Supporting Information

Intramolecular Nonbonding Interactions and Geared Phenyl Twisting in Para-Disubstituted 1,4-Diphenylazines. Electron Correlation Effects on Molecular Conformations and Enantiomerization

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TABLE S1. Total Energies and Thermochemical Data of Toluene

Toluene	Vib. anal.	E_{tot}	VZPE	TE$_{298}$	S_{298}	μ	NSS
			APFD/6-311G*				
Stag., C_s	harm.	-271.383387	80.47	84.38	80.43	0.35	M
	harm., HR			84.13	78.68		
Ecl., C_s	harm.	-271.383370	80.44	83.79	74.12	0.35	TS
			MP2(full)/6-311G*				
Stag., C_s	harm.	-270.849862	79.96	84.03	79.65	0.31	M
	harm., HR			83.84	78.98		
Ecl., C_s	harm.	-270.849772	79.84	83.41	75.30	0.32	TS
			MP2(full)/6-311+G(2df,p)				
Stag., C_s	harm.	-271.068128	80.71	84.60	78.79	0.39	M
	harm., HR			84.40	78.00		
Ecl., C_s	harm.	-271.068043	80.60	83.98	74.28	0.39	TS
			MP2(full)/6-311+G(3df,3dp)				
Stag., C_s	harm.	-271.115884	80.42	84.35	79.85	0.41	M
	harm., HR			84.11	78.38		
Ecl., C_s	harm.	-271.115855	80.34	83.75	74.39	0.41	TS

[a]Harmonic vibrational frequencies (harm.) and without or with methyl rotation treated as a hindered rotor (HR).
[b]Total energy E_{tot} in Hartree, vibrational zero-point energy (VZPE) and thermal energy TE in kcal/mol, entropy S in cal/(mol·K), and dipole moment μ in Debye.

TABLE S2. Higher Level MPx Energies of Toluene

Molecule	MP3	MP4(DQ)	MP4(SDQ)	MP4(SDTQ)
MPx(full)/6-311G*//MP2(full)/6-311G*				
Staggered, C_s	-270.889167	-270.887947	-270.897549	-270.948172
Eclipsed, C_s	-270.889094	-270.887876	-270.897480	-270.948088
MPx(full)/6-311+G(2df,p)//MP2(full)/6-311+G(2df,p)				
Staggered, C_s	-271.109131	-271.100043	-271.109640	-271.175932
Eclipsed, C_s	-271.109056	-271.099973	-271.109572	-271.175845
MPx(full)/6-311+G(3df,3pd)//MP2(full)/6-311+G(3df,3pd)				
Staggered, C_s	-271.109131	-271.100043	-271.109640	-271.175932
Eclipsed, C_s	-271.109056	-271.099973	-271.109572	-271.175845

[a]All energies in Hartree.

TABLE S3. Conformation Preference Energies of Toluene[a]

Level of Optimization (LoO)	ΔE^b LoO	ΔG^c LoO	$\Delta G_{HR}{}^d$ LoO	ΔE^e MP3	ΔE^e MP4 (SD)	ΔE^e MP4 (SDQ)	ΔE^e MP4 (SDTQ)	$\Delta G'_{HR}{}^f$
APFD/6-311G*	10.7	1302.0	1030.2					
MP2(full)/6-311G*	56.5	733.4	723.7	45.8	44.6	43.3	52.7	719.9
MP2(full)/6-311+G(2df,p)	53.3	778.0	742.5	47.1	43.9	42.7	54.6	743.7
MP2(full)/6-311+G(3df,3pd)	18.2	1046.1	847.8	47.1	43.9	42.7	54.6	884.2

[a]All data in cal/mol.

[b]Relative energies ΔE determined with total energies E_{tot} computed at the level used for the structure optimization (LoO).

[c]Relative free enthalpies ΔG determined with total energies E_{tot} and thermochemical data TE_{298} and S_{298} computed by harmonic vibrational analysis at the level used for the structure optimization (LoO).

[d]Relative free enthalpies ΔG_{HR} determined with total energies E_{tot} and thermochemical data TE_{298} and S_{298} corrected for hindered rotation (HR).

[e]Relative energies ΔE determined with MPx energies computed at MPx(full)/6-311G*//MP2(full)/6-311G*, MPx(full)/6-311+G(2df,p)//MP2(full)/6-311+G(2df,p), and MPx(full)/6-311+G(3df,3pd)//MP2(full)/6-311+G(3df,3pd). Relative energies determined using fourth-order Møller-Plesset perturbation theory (MP4) include single and double excitations (SD), single, double and quadruple excitations (SDQ), and single, double, triple, and quadruple excitations (SDTQ).

[f]Relative free enthalpies $\Delta G'_{HR}$ determined with the $E(MP4[SDTQ])$ energies and thermochemical data TE_{298} and S_{298} corrected for hindered rotation (HR).

Stationary Structures of Toluene Computed at APFD/6-311G* Level

Toluene, staggered, C_s at APFD/6-311G*

```
                        Standard orientation:
---------------------------------------------------------------------
 Center     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number       Type         X           Y           Z
---------------------------------------------------------------------
    1          6           0       -0.007369   -1.196096    1.201644
    2          6           0       -0.007369    0.194847    1.198455
    3          6           0       -0.005140    0.910637    0.000000
    4          6           0       -0.007369    0.194847   -1.198455
    5          6           0       -0.007369   -1.196096   -1.201644
    6          6           0       -0.006830   -1.897534   -0.000000
    7          1           0       -0.011708   -1.733903    2.146029
    8          1           0       -0.010595    0.735556    2.142341
    9          1           0       -0.010595    0.735556   -2.142341
   10          1           0       -0.011708   -1.733903   -2.146029
   11          1           0       -0.009975   -2.983947   -0.000000
   12          6           0        0.028572    2.412860    0.000000
   13          1           0        1.059800    2.783895    0.000000
   14          1           0       -0.463987    2.827974   -0.883171
   15          1           0       -0.463987    2.827974    0.883171
---------------------------------------------------------------------
 Rotational constants (GHZ):         5.5658143              2.5297444
1.7582176
 Standard basis: 6-311G(d) (5D, 7F)
```

Toluene, eclipsed, C_s at APFD/6-311G*

```
                        Standard orientation:
---------------------------------------------------------------------
 Center     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number       Type         X           Y           Z
---------------------------------------------------------------------
    1          6           0       -1.208785   -1.192007    0.000000
    2          6           0       -1.200028    0.200424    0.000000
    3          6           0       -0.000000    0.910539    0.000000
    4          6           0        1.196834    0.189104    0.000000
    5          6           0        1.194520   -1.200325    0.000000
    6          6           0       -0.011140   -1.897582    0.000000
    7          1           0       -2.155581   -1.725536    0.000000
    8          1           0       -2.142060    0.744012    0.000000
    9          1           0        2.142537    0.727079    0.000000
   10          1           0        2.136502   -1.742388    0.000000
   11          1           0       -0.015089   -2.983995    0.000000
   12          6           0        0.019395    2.413120    0.000000
   13          1           0       -0.989937    2.831021    0.000000
   14          1           0        0.539429    2.805088    0.880131
   15          1           0        0.539429    2.805088   -0.880131
---------------------------------------------------------------------
 Rotational constants (GHZ):         5.5662468              2.5295250
1.7580676
 Standard basis: 6-311G(d) (5D, 7F)
```

