743000    -2.9743000    -2.9743000    -2.9743000    -2.9743000    -2.9743000    -2.9743000	C	-0.12373200	3 50010500	0 28834100	С	1.05735700	1.18308900	0.15891600
$ \begin{array}{c} \mbox{C} & -0.9949300 & 2.66197500 & -1.45736700 & C & 2.95948500 & -0.27544700 & 0.7235800 & 0.7235800 & 0.7235800 & 0.7235800 & 0.7357500 & 0.7415300 & C & 0.54531100 & -0.04048700 & 0.4833500 & 0.8789500 & 0.5553200 & 0.66349100 & 0.94357100 & C & -0.88657600 & -0.38526500 & 0.4628700 & 1.98611800 & 0.9123200 & C & -2.82106400 & -0.52552300 & 2.23171700 & C & -0.63646500 & -0.9348200 & -0.24987600 & 0.35196400 & -1.20271800 & -0.35196400 & -1.56780300 & -1.46287700 & 1.9661800 & -0.924987600 & -3.54088100 & -1.20271800 & -0.4201800 & -1.8792100 & -2.41120300 & -1.76393800 & C & -2.99006600 & -1.45340800 & -0.92359400 & -2.96147700 & -2.39338200 & -0.82082900 & C & -2.90026600 & -1.45340800 & -0.9223900 & -1.65603900 & -2.36685700 & -0.9743000 & -3.39485300 & -0.9317010 & 3.30122100 & -2.96147700 & -2.95734300 & 2.76818800 & -3.39845500 & -0.33170100 & 3.30122100 & -2.989259400 & -1.775734300 & 2.78924600 & -3.39845500 & -2.38769400 & -2.24875400 & -3.39845500 & -0.33170100 & 3.30122100 & -2.982592400 & -3.39845500 & -0.33170100 & 3.30122100 & -2.989259400 & -1.76743000 & 2.78924600 & 0.339452500 & -2.38945500 & -0.33170100 & 3.30122100 & -2.98259400 & -1.76342000 & 0.7433800 & -2.78924600 & -3.39845500 & -0.33170100 & 3.30122100 & -2.989259400 & -1.6640200 & -2.989259400 & -3.39845500 & -0.33170100 & 3.03022100 & -2.98925900 & -2.68633800 & 2.967733300 & -2.78924600 & 0.33501000 & -2.24875400 & -2.28828200 & -0.6044200 & 0.74313200 & -1.1447800 & 0.4851200 & -2.94674100 & -1.6659300 & -1.76503300 & -1.67594100 & -2.47889700 & 3.75530700 & -1.83507000 & -1.76342200 & -1.4623300 & -1.64593300 & -1.4625300 & -1.4625300 & -1.4602300 & -1.64643300 & -1.6659300 & H & 3.49240300 & -1.7634200 & 0.96851800 & -1.6643300 & 1.67594100 & -2.85818800 & -1.6402300 & -1.64643300 & -1.6659300 & H & 3.8924000 & -0.74313200 & -1.18055900 & H & 3.8936900 & -1.2887700 & -2.33898500 & -1.6282500 & -1.4623300 & H & 6.6853300 & -1.6663300 & H & 6.8189700 & -2.8887700 & -2.8385700 & -1.8755000 & H & 3.8935000 & -1.67769300 &$	C	-0.11623500	2 25170300	-0.37058000	С	2.55160000	1.11097900	0.24030500
$ \begin{array}{c} \begin{tabular}{lllllllllllllllllllllllllllllllllll$	C	-0 99498300	2.06197500	-1 45736700	С	2.95948500	-0.27544700	0.72353600
$ \begin{array}{c} c \\ 2. 17990800 & 1. 17583900 & 0. 959519400 \\ C \\ 2. 8545900 & 0. 16529400 & 0. 97327100 \\ C \\ 0. 6079490 & -0. 16581000 & 0. 9123200 \\ C \\ 0. 6079490 & -0. 16581000 & 0. 9123200 \\ C \\ 0. 6079490 & -0. 16581000 & 0. 9123200 \\ C \\ -0. 703700 & -1. 6252300 & -1. 16531400 \\ C \\ -0. 63646500 & -0. 90348200 & -0. 24987600 \\ C \\ -0. 703700 & -1. 6225300 & -1. 16531400 \\ C \\ -1. 89792100 & -2. 4112030 & -1. 76393800 \\ C \\ -2. 96147700 & -2. 39338200 & -0. 82082900 \\ C \\ -1. 7633300 & -0. 13635500 & 0. 69337900 \\ C \\ -2. 9805600 & -0. 27754300 & 2. 76818800 \\ C \\ -3. 98295000 & -1. 67866000 \\ 0. 36429500 \\ C \\ -3. 98295000 & -1. 67866000 \\ 0. 36429500 \\ C \\ -3. 9829500 & -1. 67866000 \\ 0. 36429500 \\ C \\ -3. 9829500 & -1. 10773300 & -2. 4875400 \\ C \\ -3. 9829500 & -1. 10773300 & -2. 87818500 \\ C \\ -3. 9829500 & -1. 10784300 \\ -2. 41126000 \\ C \\ -3. 9829500 & -1. 10784300 \\ -2. 41126000 \\ -2. 4112600 \\ -2. 68633800 \\ -2. 9685700 & -0. 2111400 \\ C \\ -3. 982950 & -1. 10784300 \\ -2. 4112600 \\ -2. 4112600 \\ -2. 2680220 \\ -1. 153820 \\ -1. 10743300 \\ -2. 4112600 \\ -2. 4112600 \\ -2. 4112600 \\ -2. 4112600 \\ -2. 4112600 \\ -2. 553820 \\ -1. 685470 \\ -2. 55384200 \\ -1. 5613300 \\ -1. 7634700 \\ -2. 4112600 \\ -2. 4188710 \\ -2. 4188710 \\ -2. 4188710 \\ -2. 4188710 \\ -2. 4188710 \\ -2. 4188710 \\ -2. 4188710 \\ -2. 4188710 \\ -2. 4188710 \\ -2. 4188710 \\ -2. 4188710 \\ -2. 418870 \\ -2. 418870 \\ -2. 4188710 \\ -2. 418870 \\ -2. 418870 \\ -2. 418870 \\ -2. 418870 \\ -2. 418870 \\ -2. 418870 \\ -2. 418870 \\ -2. 418870 \\ -2. 418870 \\ -2. 418870 \\ -2. 4188710 \\ -2. 418870 \\ -2. 418870 \\ -2. 418870 \\ -2. 418870 \\ -2. 41887$	C	0.80480800	1 18529700	0.07143500	С	1.62032500	-1.06880900	0.83789500
C 2.8545000 0.16529400 0.97327100 C $-0.88657600$ 0.39852600 0.68349100 C $-1.865300$ 0.9132300 C $-1.4655300$ 0.14628700 1.89611800 C $-0.63646500$ 0.90348200 $-0.24987600$ C $-2.82106100$ 0.52552300 2.23171700 C $-0.63646500$ 0.90348200 $-0.24987600$ C $-3.54088100$ $-1.06947600$ $-0.35196100$ C $-1.8702100$ $-2.41120300$ $-1.76393800$ C $-2.99008600$ $-1.45340800$ $-0.04201800$ $-2.96147700$ $-2.39938200$ $-0.82082900$ C $-1.19251500$ $-1.33651500$ $-1.65603900$ $-2.92959400$ C $-2.89259400$ $-2.47856000$ $0.36429500$ C $-3.3013140$ $-2.35769400$ $-2.29259400$ C $-3.80285000$ $-0.27754300$ $-2.28025900$ C $-3.80868000$ $-2.09685700$ $-0.97130000$ $-2.9745000$ $-2.9745000$ $-2.2872400$ $-2.4875400$ $-2.2872400$ $-0.03170100$ $-3.0122100$ $-2.411256800$ $0.33501000$ $-2.28121900$ $-2.28782400$ $-0.33170100$ $-3.0122100$ $-2.411256800$ $0.335010000$ $-2.28628200$ $-0.034730000$ $-2.78924600$ C $-3.80286000$ $-2.27822600$ $-1.6743000$ $-2.78924600$ C $-3.80286000$ $-2.27822600$ $-1.674200$ C $-3.80286000$ $-2.27822600$ $-0.97733000$ $-2.7782400$ C $-3.828371000$ $-3.21136000$ $-0.3614400$ C $-4.00238600$ $-1.77541300$ $-2.78924600$ C $-2.88371000$ $-3.21136000$ $-0.9952700$ $-2.9760300$ $-0.17871000$ $0.68253000$ H $-2.4789700$ $-3.21184000$ $-2.4887100$ $-1.65603300$ $-1.27603200$ H $-2.55384200$ $-0.1694200$ $-2.88371000$ $-3.71952100$ $-0.7854300$ $-1.9458100$ $-2.9553700$ H $-2.55384200$ $-0.1694200$ $-2.13608000$ H $-2.2789800$ $-1.0458100$ $-1.9458100$ $-1.9458100$ $-1.9458100$ $-2.9799800$ $-1.9458100$ $-1.9458300$ $-1.$	C	2 17690800	1 47583900	0.59519400	С	0.54531100	-0.04048700	0.48435300
C1.81633100-0.943552000.61230200C-1.46055300-0.146287001.89611800C0.60734900-0.16581000.09123200C-2.82106400-0.525523001.20531200C-0.73073000-1.66625300-1.40531400C-2.82106400-0.525523001.20531200C-0.73073000-1.66263500-1.40531400C-1.66668300-1.005947600-0.35196400-0.35196400C-1.8752100-2.31938200-0.82082900C-1.9251500-1.33651500-1.65603900C-2.8820000-1.678660000.36129500C-3.30113400-2.35769400-2.94875400C-2.8808600-0.217139001.91925000C-3.8088800-2.09685700-0.9733000C-2.8808600-0.277543002.78924600C3.350100002.02161300-0.30640400C-2.8808600-0.277543002.78924600C3.3541300-0.331761003.30122100C-3.8924500-1.076370001.756740001.2974200C2.8837100-2.11426000.3095700C-2.66853000.7114700C2.8837100-2.1142600-0.3640400-2.25828200-0.16044200C2.698338002.597613000.71144700C2.8837100-1.7763020-1.7634200C2.5926200-1.81358200-0.3655700-1.7634200-1.7634200-1.7634200C2.5926200-1.81358200-0.4655300H3.49240300 <t< th=""><th>C</th><th>2 85450900</th><th>0 16529400</th><th>0.97327100</th><th>С</th><th>-0.88657600</th><th>-0.39852600</th><th>0.68349100</th></t<>	C	2 85450900	0 16529400	0.97327100	С	-0.88657600	-0.39852600	0.68349100