Stationary Structures of Toluene Computed at MP2(full)/6-311G* Level

Toluene, staggered, C_s at MP2(full)/6-311G*

```
                        Standard orientation:
---------------------------------------------------------------------
```

```
Center      Atomic      Atomic              Coordinates (Angstroms)
Number      Number      Type            X            Y            Z
---------------------------------------------------------------------
    1          6           0        -0.007309    -1.200347     1.206955
    2          6           0        -0.007309     0.196678     1.203406
    3          6           0        -0.008393     0.915164     0.000000
    4          6           0        -0.007309     0.196678    -1.203406
    5          6           0        -0.007309    -1.200347    -1.206955
    6          6           0        -0.005901    -1.904224    -0.000000
    7          1           0        -0.010841    -1.738266     2.151420
    8          1           0        -0.011519     0.736694     2.148245
    9          1           0        -0.011519     0.736694    -2.148245
   10          1           0        -0.010841    -1.738266    -2.151420
   11          1           0        -0.008777    -2.990728    -0.000000
   12          6           0         0.030172     2.421244     0.000000
   13          1           0         1.062440     2.784838     0.000000
   14          1           0        -0.464395     2.829984    -0.884091
   15          1           0        -0.464395     2.829984     0.884091
---------------------------------------------------------------------
 Rotational constants (GHZ):        5.5231407              2.5138406
1.7463748
 Standard basis: 6-311G(d) (5D, 7F)
```

Toluene, eclipsed, C_s at MP2(full)/6-311G*
```
                            Standard orientation:
---------------------------------------------------------------------
Center      Atomic      Atomic              Coordinates (Angstroms)
Number      Number      Type            X            Y            Z
---------------------------------------------------------------------
    1          6           0        -1.213493    -1.196551     0.000000
    2          6           0        -1.204990     0.201584     0.000000
    3          6           0         0.000000     0.915094     0.000000
    4          6           0         1.201725     0.191447     0.000000
    5          6           0         1.200364    -1.204454     0.000000
    6          6           0        -0.010028    -1.904391     0.000000
    7          1           0        -2.160032    -1.730792     0.000000
    8          1           0        -2.148021     0.744288     0.000000
    9          1           0         2.148461     0.728711     0.000000
   10          1           0         2.142801    -1.745957     0.000000
   11          1           0        -0.013735    -2.990891     0.000000
   12          6           0         0.018278     2.421830     0.000000
   13          1           0        -0.994281     2.830512     0.000000
   14          1           0         0.536839     2.808384     0.881810
   15          1           0         0.536839     2.808384    -0.881810
---------------------------------------------------------------------
 Rotational constants (GHZ):        5.5238925              2.5132185
1.7460379
 Standard basis: 6-311G(d) (5D, 7F)
```

Stationary Structures of Toluene Computed at MP2(full)/6-311+G(2df,p) Level

Toluene, staggered, C_s at MP2(full)/6-311+G(2df,p)
```
                            Standard orientation:
---------------------------------------------------------------------
Center      Atomic      Atomic              Coordinates (Angstroms)
Number      Number      Type            X            Y            Z
---------------------------------------------------------------------
    1          6           0        -0.007875    -1.194378     1.200738
    2          6           0        -0.007875     0.195432     1.196549
    3          6           0        -0.005129     0.910247     0.000000
    4          6           0        -0.007875     0.195432    -1.196549
```

```
    5            6            0        -0.007875    -1.194378    -1.200738
    6            6            0        -0.006932    -1.894433    -0.000000
    7            1            0        -0.012599    -1.731003     2.143123
    8            1            0        -0.012448     0.735693     2.138521
    9            1            0        -0.012448     0.735693    -2.138521
   10            1            0        -0.012599    -1.731003    -2.143123
   11            1            0        -0.009989    -2.978511    -0.000000
   12            6            0         0.030771     2.408943     0.000000
   13            1            0         1.061241     2.773910     0.000000
   14            1            0        -0.462208     2.817013    -0.883544
   15            1            0        -0.462208     2.817013     0.883544
 -------------------------------------------------------------------
 Rotational constants (GHZ):          5.5792185              2.5386289
 1.7638514
 Standard basis: 6-311+G(2df,p) (5D, 7F)
```

Toluene, eclipsed, C_s at MP2(full)/6-311+G(2df,p)

```
                         Standard orientation:
 -------------------------------------------------------------------
 Center     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number      Type          X            Y            Z
 -------------------------------------------------------------------
    1            6            0        -1.206877    -1.190972     0.000000
    2            6            0        -1.197931     0.199971     0.000000
    3            6            0        -0.000000     0.910177     0.000000
    4            6            0         1.195081     0.190642     0.000000
    5            6            0         1.194540    -1.198035     0.000000
    6            6            0        -0.009358    -1.894587     0.000000
    7            1            0        -2.151250    -1.724093     0.000000
    8            1            0        -2.137954     0.743145     0.000000
    9            1            0         2.139072     0.727937     0.000000
   10            1            0         2.135022    -1.738039     0.000000
   11            1            0        -0.012751    -2.978663     0.000000
   12            6            0         0.016681     2.409395     0.000000
   13            1            0        -0.994870     2.816554     0.000000
   14            1            0         0.534959     2.796806     0.879992
   15            1            0         0.534959     2.796806    -0.879992
 -------------------------------------------------------------------
 Rotational constants (GHZ):          5.5799527              2.5381627
 1.7636011
 Standard basis: 6-311+G(2df,p) (5D, 7F)
```

Stationary Structures of Toluene Computed at MP2(full)/6-311+G(3df,3pd) Level

Toluene, staggered, Cs at MP2(full)/6-311+G(3df,3pd)

```
                         Standard orientation:
 -------------------------------------------------------------------
 Center     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number      Type          X            Y            Z
 -------------------------------------------------------------------
    1            6            0         0.005871     0.911029     0.000000
    2            6            0         0.007740     0.195124     1.196112
    3            6            0         0.007740    -1.194756     1.201480
    4            6            0         0.006449    -1.893231     0.000000
    5            6            0         0.007740    -1.194756    -1.201480
    6            6            0         0.007740     0.195124    -1.196112
    7            1            0         0.012128    -1.729763    -2.141769
    8            1            0         0.012738     0.735365    -2.135371
```

```
    9          1          0          0.012128   -1.729763    2.141769
   10          1          0          0.009098   -2.974942    0.000000
   11          6          0         -0.030257    2.409025    0.000000
   12          1          0          0.461149    2.814936   -0.881860
   13          1          0         -1.059266    2.768510    0.000000
   14          1          0          0.461149    2.814936    0.881860
   15          1          0          0.012738    0.735365    2.135371
 ----------------------------------------------------------------------
```

Toluene, eclipsed, C_s at MP2(full)/6-311+G(3df,3pd)

```
                        Standard orientation:
 ----------------------------------------------------------------------
 Center     Atomic     Atomic            Coordinates (Angstroms)
 Number     Number     Type           X           Y           Z
 ----------------------------------------------------------------------
    1          6          0         -1.207845   -1.191285    0.000000
    2          6          0         -1.197576    0.199708    0.000000
    3          6          0          0.000000    0.910862    0.000000
    4          6          0          1.194723    0.190359    0.000000
    5          6          0          1.194997   -1.198469    0.000000
    6          6          0         -0.009599   -1.893488    0.000000
    7          1          0         -2.150091   -1.722704    0.000000
    8          1          0         -2.134649    0.743295    0.000000
    9          1          0          2.135983    0.727382    0.000000
   10          1          0          2.133384   -1.736780    0.000000
   11          1          0         -0.013054   -2.975117    0.000000
   12          6          0          0.017131    2.409483    0.000000
   13          1          0         -0.991920    2.815261    0.000000
   14          1          0          0.534676    2.792819    0.878291
   15          1          0          0.534676    2.792819   -0.878291
 ----------------------------------------------------------------------
 Rotational constants (GHZ):          5.5819046              2.5394337
1.7643354
 Standard basis: 6-311+G(3df,3pd)  (5D, 7F)
```