$ \begin{array}{c} \mbox{C} 0. 60794900 & -0. 16581000 & 0. 09123200 \\ \mbox{C} -0. 63646500 & -0. 90348200 & -0. 24987600 \\ \mbox{C} -0. 73073000 & -1. 62623500 & -1. 40531400 \\ \mbox{C} -1. 8792100 & -2. 41120300 & -1. 76393800 \\ \mbox{C} -2. 8910700 & -2. 41120300 & -1. 76393800 \\ \mbox{C} -2. 99008600 & -1. 45340800 & -0. 4201800 \\ \mbox{C} -2. 99008600 & -1. 45340800 & -0. 4201800 \\ \mbox{C} -2. 89250000 & -1. 67866000 & 0. 36429500 \\ \mbox{C} -1. 76931800 & -0. 21213900 & 1. 91925000 \\ \mbox{C} -3. 88294500 & -0. 04788400 & 2. 41258800 \\ \mbox{C} -3. 88294500 & -1. 04788400 & 2. 41258800 \\ \mbox{C} -3. 89294500 & -1. 04788400 & 2. 41258600 \\ \mbox{C} -3. 89294500 & -1. 04788400 & 2. 41258600 \\ \mbox{C} -4. 00238600 & -1. 75047000 & 1. 20974200 \\ \mbox{C} -4. 00238600 & -1. 75047000 & 1. 20974200 \\ \mbox{C} -4. 00238600 & -1. 7871000 & 0. 8851200 \\ \mbox{C} -2. 89252000 & -1. 6187100 & 0. 68251200 \\ \mbox{C} -4. 09309000 & -0. 17871000 & 0. 68251200 \\ \mbox{C} -4. 09309000 & -0. 17871000 & 0. 68251200 \\ \mbox{C} -4. 7643400 & -1. 4567300 & 0. 68253000 \\ \mbox{H} -3. 52798800 & -1. 043654700 \\ \mbox{C} -3. 5185900 & -1. 04365300 \\ \mbox{H} -3. 5437200 & -2. 5799880 & 0. 34009200 \\ \mbox{H} -2. 5185900 & -1. 6647300 \\ \mbox{H} -2. 53184200 & -0. 34567300 \\ \mbox{H} -2. 53184200 & -0. 34567300 \\ \mbox{H} -2. 53184200 & -1. 6643200 \\ \mbox{H} -2. 53184900 & -1. 6643200 \\ \mbox{H} -2. 53185900 & -1. 66786700 \\ \mbox{H} -2. 5318200 & -2. 70030900 \\ \mbox{H} -2. 5318200 & -1. 637867900 \\ \mbox{H} -2. 5318200 & -2. 63192700 \\ \mbox{H} -2. 5318200 & -1. 637867900 \\ \mbox{H} -2. 5318200 & -2. 63192700 \\ \mbox{H} -2. 5318200 & -1. 637867900 \\ \mbox{H} -2. 5318200 & -1. 637867900 \\ \mbox{H} -2. 5318200 & -2. 63192700 \\ \mbox{H} -2. 5318200 & -1. 6587500 \\ \mbox{H} -2. 8508700 \\ \mbox{H} -2. 8508700 \\ \mbox{H} -2. 85387700 \\ \mbox{H} -2. 8318700 \\ \mbox{H} -2. 8318700 \\ \mbox{H} -2. 8$	C	1 81633100	-0.94355200	0.61230200	С	-1.46055300	-0.14628700	1.89611800
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	C	0 60794900	-0.16581000	0.09123200	С	-2.82106400	-0.52552300	2.23171700
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C	-0 63646500	-0.90348200	-0.24987600	0	-3.54088100	-1.20271800	1.20631200
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C	-0.73073000	-1.62623500	-1 40531400	С	-1.66686300	-1.06947600	-0.35196400
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C	-1 89792100	-2 41120300	-1 76393800	С	-2.99008600	-1.45340800	-0.04201800
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0	-2,96147700	-2 39938200	-0.82082900	С	-1.19251500	-1.33651500	-1.65603900
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Č	-1 75233300	-0.91363500	0.69337900	С	-2.00127600	-1.97328100	-2.59259400
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C	-2 89250000	-1.67866000	0.36429500	С	-3.31013400	-2.35769400	-2.24875400
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C	-1.76091800	-0.21213900	1.91925000	С	-3.80868000	-2.09685700	-0.97430000
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Ĉ	-2.86086600	-0.27754300	2. 76818800	0	-3.39483500	-0.33170100	3.30122100
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C	-3 98294500	-1 04788400	2 41256800	0	3.35010000	2.02161300	-0.03640400
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	С	-4 00238600	-1 75047000	1,20974200	С	3.79525200	-1.08928300	-0.30952700
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	0	-2 04657100	-3,07433600	-2 78924600	С	1.84126000	-2.25828200	-0.16044200
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	0	2 69833800	2 59761300	0 71144700	С	4.23099100	-2.41142600	0.38019400
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Č	4 09309000	-0.17871000	0.08851200	С	2.88371000	-3.21136000	0.49581800
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C	2.59226200	-1.81358200	-0.43654700	С	2.69103500	-1.59503300	-1.27760300
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C	4 74694900	-1 45679300	0.68253000	Н	3.49240300	-0.17443000	1.67594100
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Ĉ	3. 70347200	-2.57998800	0.34009200	Н	1.42193800	-1.46023100	1.84387100
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	C	3. 42194300	-0. 74313200	-1.19405500	Н	-2.47889700	3.55307000	-1.76304200
$\begin{array}{c c c c c c c c c c c c c c c c c c c $	Н	3. 12218500	0. 19367300	2. 03532900	Н	-1.54062800	5.74618900	-1.04543500
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Н	1.51444400	-1.56433300	1. 46559300	Н	0.61860400	5.81285000	0.19323700
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Н	-2.53158900	2.91079500	-2.70030900	Н	1.82230000	3.71952100	0.70855300
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Н	-2.55384200	5. 09230700	-1.49802100	Н	-1.28489800	1.46402800	-1.24508800
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	-0.99439000	5.46262900	0.40711800	Н	-0.91369200	0.35692900	2.68321400
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Н	0.56812400	3.67867900	1.10098500	Н	-0.18804800	-1.03004700	-1.92372700
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Н	-0.98320900	1.12531800	-2.00161000	Н	-1.62247900	-2.16952500	-3.58943000
$\begin{array}{llllllllllllllllllllllllllllllllllll$	Н	0.06925000	-1.63772000	-2.13366900	Н	-3.93908900	-2.85443200	-2.97954000
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	-0.90052900	0.38877700	2.18829300	Н	-4.81433700	-2.37163400	-0.68119600
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	-2.85369300	0.26934900	3.70439700	Н	4.70093800	-2.23202700	1.35318100
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	-4.83983700	-1.09627300	3.07581700	Н	4.95671800	-2.94747100	-0.24158900
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	-4.85022000	-2.35192700	0.90617600	Н	2.62230400	-3.45093200	1.53239700
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	4.93110000	-1.36367000	1.75831300	Н	2.93494100	-4.15681800	-0.05528700
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	5.71078300	-1.65296500	0.19965500	Н	3.06464400	-2.31671700	-2.01170800
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	3.30988300	-3.07756800	1.23345300	Н	2.17943800	-0.78720600	-1.81118000
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	4.14689900	-3.35372700	-0.29595400	Н	4.60857500	-0.50943000	-0.75025200
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	4.14233200	-1.18036800	-1.89315400	Н	0.92214800	-2.75817700	-0.47125700
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	2.81277400	-0.00974400	-1.73145200				
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	4.77102400	0.66730400	-0.04088800	TS	$-1 (7\beta_A \rightarrow$	7 <b>β</b> <sub>B</sub> )	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	Н	1.95305100	-2.46192500	-1.03825200	E =	-1190.04409	a. u.	
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$					С	3.93759500	-1.87585000	1.39381800
$\begin{array}{l} F^{F}\\ E = -1190.\ 0607954 \ \text{a. u.}\\ C = -1.\ 54526000 \ 3.\ 59247400 \ -1.\ 21087300 \end{array} \qquad \begin{array}{l} C \qquad 4.\ 35463500 \ -1.\ 96607600 \ -0.\ 98907000 \\ C \qquad 3.\ 30566400 \ -1.\ 06768900 \ -1.\ 20877700 \end{array}$	7 <b>R</b>	n			С	4.67246900	-2.37344800	0.31090700
C $-1.54526000$ $3.59247400$ $-1.21087300$ C $3.30566400$ $-1.06768900$ $-1.20877700$	<b>י</b> ק קי	18 = -1190 060705/	1 9 11		С	4.35463500	-1.96607600	-0.98907000
	C -	-1.54526000	3. 59247400	-1.21087300	С	3.30566400	-1.06768900	-1.20877700