Stationary Structures of Benzaldehyde Azines Computed at APFD/6-311G* Level

1(H, Cl, Cl), C_{2h} at APFD/6-311G*

```
                        Standard orientation:
 ----------------------------------------------------------------------
 Center     Atomic     Atomic            Coordinates (Angstroms)
 Number     Number     Type           X           Y           Z
 ----------------------------------------------------------------------
    1         17          0          1.639758    7.222158    0.000000
    2          7          0         -0.060186    0.685803    0.000000
    3          6          0          2.607089    4.694921    0.000000
    4          1          0          3.591607    5.149625    0.000000
    5          6          0          2.459334    3.314593    0.000000
    6          1          0          3.344797    2.684245    0.000000
    7          6          0          0.194370    4.931596    0.000000
    8          1          0         -0.679199    5.574523    0.000000
    9          6          0          1.191046    2.726503    0.000000
   10          6          0          0.060186    3.554678    0.000000
   11          1          0         -0.922710    3.095833    0.000000
   12          6          0          1.076589    1.276418    0.000000
   13          6          0          1.470186    5.492769    0.000000
   14         17          0         -1.639758   -7.222158   -0.000000
   15          7          0          0.060186   -0.685803    0.000000
   16          6          0         -2.607089   -4.694921   -0.000000
   17          1          0         -3.591607   -5.149625   -0.000000
```

```
  18          6          0      -2.459334    -3.314593    -0.000000
  19          1          0      -3.344797    -2.684245    -0.000000
  20          6          0      -0.194370    -4.931596    -0.000000
  21          1          0       0.679199    -5.574523     0.000000
  22          6          0      -1.191046    -2.726503    -0.000000
  23          6          0      -0.060186    -3.554678    -0.000000
  24          1          0       0.922710    -3.095833     0.000000
  25          6          0      -1.076589    -1.276418    -0.000000
  26          6          0      -1.470186    -5.492769    -0.000000
  27          1          0       1.997395     0.684339     0.000000
  28          1          0      -1.997395    -0.684339    -0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):        2.4147615               0.0733035
 0.0711438
```

2(H, Br, Br), C_{2h} at APFD/6-311G*

```
                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type          X           Y           Z
 ---------------------------------------------------------------------
    1          7          0      -0.060125     0.685942     0.000000
    2          6          0       2.607884     4.694905     0.000000
    3          1          0       3.594077     5.145605     0.000000
    4          6          0       2.459198     3.314285     0.000000
    5          1          0       3.344553     2.683569     0.000000
    6          6          0       0.193280     4.931646     0.000000
    7          1          0      -0.682871     5.570758     0.000000
    8          6          0       1.190997     2.726490     0.000000
    9          6          0       0.060125     3.554139     0.000000
   10          1          0      -0.922753     3.095013     0.000000
   11          6          0       1.076793     1.276387     0.000000
   12          6          0       1.470120     5.494231     0.000000
   13          7          0       0.060125    -0.685942     0.000000
   14          6          0      -2.607884    -4.694905     0.000000
   15          1          0      -3.594077    -5.145605     0.000000
   16          6          0      -2.459198    -3.314285     0.000000
   17          1          0      -3.344553    -2.683569     0.000000
   18          6          0      -0.193280    -4.931646     0.000000
   19          1          0       0.682871    -5.570758     0.000000
   20          6          0      -1.190997    -2.726490     0.000000
   21          6          0      -0.060125    -3.554139     0.000000
   22          1          0       0.922753    -3.095013     0.000000
   23          6          0      -1.076793    -1.276387     0.000000
   24          6          0      -1.470120    -5.494231     0.000000
   25          1          0       1.997449     0.684223     0.000000
   26          1          0      -1.997449    -0.684223     0.000000
   27         35          0       1.655733     7.385116     0.000000
   28         35          0      -1.655733    -7.385116     0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):        2.3407195               0.0417909
 0.0410579
```

8_{tt}(H, Me, Me), C_{2h} at APFD/6-311G*

```
                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type          X           Y           Z
 ---------------------------------------------------------------------
    1          7          0       0.062018     0.686266     0.000000
    2          6          0      -2.598020     4.699870     0.000000
    3          1          0      -3.592792     5.138420     0.000000
```

```
    4          6          0        -2.457118    3.317287    0.000000
    5          1          0        -3.341211    2.683963    0.000000
    6          6          0        -0.210768    4.938278    0.000000
    7          1          0         0.672058    5.573771    0.000000
    8          6          0        -1.189903    2.729868    0.000000
    9          6          0        -0.062018    3.564104    0.000000
   10          1          0         0.922131    3.107112    0.000000
   11          6          0        -1.073304    1.280558    0.000000
   12          6          0        -1.480294    5.532334    0.000000
   13          7          0        -0.062018   -0.686266    0.000000
   14          6          0         2.598020   -4.699870    0.000000
   15          1          0         3.592792   -5.138420    0.000000
   16          6          0         2.457118   -3.317287    0.000000
   17          1          0         3.341211   -2.683963    0.000000
   18          6          0         0.210768   -4.938278    0.000000
   19          1          0        -0.672058   -5.573771    0.000000
   20          6          0         1.189903   -2.729868    0.000000
   21          6          0         0.062018   -3.564104    0.000000
   22          1          0        -0.922131   -3.107112    0.000000
   23          6          0         1.073304   -1.280558    0.000000
   24          6          0         1.480294   -5.532334    0.000000
   25          1          0        -1.994454    0.688348    0.000000
   26          1          0         1.994454   -0.688348    0.000000
   27          6          0        -1.616176    7.027143    0.000000
   28          1          0        -1.136811    7.469188    0.879769
   29          1          0        -1.136811    7.469188   -0.879769
   30          1          0        -2.662514    7.340250    0.000000
   31          6          0         1.616176   -7.027143    0.000000
   32          1          0         1.136811   -7.469188    0.879769
   33          1          0         1.136811   -7.469188   -0.879769
   34          1          0         2.662514   -7.340250    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):        2.4362043              0.1079344
0.1034874
```

8ct(H, Me, Me), C_s at APFD/6-311G*

```
                        Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic            Coordinates (Angstroms)
 Number     Number     Type          X           Y           Z
 ---------------------------------------------------------------------
    1          7          0         0.007577   -0.689639    0.000000
    2          6          0        -2.986592   -4.460315    0.000000
    3          1          0        -4.015030   -4.814069    0.000000
    4          6          0        -2.728464   -3.097862    0.000000
    5          1          0        -3.554457   -2.390404    0.000000
    6          6          0        -0.629378   -4.905828    0.000000
    7          1          0         0.196877   -5.612688    0.000000
    8          6          0        -1.413077   -2.620306    0.000000
    9          6          0        -0.363053   -3.546530    0.000000
   10          1          0         0.657043   -3.176677    0.000000
   11          6          0        -1.173837   -1.185867    0.000000
   12          6          0        -1.942160   -5.387705    0.000000
   13          7          0         0.000000    0.688464    0.000000
   14          6          0         2.990475    4.462592    0.000000
   15          1          0         4.018613    4.815855    0.000000
   16          6          0         2.732924    3.097212    0.000000
   17          1          0         3.559909    2.391019    0.000000
   18          6          0         0.632050    4.902406    0.000000
   19          1          0        -0.194251    5.609914    0.000000
   20          6          0         1.420157    2.619057    0.000000
   21          6          0         0.367281    3.545593    0.000000
   22          1          0        -0.652286    3.174202    0.000000
```

```
   23          6          0       1.181471    1.184719    0.000000
   24          6          0       1.946970    5.386725    0.000000
   25          1          0      -2.041460   -0.517661    0.000000
   26          1          0       2.049293    0.516829    0.000000
   27          6          0      -2.233279   -6.860289    0.000000
   28          1          0      -2.816939   -7.149946    0.879914
   29          1          0      -2.816939   -7.149946   -0.879914
   30          1          0      -1.317213   -7.454921    0.000000
   31          6          0       2.208506    6.864408    0.000000
   32          1          0       1.768144    7.345322   -0.879640
   33          1          0       1.768144    7.345322    0.879640
   34          1          0       3.277547    7.088012    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):       2.4412884               0.1078810
 0.1034474
```