С	2.54737800	-0.57924000	-0.12976600	С	0.07381800	-2.51397400	-0.37193700
С	2.88464600	-0.98340200	1.17692800	С	0.90880300	-3.69500900	-0.31275500
С	1.48779300	0.43667600	-0.35586600	0	2.27245100	-3.46809000	-0.08268500
С	1.95227900	1.81870200	-0.67246400	С	1.94959200	-1.02113700	-0.02347300
С	0.75169800	2.73228100	-0.78635500	С	2.77310600	-2.17732900	0.04722100
С	-0.46561800	1.80418400	-0.48858000	С	2.62885700	0.20867600	0.11231200
С	0.11101400	0.39160800	-0.31492600	С	4.00486000	0.28343800	0.31045700
С	-0.73877800	-0.83366100	-0.15410900	С	4.77786600	-0.88373200	0.38268300
С	-0.10451800	-2.04186000	0.00570300	С	4.15417400	-2.11877000	0.24848000
С	-0.75158100	-3.32318500	0.18064000	0	0.51670500	-4.85753900	-0. 43927500
0	-2.15964300	-3.29942200	0.19139100	0	-2.35204800	2.88344000	-0.69975700
С	-2.22611300	-0.86414400	-0.18891900	С	-4.03019800	0.43475100	0.34946200
С	-2.86457700	-2.12056700	-0.00591600	С	-2.68167500	-1.35128300	0.77817200
С	-3.10743000	0.22598500	-0.40293800	С	-4.94791900	-0.77958500	0.03595300
С	-4. 49134500	0.07561500	-0.41913100	С	-4.02084900	-2.01239600	0.33763100
С	-5.07519400	-1.18326200	-0.21959600	С	-3.19540500	-0.10211800	1.54096300
С	-4.25319600	-2.28354100	-0.01389200	Н	-3.40233700	0.52035300	-1.76720100
0	-0.18646700	-4.40793900	0.32855000	Н	-2.07789800	-1.42528400	-1.34899800
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С	0.69602200	3.81507600	0.33239600	Н	2.68118300	5.38832500	0.38414800
С	-1.06249900	2.44843000	0.82044200	Н	2.17797000	4.58586100	-1.91764000
С	-0.53737500	4.71861700	0.05545000	Н	0.68230000	2.63838800	-2.25692500
С	-1.75071900	3.78046900	0.39957000	Н	0.17379700	2.28544600	2.00217100
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Н	0.72382300	3.18430100	-1.78401400	Н	2.07640100	1.12495200	0.06012500
Н	-1.18416600	1.83311300	-1.31117700	Н	4.47170300	1.25722900	0.40808100
Н	4. 18378400	-2.18138800	2.40556300	Н	5.84981800	-0.82913300	0.53830500
Н	5.48721100	-3.06981500	0.48009500	Н	4.70129100	-3.05238000	0.29057200
Н	4.92560500	-2.34141500	-1.83205600	Н	-5.30794600	-0.76566300	-0.99847400
Н	3.07241000	-0.74219600	-2.21700900	Н	-5.82733000	-0.77641200	0.68957900
Н	2.31701500	-0.59870400	2.01871200	Н	-3.89271400	-2.66679000	-0.53195200
Н	0.96853700	-2.11340300	0.01893500	Н	-4.42737800	-2.62508400	1.14952000
Н	-2.72305700	1.21504000	-0.56231800	Н	-3.80743400	-0.36357300	2.41058600
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Н	-6.15313300	-1.30096000	-0.22952100	Н	-4.55320900	1.38163600	0.49744500
Н	-4.64652500	-3.28103700	0.13776500	Н	-2.02038600	-2.01408700	1.33798600
Н	-0.56072400	5.07539300	-0.97991600				
Н	-0.52321200	5.59991700	0.70637000	7α	Å		
Н	-2.43065000	3.64784500	-0.45031200	E =	-1190.065355	2 a.u.	
Н	-2.34087700	4.18357800	1.22977000	Ċ	-1. 14907800	-0.96263100	0.10853300
Н	-0.03575000	3.58746400	2.41802000	Ċ	-1. 47610400	-1.88873200	1.05849400
Н	0.90286300	2.19114100	1.84610800	Ċ	-2.84132700	-2.19671200	1. 43942400
Н	1.63998700	4.35051100	0.45215100	0	-3.85212700	-1.47625600	0.74320900
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				0	0 55050400	0 57101500	0.00004000