8cc(H, Me, Me), C_{2h} at APFD/6-311G*

```
                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic            Coordinates (Angstroms)
 Number     Number      Type         X           Y           Z
 ---------------------------------------------------------------------
    1          7          0      -0.062505    0.686213    0.000000
    2          6          0       2.598101    4.698914    0.000000
    3          1          0       3.592858    5.138681    0.000000
    4          6          0       2.457605    3.319135    0.000000
    5          1          0       3.341461    2.685390    0.000000
    6          6          0       0.211433    4.940969    0.000000
    7          1          0      -0.671939    5.574938    0.000000
    8          6          0       1.188229    2.730934    0.000000
    9          6          0       0.062505    3.564127    0.000000
   10          1          0      -0.921969    3.107895    0.000000
   11          6          0       1.072315    1.281341    0.000000
   12          6          0       1.478477    5.533476    0.000000
   13          7          0       0.062505   -0.686213    0.000000
   14          6          0      -2.598101   -4.698914    0.000000
   15          1          0      -3.592858   -5.138681    0.000000
   16          6          0      -2.457605   -3.319135    0.000000
   17          1          0      -3.341461   -2.685390    0.000000
   18          6          0      -0.211433   -4.940969    0.000000
   19          1          0       0.671939   -5.574938    0.000000
   20          6          0      -1.188229   -2.730934    0.000000
   21          6          0      -0.062505   -3.564127    0.000000
   22          1          0       0.921969   -3.107895    0.000000
   23          6          0      -1.072315   -1.281341    0.000000
   24          6          0      -1.478477   -5.533476    0.000000
   25          1          0       1.993771    0.689568    0.000000
   26          1          0      -1.993771   -0.689568    0.000000
   27          6          0       1.643159    7.025449    0.000000
   28          1          0       2.200033    7.363994    0.879808
   29          1          0       2.200033    7.363994   -0.879808
   30          1          0       0.679668    7.539680    0.000000
   31          6          0      -1.643159   -7.025449    0.000000
   32          1          0      -2.200033   -7.363994    0.879808
   33          1          0      -2.200033   -7.363994   -0.879808
   34          1          0      -0.679668   -7.539680    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):       2.4463109               0.1078399
 0.1034187
```

S12

Stationary Structures of Acetophenone Azines Computed at APFD/6-311G* Level

1(Me, Cl, Cl), C_2 at APFD/6-311G*

```
                      Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number       Type         X           Y           Z
 ---------------------------------------------------------------------
    1         17           0       -0.355746    7.336601    -0.311105
    2          7           0       -0.134182    0.662922    -0.271802
    3          6           0        0.964071    5.200682     0.703631
    4          1           0        1.527361    5.918540     1.289926
    5          6           0        1.222601    3.839407     0.810193
    6          1           0        1.994943    3.511365     1.498415
    7          6           0       -0.764734    4.726529    -0.919106
    8          1           0       -1.533502    5.082596    -1.596555
    9          6           0        0.497851    2.904315     0.065656
   10          6           0       -0.501311    3.373131    -0.797827
   11          1           0       -1.066836    2.652573    -1.378460
   12          6           0        0.764734    1.458345     0.187249
   13          6           0        2.032330    0.988010     0.837525
   14          1           0        2.225609   -0.049419     0.562180
   15          1           0        1.954905    1.029564     1.929860
   16          1           0        2.884574    1.605202     0.543985
   17          6           0       -0.027881    5.634644    -0.163647
   18         17           0        0.355746   -7.336601    -0.311105
   19          7           0        0.134182   -0.662922    -0.271802
   20          6           0       -0.964071   -5.200682     0.703631
   21          1           0       -1.527361   -5.918540     1.289926
   22          6           0       -1.222601   -3.839407     0.810193
   23          1           0       -1.994943   -3.511365     1.498415
   24          6           0        0.764734   -4.726529    -0.919106
   25          1           0        1.533502   -5.082596    -1.596555
   26          6           0       -0.497851   -2.904315     0.065656
   27          6           0        0.501311   -3.373131    -0.797827
   28          1           0        1.066836   -2.652573    -1.378460
   29          6           0       -0.764734   -1.458345     0.187249
   30          6           0       -2.032330   -0.988010     0.837525
   31          1           0       -2.225609    0.049419     0.562180
   32          1           0       -2.884574   -1.605202     0.543985
   33          1           0       -1.954905   -1.029564     1.929860
   34          6           0        0.027881   -5.634644    -0.163647
 ---------------------------------------------------------------------
 Rotational constants (GHZ):        1.3424285           0.0731041
 0.0716058
```

1(Me, Cl, Cl), C_{2h} at APFD/6-311G*

```
 Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number       Type         X           Y           Z
 ---------------------------------------------------------------------
    1         17           0        1.231797    7.247312     0.000000
    2          7           0       -0.000058    0.683824     0.000000
    3          6           0        2.417177    4.812733     0.000000
    4          1           0        3.358921    5.350737     0.000000
    5          6           0        2.395161    3.423625     0.000000
    6          1           0        3.342726    2.895961     0.000000
    7          6           0        0.000058    4.832590     0.000000
    8          1           0       -0.930132    5.390693     0.000000
    9          6           0        1.188738    2.714689     0.000000
   10          6           0       -0.006339    3.449157     0.000000
```

```
  11            1            0       -0.945871    2.909231    0.000000
  12            6            0        1.165382    1.238243    0.000000
  13            6            0        2.468377    0.494976    0.000000
  14            1            0        2.292741   -0.577110    0.000000
  15            1            0        3.063637    0.755115    0.881089
  16            1            0        3.063637    0.755115   -0.881089
  17            6            0        1.217171    5.508679    0.000000
  18           17            0       -1.231797   -7.247312    0.000000
  19            7            0        0.000058   -0.683824    0.000000
  20            6            0       -2.417177   -4.812733    0.000000
  21            1            0       -3.358921   -5.350737    0.000000
  22            6            0       -2.395161   -3.423625    0.000000
  23            1            0       -3.342726   -2.895961    0.000000
  24            6            0       -0.000058   -4.832590    0.000000
  25            1            0        0.930132   -5.390693    0.000000
  26            6            0       -1.188738   -2.714689    0.000000
  27            6            0        0.006339   -3.449157    0.000000
  28            1            0        0.945871   -2.909231    0.000000
  29            6            0       -1.165382   -1.238243    0.000000
  30            6            0       -2.468377   -0.494976    0.000000
  31            1            0       -2.292741    0.577110    0.000000
  32            1            0       -3.063637   -0.755115   -0.881089
  33            1            0       -3.063637   -0.755115    0.881089
  34            6            0       -1.217171   -5.508679    0.000000
 -------------------------------------------------------------------
 Rotational constants (GHZ):        1.3033251              0.0741154
 0.0701885
```