# TS-2 $(7\beta_{\text{A}} \rightarrow 7\beta_{\text{B}})$

E	= -1190.0397672	a.u.	
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С	0.35317000	2.30478100	-0.14987000
С	0.61913100	2.78342600	1.14678200
С	-0.62420100	1.20371900	-0.35390400
С	-2.01960900	1.69001400	-0.62133200
С	-2.94816800	0.50951300	-0.77013700
С	-2.03571800	-0.72082300	-0.51362300
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0	-3.85212700	-1.47625600	0.74320900
С	-2.21757600	-0.28003900	-0.62181600
С	-3.55252400	-0.57191500	-0.26694800
С	-2.00709200	0.63010500	-1.68029600
С	-3.08010600	1.22690800	-2.33454400
С	-4.39861100	0.92730000	-1.94762700
С	-4.63797000	0.02491800	-0.91409800
0	-3.20130600	-2.99295300	2.30517500
Н	-0.71362700	-2.44762900	1.58339100
Н	-0.99305500	0.85787300	-1.98383200
Н	-2.89806500	1.92257000	-3.14631500
Н	-5.23430400	1.39372100	-2.45827000
Н	-5.63976100	-0.23779500	-0.59742000
С	0.27542200	-0.73371600	-0.21933900
С	1.12708300	-1.86786800	-0.67610700
С	2.50470600	-1.32676200	-1.03588800
С	2.44064400	0.19153700	-0.67858900