2(Me, Br, Br), C_2 at APFD/6-311G*

```
                         Standard orientation:
 -------------------------------------------------------------------
 Center     Atomic     Atomic            Coordinates (Angstroms)
 Number     Number      Type         X            Y            Z
 -------------------------------------------------------------------
    1          7          0       -0.116553    0.666068   -0.212386
    2          6          0        1.094769    5.173779    0.769818
    3          1          0        1.676391    5.872966    1.360579
    4          6          0        1.317580    3.805777    0.875680
    5          1          0        2.078906    3.457843    1.566543
    6          6          0       -0.640715    4.744828   -0.860442
    7          1          0       -1.398706    5.116361   -1.541536
    8          6          0        0.571918    2.890188    0.127908
    9          6          0       -0.411691    3.384828   -0.738626
   10          1          0       -0.993580    2.679524   -1.321977
   11          6          0        0.801340    1.437713    0.249524
   12          6          0        2.054518    0.934496    0.903036
   13          1          0        2.222544   -0.107034    0.626490
   14          1          0        1.974656    0.976110    1.995189
   15          1          0        2.922979    1.530478    0.613299
   16          6          0        0.116553    5.635228   -0.101268
   17          7          0        0.116553   -0.666068   -0.212386
   18          6          0       -1.094769   -5.173779    0.769818
   19          1          0       -1.676391   -5.872966    1.360579
   20          6          0       -1.317580   -3.805777    0.875680
   21          1          0       -2.078906   -3.457843    1.566543
   22          6          0        0.640715   -4.744828   -0.860442
   23          1          0        1.398706   -5.116361   -1.541536
   24          6          0       -0.571918   -2.890188    0.127908
   25          6          0        0.411691   -3.384828   -0.738626
   26          1          0        0.993580   -2.679524   -1.321977
   27          6          0       -0.801340   -1.437713    0.249524
   28          6          0       -2.054518   -0.934496    0.903036
```

```
      29             1            0         -2.222544      0.107034      0.626490
      30             1            0         -2.922979     -1.530478      0.613299
      31             1            0         -1.974656     -0.976110      1.995189
      32             6            0         -0.116553     -5.635228     -0.101268
      33            35            0          0.193412     -7.504323     -0.261876
      34            35            0         -0.193412      7.504323     -0.261876
 ----------------------------------------------------------------------
 Rotational constants (GHZ):          1.2829600               0.0420063
 0.0414997
```

2(Me, Br, Br), C_{2h} at APFD/6-311G*

```
                        Standard orientation:
 ----------------------------------------------------------------------
 Center     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number      Type         X           Y           Z
 ----------------------------------------------------------------------
      1          7           0       0.000105     0.683789     0.000000
      2          6           0       2.418979     4.812523     0.000000
      3          1           0       3.362887     5.346418     0.000000
      4          6           0       2.395847     3.422964     0.000000
      5          1           0       3.343374     2.895100     0.000000
      6          6           0       0.000105     4.832724     0.000000
      7          1           0      -0.932204     5.386960     0.000000
      8          6           0       1.189416     2.714414     0.000000
      9          6           0      -0.005427     3.448812     0.000000
     10          1           0      -0.945085     2.908957     0.000000
     11          6           0       1.165845     1.237731     0.000000
     12          6           0       2.468823     0.494017     0.000000
     13          1           0       2.293608    -0.578064     0.000000
     14          1           0       3.063649     0.754539     0.881173
     15          1           0       3.063649     0.754539    -0.881173
     16          6           0       1.218227     5.510147     0.000000
     17          7           0      -0.000105    -0.683789     0.000000
     18          6           0      -2.418979    -4.812523     0.000000
     19          1           0      -3.362887    -5.346418     0.000000
     20          6           0      -2.395847    -3.422964     0.000000
     21          1           0      -3.343374    -2.895100     0.000000
     22          6           0      -0.000105    -4.832724     0.000000
     23          1           0       0.932204    -5.386960     0.000000
     24          6           0      -1.189416    -2.714414     0.000000
     25          6           0       0.005427    -3.448812     0.000000
     26          1           0       0.945085    -2.908957     0.000000
     27          6           0      -1.165845    -1.237731     0.000000
     28          6           0      -2.468823    -0.494017     0.000000
     29          1           0      -2.293608     0.578064     0.000000
     30          1           0      -3.063649    -0.754539    -0.881173
     31          1           0      -3.063649    -0.754539     0.881173
     32          6           0      -1.218227    -5.510147     0.000000
     33         35           0       1.234878     7.410848     0.000000
     34         35           0      -1.234878    -7.410848     0.000000
 ----------------------------------------------------------------------
 Rotational constants (GHZ):          1.2558894               0.0423467
 0.0409862
 Standard basis: 6-311G(d) (5D, 7F)
```

8cc(Me, Me, Me), C_2 at APFD/6-311G*

```
                        Standard orientation:
 ----------------------------------------------------------------------
 Center     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number      Type         X           Y           Z
 ----------------------------------------------------------------------
      1          7           0       0.151791     0.660187    -0.305945
```

```
    2           7           0         -0.151791   -0.660187   -0.305945
    3           6           0         -0.733436    1.477398    0.142451
    4           6           0         -0.436244    2.917666    0.025811
    5           6           0         -1.146612    3.868442    0.767153
    6           6           0         -0.853219    5.221057    0.658612
    7           6           0          0.151791    5.674607   -0.196263
    8           6           0          0.858797    4.724008   -0.936783
    9           6           0          0.576057    3.371689   -0.827780
   10           6           0         -2.019026    1.033833    0.777835
   11           6           0          0.733436   -1.477398    0.142451
   12           6           0          0.436244   -2.917666    0.025811
   13           6           0         -0.576057   -3.371689   -0.827780
   14           6           0         -0.858797   -4.724008   -0.936783
   15           6           0         -0.151791   -5.674607   -0.196263
   16           6           0          0.853219   -5.221057    0.658612
   17           6           0          1.146612   -3.868442    0.767153
   18           6           0          2.019026   -1.033833    0.777835
   19           1           0         -1.930101    3.553253    1.449629
   20           1           0         -1.416020    5.939808    1.250230
   21           1           0          1.643948    5.051865   -1.614175
   22           1           0          1.131678    2.641917   -1.407079
   23           1           0         -2.852980    1.672889    0.478481
   24           1           0         -2.232456    0.001906    0.496554
   25           1           0         -1.951809    1.069883    1.871107
   26           1           0         -1.131678   -2.641917   -1.407079
   27           1           0         -1.643948   -5.051865   -1.614175
   28           1           0          1.416020   -5.939808    1.250230
   29           1           0          1.930101   -3.553253    1.449629
   30           1           0          2.852980   -1.672889    0.478481
   31           1           0          2.232456   -0.001906    0.496554
   32           1           0          1.951809   -1.069883    1.871107
   33           6           0         -0.456224   -7.140622   -0.308015
   34           1           0          0.425410   -7.708399   -0.622718
   35           1           0         -0.776683   -7.554974    0.653620
   36           1           0         -1.250536   -7.335052   -1.032159
   37           6           0          0.456224    7.140622   -0.308015
   38           1           0         -0.425410    7.708399   -0.622718
   39           1           0          0.776683    7.554974    0.653620
   40           1           0          1.250536    7.335052   -1.032159
 ----------------------------------------------------------------------
 Rotational constants (GHZ):       1.3856439              0.1066495
0.1035435
```