С	1.01781800	0.41666200	-0. 16862100
0	0.79098800	-3.06254100	-0.72845500
С	3.64909100	-1.87163800	-0.12589200
С	3.56728600	0.34670100	0.39851700
С	4.99137600	-1.32747400	-0.68983000
С	4.93149500	0.20306300	-0.33662400
С	3.47831600	-1.00709600	1.15241800
Н	2.70721700	-1.53042100	-2.09318800
Н	2.64383100	0.84060100	-1.53926000
Н	5.08936500	-1.50932300	-1.76553400
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Н	4.98976100	0.84287100	-1.22464000
Н	5.75503800	0.48895400	0.32687600
Н	4.29206500	-1.14584100	1.87193700
Н	2.52618200	-1.16266200	1.66886200
Н	3.60936200	-2.95518600	0.00176600
Н	3.47623600	1.25079700	1.00422800
С	-0.71888400	3.12021700	1.85601500
С	-0.14418000	4.27937500	1.32065800
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С	1.19174400	2.91536300	-0. 17272100
С	0.60685100	1.73706800	0.34199000
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Н	-1.45103100	3.19403100	2.65335700
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Н	-0.78850700	0.97398800	1.80791200

### 7α₀

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С	-1.36568900	0.25825500	1.81830300
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0	-4.06543700	-2.07037600	-2.39239400
Н	-1.43506000	-1.77897000	-2.38319800
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Н	-4.11122000	0.78715400	3.76422900
Н	-5.21966600	-0.25687400	1.77162000
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С	2.52870000	-0.04179500	-0.53751600
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С	4.76930800	-1.76876400	0.32873700
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С	2.81830600	-1.17687700	1.61087200
Н	2.93987000	-1.92408100	-1.67823600

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Н	5.15243800	-2.03060900	-0.66344100
Н	5.38605000	-2.29245400	1.06751300
Н	5.16870200	0.34992800	-0.26082600
Н	5. 37226200	0.03607100	1. 46545700
Н	3 36148700	-1 31616600	2 55163600
н	1 74498900	-1 21747100	1 81949500
н	3 08743200	-3 21621300	0.66452500
и П	3.00745200	1 04408500	1 26405200
	0. 07500000	2 60208000	1.00400000
C	-0.010000	3.00208000	-1.22320300
C	0.09192000	4. 57457800	-0.94384800
C	1. 37312800	4.17573200	-0.54785900
C	1.68052900	2.81961200	-0. 42315800
C	0.71010600	1.82189200	-0.67450100
С	-0.57276500	2.24682900	-1.09226000
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Н	2.13580500	4.91963800	-0.34152000
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C	-1.54582000	1 3074400	-0.06562400
C	-2 77443800	2 15/18800	0.00302400
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C	-2 70500200	-0 73283700	-0.01004000
C	-3 01770200	0.01052600	0.01994900
C	-2 86740900	-2 13949100	-0.05320200
C	-4 12228600	-2.74255300	-0.04276600
C	-5 20054700	-1 96984800	0.04210000
C	-5 181/1900	-0 58534600	0.00303700
0	-2 86342000	3 38557800	0.01764900
н	-0.68935100	2 04075200	-0 12934000
Ц	-1 00303800	-2 76796300	-0.04941900
и П	-4 18517000	-2 82527000	-0.06520000
11	-4. 10517500 6. 26705500	-3.82521900	-0.00329000
п	-0.20795500	-2.44042300	0.01490200
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C	-0.02570700		-0.17747100
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C	1.00427200	-2.08382700	-0.00740200
C	2.3000000	-0.02512500	-0.07414400
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0	-0.19174700	-2.99068000	0.21223100
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C	3. 52089300	-0.64434300	0.37752400
C	4. 19629000	-2.90431000	-0. 29169800
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U	3.00546000	-1.68460800	1.40822400
H	1.80838500	-2.5/5/4300	-1.04/10200
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H	4.94310600	-1.03897000	-1.27317400
H	5.60787700	-1.31449000	0.33913500
H	3. 75855500	-1.94700900	2.15840900
H	2.08874800	-1.38210400	1.92473700