8tt(Me, Me, Me), C_2 at APFD/6-311G*

```
                       Standard orientation:
 ----------------------------------------------------------------------
 Center     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number       Type        X           Y           Z
 ----------------------------------------------------------------------
      1           7           0         -0.658135    0.160139   -0.301704
      2           7           0          0.658135   -0.160139   -0.301704
      3           6           0         -1.486941   -0.714919    0.145684
      4           6           0         -2.922883   -0.398156    0.029753
      5           6           0         -3.883107   -1.101090    0.760956
      6           6           0         -5.234245   -0.787143    0.653017
      7           6           0         -5.670926    0.230315   -0.190795
      8           6           0         -4.706973    0.933446   -0.923634
      9           6           0         -3.361815    0.631376   -0.815731
     10           6           0         -1.060455   -2.006930    0.779644
     11           6           0          1.486941    0.714920    0.145684
     12           6           0          2.922883    0.398156    0.029753
     13           6           0          3.361814   -0.631376   -0.815731
     14           6           0          4.706972   -0.933446   -0.923634
```

```
     15           6           0        5.670926   -0.230316   -0.190795
     16           6           0        5.234245    0.787143    0.653016
     17           6           0        3.883107    1.101091    0.760956
     18           6           0        1.060455    2.006930    0.779644
     19           1           0       -3.581167   -1.895202    1.437040
     20           1           0       -5.960176   -1.346243    1.238633
     21           1           0       -5.024611    1.730719   -1.592299
     22           1           0       -2.622386    1.182709   -1.386796
     23           1           0       -1.707294   -2.832924    0.474944
     24           1           0       -0.029745   -2.231244    0.502612
     25           1           0       -1.101300   -1.942160    1.872867
     26           1           0        2.622386   -1.182709   -1.386796
     27           1           0        5.024611   -1.730720   -1.592299
     28           1           0        5.960176    1.346243    1.238633
     29           1           0        3.581168    1.895202    1.437040
     30           1           0        1.707294    2.832924    0.474944
     31           1           0        0.029745    2.231244    0.502612
     32           1           0        1.101301    1.942161    1.872867
     33           6           0        7.127027   -0.568498   -0.327032
     34           1           0        7.486799   -0.370208   -1.342355
     35           1           0        7.744893    0.012928    0.361050
     36           1           0        7.310983   -1.628545   -0.124946
     37           6           0       -7.127028    0.568497   -0.327032
     38           1           0       -7.486800    0.370201   -1.342354
     39           1           0       -7.744893   -0.012925    0.361054
     40           1           0       -7.310983    1.628545   -0.124953
 ----------------------------------------------------------------------
 Rotational constants (GHZ):        1.3809806        0.1067882
 0.1035871
```

8_{ct}(Me, Me, Me), C_1 at APFD/6-311G*

```
                         Standard orientation:
 ----------------------------------------------------------------------
 Center     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number      Type         X           Y           Z
 ----------------------------------------------------------------------
      1           7           0       -0.659011    0.158749   -0.302215
      2           7           0        0.657005   -0.163031   -0.303518
      3           6           0       -1.488339   -0.716616    0.143628
      4           6           0       -2.924065   -0.398287    0.029303
      5           6           0       -3.884450   -1.101842    0.759701
      6           6           0       -5.235368   -0.786427    0.653318
      7           6           0       -5.671677    0.233153   -0.188129
      8           6           0       -4.707567    0.936910   -0.920152
      9           6           0       -3.362612    0.633386   -0.813763
     10           6           0       -1.062630   -2.010540    0.774198
     11           6           0        1.486811    0.710597    0.144561
     12           6           0        2.922708    0.393531    0.026375
     13           6           0        3.361686   -0.625535   -0.827058
     14           6           0        4.709831   -0.926973   -0.937536
     15           6           0        5.671018   -0.232604   -0.198726
     16           6           0        5.232439    0.779189    0.655958
     17           6           0        3.884131    1.091255    0.766003
     18           6           0        1.061806    2.001854    0.781124
     19           1           0       -3.582771   -1.897607    1.433956
     20           1           0       -5.961424   -1.346051    1.238280
     21           1           0       -5.024918    1.735844   -1.586970
     22           1           0       -2.623050    1.185207   -1.384181
     23           1           0       -1.710636   -2.835143    0.468218
     24           1           0       -0.032409   -2.235237    0.495639
     25           1           0       -1.102344   -1.948254    1.867611
     26           1           0        2.623608   -1.171469   -1.405037
     27           1           0        5.025979   -1.717081   -1.614729
```

```
    28          1           0        5.959621    1.332459    1.246260
    29          1           0        3.580670    1.879502    1.448306
    30          1           0        1.711100    2.827309    0.480209
    31          1           0        0.032117    2.228985    0.502465
    32          1           0        1.099793    1.934062    1.874290
    33          6           0        7.132552   -0.557305   -0.312070
    34          1           0        7.543751   -0.882299    0.649394
    35          1           0        7.315067   -1.355058   -1.035531
    36          1           0        7.711971    0.316073   -0.628577
    37          6           0       -7.127586    0.572764   -0.322874
    38          1           0       -7.488605    0.374645   -1.337796
    39          1           0       -7.745304   -0.007981    0.365918
    40          1           0       -7.310313    1.633014   -0.120775
 ----------------------------------------------------------------------
 Rotational constants (GHZ):       1.3830920             0.1067243
 0.1035557
```

8cc(Me, Me, Me), C_{2h} at APFD/6-311G*

```
                         Standard orientation:
 ----------------------------------------------------------------------
 Center     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number       Type         X           Y           Z
 ----------------------------------------------------------------------
     1          7           0       -0.000368    0.684287    0.000000
     2          6           0        2.413847    4.814097    0.000000
     3          1           0        3.367573    5.336458    0.000000
     4          6           0        2.398528    3.423257    0.000000
     5          1           0        3.345250    2.893063    0.000000
     6          6           0        0.022231    4.838921    0.000000
     7          1           0       -0.916437    5.389001    0.000000
     8          6           0        1.192738    2.715458    0.000000
     9          6           0        0.000368    3.456835    0.000000
    10          1           0       -0.941073    2.919506    0.000000
    11          6           0        1.164871    1.239501    0.000000
    12          6           0        2.467117    0.492552    0.000000
    13          1           0        2.289078   -0.579188    0.000000
    14          1           0        3.062599    0.752818    0.880852
    15          1           0        3.062599    0.752818   -0.880852
    16          6           0        1.230304    5.546949    0.000000
    17          7           0        0.000368   -0.684287    0.000000
    18          6           0       -2.413847   -4.814097    0.000000
    19          1           0       -3.367573   -5.336458    0.000000
    20          6           0       -2.398528   -3.423257    0.000000
    21          1           0       -3.345250   -2.893063    0.000000
    22          6           0       -0.022231   -4.838921    0.000000
    23          1           0        0.916437   -5.389001    0.000000
    24          6           0       -1.192738   -2.715458    0.000000
    25          6           0       -0.000368   -3.456835    0.000000
    26          1           0        0.941073   -2.919506    0.000000
    27          6           0       -1.164871   -1.239501    0.000000
    28          6           0       -2.467117   -0.492552    0.000000
    29          1           0       -2.289078    0.579188    0.000000
    30          1           0       -3.062599   -0.752818   -0.880852
    31          1           0       -3.062599   -0.752818    0.880852
    32          6           0       -1.230304   -5.546949    0.000000
    33          6           0        1.233554    7.047635    0.000000
    34          1           0        0.717452    7.446034   -0.879757
    35          1           0        0.717452    7.446034    0.879757
    36          1           0        2.248368    7.451712    0.000000
    37          6           0       -1.233554   -7.047635    0.000000
    38          1           0       -0.717452   -7.446034   -0.879757
    39          1           0       -0.717452   -7.446034    0.879757
    40          1           0       -2.248368   -7.451712    0.000000
```

```
-------------------------------------------------------------------
Rotational constants (GHZ):          1.3396665          0.1087718
0.1008544
```

8tt(Me, Me, Me), C_{2h} at APFD/6-311G*

```
                     Standard orientation:
-------------------------------------------------------------------
Center     Atomic      Atomic           Coordinates (Angstroms)
Number     Number      Type          X           Y           Z
-------------------------------------------------------------------
    1          7          0      -0.001238    0.684156    0.000000
    2          6          0       2.414710    4.813281    0.000000
    3          1          0       3.368216    5.336885    0.000000
    4          6          0       2.399151    3.425374    0.000000
    5          1          0       3.345337    2.894226    0.000000
    6          6          0       0.023480    4.842409    0.000000
    7          1          0      -0.915608    5.391004    0.000000
    8          6          0       1.190857    2.716704    0.000000
    9          6          0       0.001238    3.457475    0.000000
   10          1          0      -0.940831    2.921289    0.000000
   11          6          0       1.163499    1.240511    0.000000
   12          6          0       2.465936    0.493950    0.000000
   13          1          0       2.288121   -0.577847    0.000000
   14          1          0       3.061320    0.754365    0.880888
   15          1          0       3.061320    0.754365   -0.880888
   16          6          0       1.229082    5.548495    0.000000
   17          7          0       0.001238   -0.684156    0.000000
   18          6          0      -2.414710   -4.813281    0.000000
   19          1          0      -3.368216   -5.336885    0.000000
   20          6          0      -2.399151   -3.425374    0.000000
   21          1          0      -3.345337   -2.894226    0.000000
   22          6          0      -0.023480   -4.842409    0.000000
   23          1          0       0.915608   -5.391004    0.000000
   24          6          0      -1.190857   -2.716704    0.000000
   25          6          0      -0.001238   -3.457475    0.000000
   26          1          0       0.940831   -2.921289    0.000000
   27          6          0      -1.163499   -1.240511    0.000000
   28          6          0      -2.465936   -0.493950    0.000000
   29          1          0      -2.288121    0.577847    0.000000
   30          1          0      -3.061320   -0.754365   -0.880888
   31          1          0      -3.061320   -0.754365    0.880888
   32          6          0      -1.229082   -5.548495    0.000000
   33          6          0       1.260318    7.049252    0.000000
   34          1          0       1.784406    7.436459    0.879937
   35          1          0       1.784406    7.436459   -0.879937
   36          1          0       0.254642    7.475521    0.000000
   37          6          0      -1.260318   -7.049252    0.000000
   38          1          0      -1.784406   -7.436459    0.879937
   39          1          0      -1.784406   -7.436459   -0.879937
   40          1          0      -0.254642   -7.475521    0.000000
-------------------------------------------------------------------
Rotational constants (GHZ):          1.3449342          0.1086304
0.1007625
```

8ct(Me, Me, Me), C_s at APFD/6-311G*

```
                     Standard orientation:
-------------------------------------------------------------------
Center     Atomic      Atomic           Coordinates (Angstroms)
Number     Number      Type          X           Y           Z
-------------------------------------------------------------------
    1          7          0       0.006657    0.684252    0.000000
    2          6          0       2.443188    4.801069    0.000000
```

```
    3            1            0          3.399753    5.318224    0.000000
    4            6            0          2.420327    3.410302    0.000000
    5            1            0          3.364151    2.875006    0.000000
    6            6            0          0.051795    4.838853    0.000000
    7            1            0         -0.883818    5.394120    0.000000
    8            6            0          1.210748    2.709070    0.000000
    9            6            0          0.022375    3.456965    0.000000
   10            1            0         -0.921902    2.924686    0.000000
   11            6            0          1.174961    1.233360    0.000000
   12            6            0          2.473008    0.479195    0.000000
   13            1            0          2.288949   -0.591534    0.000000
   14            1            0          3.069863    0.736163    0.880884
   15            1            0          3.069863    0.736163   -0.880884
   16            6            0          1.263718    5.540334    0.000000
   17            7            0          0.000000   -0.684101    0.000000
   18            6            0         -2.441082   -4.798186    0.000000
   19            1            0         -3.397651   -5.316153    0.000000
   20            6            0         -2.417081   -3.410474    0.000000
   21            1            0         -3.359929   -2.873425    0.000000
   22            6            0         -0.050030   -4.841870    0.000000
   23            1            0          0.885785   -5.396027    0.000000
   24            6            0         -1.204450   -2.709149    0.000000
   25            6            0         -0.019376   -3.457035    0.000000
   26            1            0          0.926016   -2.926715    0.000000
   27            6            0         -1.168225   -1.233193    0.000000
   28            6            0         -2.466200   -0.478845    0.000000
   29            1            0         -2.281997    0.591856    0.000000
   30            1            0         -3.063147   -0.735697   -0.880877
   31            1            0         -3.063147   -0.735697    0.880877
   32            6            0         -1.259886   -5.540585    0.000000
   33            6            0          1.275069    7.040986    0.000000
   34            1            0          0.761137    7.442152   -0.879765
   35            1            0          0.761137    7.442152    0.879765
   36            1            0          2.292065    7.439543    0.000000
   37            6            0         -1.299727   -7.041143    0.000000
   38            1            0         -1.826020   -7.425367    0.879938
   39            1            0         -1.826020   -7.425367   -0.879938
   40            1            0         -0.296485   -7.473059    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):        1.3420992            0.1087029
 0.1008089
```

Stationary Structures of Benzaldehyde Azines Computed at MP2(full)6-311G* Level

1(H, Cl, Cl), C_{2h} at MP2(full)/6-311G*
```
 Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number      Type         X           Y           Z
 ---------------------------------------------------------------------
    1           17           0          1.659030    7.235546   -0.000000
    2            7            0         -0.067454    0.693710   -0.000000
    3            6            0          2.626948    4.705116   -0.000000
    4            1            0          3.612076    5.160832   -0.000000
    5            6            0          2.478393    3.318898   -0.000000
    6            1            0          3.363393    2.686505   -0.000000
    7            6            0          0.207127    4.946180   -0.000000
    8            1            0         -0.665384    5.592111   -0.000000
    9            6            0          1.202787    2.732298   -0.000000
   10            6            0          0.067454    3.562505   -0.000000
   11            1            0         -0.917713    3.106375   -0.000000
```

```
    12           6            0         1.086700     1.277686    -0.000000
    13           6            0         1.487413     5.510844    -0.000000
    14          17            0        -1.659030    -7.235546     0.000000
    15           7            0         0.067454    -0.693710     0.000000
    16           6            0        -2.626948    -4.705116     0.000000
    17           1            0        -3.612076    -5.160832     0.000000
    18           6            0        -2.478393    -3.318898     0.000000
    19           1            0        -3.363393    -2.686505     0.000000
    20           6            0        -0.207127    -4.946180     0.000000
    21           1            0         0.665384    -5.592111     0.000000
    22           6            0        -1.202787    -2.732298     0.000000
    23           6            0        -0.067454    -3.562505     0.000000
    24           1            0         0.917713    -3.106375     0.000000
    25           6            0        -1.086700    -1.277686     0.000000
    26           6            0        -1.487413    -5.510844     0.000000
    27           1            0         2.000844     0.675157    -0.000000
    28           1            0        -2.000844    -0.675157    -0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):       2.3936576               0.0728968
 0.0707424
```