2. 37019600 -3. 74551700

Н

0.71217300

1.03404400 -2.07131200 -0.29287200

С

Н	3.78467900	0.34275700	0.76142400	С	2.44264600	-1.67282400	-0.68436000
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С	2.16347400	4.35299000	0.18548500	С	0.98902100	0.24952800	-0.30047900
С	1.81739100	3.57632000	1.29807700	0	0.75167600	-3.26066600	-0.06691600
С	1.44743500	2.23883200	1.13641000	С	3.51465400	-2.09543300	0.36522700
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Н	2.41156100	4.37806000	-1.95833000	С	4.89820100	-0.14165700	-0.13592700
Н	2.43913000	5.39437900	0.31312200	С	3.31757500	-1.00880000	1.45785300
Н	1.82881600	4.01291600	2.29127100	Н	2.66266300	-2.08934000	-1.67393400
Н	1.16613100	1.64381300	1.99920500	Н	2.71679800	0.35915200	-1.56504900
Н	1.78255900	2.00199300	-2.25121600	Н	5.04884100	-2.08604200	-1.22820400
				Н	5.70569000	-2.13237200	0.41030700
TS	$-2 (7\alpha \rightarrow$	7α,		Н	5.03390500	0.32800200	-1.11657000
E =	= -1190.0366235	5 a. u.		Н	5.69638000	0.22890100	0.51671800
C	-1.35563900	-1.00183700	-0.03975600	Н	4.08640900	-1.04258600	2.23668400
C	-1.81197500	-2.29971300	-0.05179400	Н	2.33333300	-1.04091100	1.93642000
C	-3.19759400	-2.71760100	-0.02797200	Н	3.41245000	-3.13588500	0.67801800
0	-4.15508000	-1.68769400	-0.01346200	Н	3.42676100	1.18504200	0.89942100
C	-2.40436200	0.05055900	0.05155900	С	0.73170200	3.90912300	-1.27034400
С	-3.76621100	-0.35729600	0.04758700	С	0.80130900	4.53906400	-0.02208000
С	-2.20521700	1.44319200	0.16007200	С	0.90551900	3.76539300	1.13999300
С	-3.25709400	2.35311900	0.23226300	С	0.93007000	2.36926600	1.05781700
С	-4.58474700	1.90697400	0.20080100	С	0.83952300	1.72690500	-0.19340000
С	-4.83381700	0.54277900	0.11177400	С	0.76270100	2.51392200	-1.35825100
0	-3.60062100	-3.88233800	-0.03779800	Н	0.65376400	4.50218900	-2.17580200
Н	-1.12405100	-3.12805100	-0.08171200	Н	0.77905100	5.62180000	0.04419300
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Н	-5.40868200	2.61044000	0.25301800	Н	0.70393700	2.03040000	-2.32827600
Н	-5.83766000	0.13652200	0.09668900				
С	0.14001000	-0.83279100	-0.18271400				

#### 2.2 Complete Reference for Ref. 15 – "Gaussian 03" details.

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, *Gaussian 03* (revision B.05), Gaussian, Inc., Pittsburgh, PA, 2003.

## 3.0 Representative NMR spectra (all run at 298 K in CDCl<sub>3</sub>).

 $^{1}$ H NMR (400 Mhz) spectrum of compound **5**.



# $^{13}\text{C}\{^{1}\text{H}\}$ (100 MHz) NMR spectrum of compound **5**.



```
<sup>13</sup>C{<sup>1</sup>H} DEPT135 (100 Mhz) NMR spectrum of compound 5.
```



<sup>1</sup>H NMR (500 Mhz) spectrum of complex **6**.





<sup>13</sup>C{<sup>1</sup>H} DEPT135 (125 MHz) NMR spectrum of complex **6**.



<sup>1</sup>H NMR (500 Mhz) spectrum of regioisomer  $7\alpha$ .\*



\* Note: trace diethyl ether impurity in this <sup>1</sup>H NMR spectrum.



 $^{13}C{^{1}H}$  (125 MHz) NMR spectrum of regioisomer 7 $\alpha$ .

<sup>13</sup>C{<sup>1</sup>H} DEPT135 (125 MHz) NMR spectrum of regioisomer 7a.



<sup>1</sup>H NMR (500 Mhz) spectrum of regioisomer  $7\beta$  (mixture of atropisomers at room temperature).







 $^{13}C{^{1}H}$  DEPT135 (125 MHz) NMR spectrum of regioisomer 7 $\beta$ .