2(H, Br, Br), C_{2h} at MP2(full)/6-311G*

```
                        Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number      Type          X           Y           Z
 ---------------------------------------------------------------------
     1           7            0        -0.067398     0.693981     0.000000
     2           6            0         2.629178     4.705368     0.000000
     3           1            0         3.616315     5.156559     0.000000
     4           6            0         2.478747     3.318643     0.000000
     5           1            0         3.363485     2.685527     0.000000
     6           6            0         0.205274     4.946842     0.000000
     7           1            0        -0.670221     5.588584     0.000000
     8           6            0         1.202996     2.732352     0.000000
     9           6            0         0.067398     3.562180     0.000000
    10           1            0        -0.917589     3.105296     0.000000
    11           6            0         1.087033     1.277614     0.000000
    12           6            0         1.487446     5.510044     0.000000
    13           7            0         0.067398    -0.693981     0.000000
    14           6            0        -2.629178    -4.705368     0.000000
    15           1            0        -3.616315    -5.156559     0.000000
    16           6            0        -2.478747    -3.318643     0.000000
    17           1            0        -3.363485    -2.685527     0.000000
    18           6            0        -0.205274    -4.946842     0.000000
    19           1            0         0.670221    -5.588584     0.000000
    20           6            0        -1.202996    -2.732352     0.000000
    21           6            0        -0.067398    -3.562180     0.000000
    22           1            0         0.917589    -3.105296     0.000000
    23           6            0        -1.087033    -1.277614     0.000000
    24           6            0        -1.487446    -5.510044     0.000000
    25           1            0         2.001164     0.675265     0.000000
    26           1            0        -2.001164    -0.675265     0.000000
    27          35            0         1.675169     7.392763     0.000000
    28          35            0        -1.675169    -7.392763     0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):       2.3185088               0.0416248
 0.0408907
```

8cc(H, Me, Me), C_{2h} at MP2(full)6-311G*

```
                        Standard orientation:
 ---------------------------------------------------------------------
```

```
 Center      Atomic      Atomic              Coordinates (Angstroms)
 Number      Number      Type            X            Y            Z
 ---------------------------------------------------------------------
     1          7          0        -0.069554     0.693946    -0.000000
     2          6          0         2.618442     4.709020    -0.000000
     3          1          0         3.615041     5.146621    -0.000000
     4          6          0         2.476556     3.322603    -0.000000
     5          1          0         3.359937     2.687037     0.000000
     6          6          0         0.223847     4.955294    -0.000000
     7          1          0        -0.660472     5.589253    -0.000000
     8          6          0         1.199826     2.736695    -0.000000
     9          6          0         0.069554     3.571311    -0.000000
    10          1          0        -0.917367     3.118291    -0.000000
    11          6          0         1.082715     1.281676    -0.000000
    12          6          0         1.495720     5.549554    -0.000000
    13          7          0         0.069554    -0.693946    -0.000000
    14          6          0        -2.618442    -4.709020     0.000000
    15          1          0        -3.615041    -5.146621     0.000000
    16          6          0        -2.476556    -3.322603     0.000000
    17          1          0        -3.359937    -2.687037     0.000000
    18          6          0        -0.223847    -4.955294     0.000000
    19          1          0         0.660472    -5.589253    -0.000000
    20          6          0        -1.199826    -2.736695     0.000000
    21          6          0        -0.069554    -3.571311     0.000000
    22          1          0         0.917367    -3.118291    -0.000000
    23          6          0        -1.082715    -1.281676     0.000000
    24          6          0        -1.495720    -5.549554     0.000000
    25          6          0         1.661880     7.046111    -0.000000
    26          1          0         2.216561     7.379319     0.881764
    27          1          0         2.216561     7.379319    -0.881764
    28          1          0         0.694575     7.552360    -0.000000
    29          6          0        -1.661880    -7.046111     0.000000
    30          1          0        -2.216561    -7.379319     0.881764
    31          1          0        -2.216561    -7.379319    -0.881764
    32          1          0        -0.694575    -7.552360     0.000000
    33          1          0         1.997784     0.680105     0.000000
    34          1          0        -1.997784    -0.680105     0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):        2.4235728           0.1071637
0.1027567
 Standard basis: 6-311G(d) (5D, 7F)
```

8tt(H, Me, Me), *C*2h at MP2(full)6-311G*
```
                    Standard orientation:
 ---------------------------------------------------------------------
 Center      Atomic      Atomic              Coordinates (Angstroms)
 Number      Number      Type            X            Y            Z
 ---------------------------------------------------------------------
     1          7          0         0.069203     0.694240    -0.000000
     2          6          0        -2.618923     4.709299    -0.000000
     3          1          0        -3.615466     5.145736    -0.000000
     4          6          0        -2.476353     3.320793    -0.000000
     5          1          0        -3.359718     2.685171    -0.000000
     6          6          0        -0.223750     4.952975    -0.000000
     7          1          0         0.660015     5.588579    -0.000000
     8          6          0        -1.201278     2.735797    -0.000000
     9          6          0        -0.069203     3.571242    -0.000000
    10          1          0         0.917463     3.117680    -0.000000
    11          6          0        -1.083571     1.281171    -0.000000
    12          6          0        -1.497901     5.548114    -0.000000
    13          7          0        -0.069203    -0.694240    -0.000000
    14          6          0         2.618923    -4.709299    -0.000000
```

```
      15          1          0        3.615466   -5.145736   -0.000000
      16          6          0        2.476353   -3.320793   -0.000000
      17          1          0        3.359718   -2.685171   -0.000000
      18          6          0        0.223750   -4.952975   -0.000000
      19          1          0       -0.660015   -5.588579   -0.000000
      20          6          0        1.201278   -2.735797   -0.000000
      21          6          0        0.069203   -3.571242   -0.000000
      22          1          0       -0.917463   -3.117680   -0.000000
      23          6          0        1.083571   -1.281171   -0.000000
      24          6          0        1.497901   -5.548114   -0.000000
      25          6          0       -1.637611    7.047086   -0.000000
      26          1          0       -1.160940    7.484969    0.881653
      27          1          0       -1.160940    7.484969   -0.881653
      28          1          0       -2.687102    7.348233   -0.000000
      29          6          0        1.637611   -7.047086   -0.000000
      30          1          0        1.160940   -7.484969    0.881653
      31          1          0        1.160940   -7.484969   -0.881653
      32          1          0        2.687102   -7.348233   -0.000000
      33          1          0       -1.998231    0.679048   -0.000000
      34          1          0        1.998231   -0.679048   -0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):          2.4145925              0.1072549
 0.1028243
 Standard basis: 6-311G(d) (5D, 7F)
```

8_{ct}(H, Me, Me), C_s at MP2(full)6-311G*

```
                        Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic             Coordinates (Angstroms)
 Number     Number     Type          X           Y           Z
 ---------------------------------------------------------------------
       1          7          0        0.280654    0.638245    0.000000
       2          6          0       -1.014228    5.293481   -0.000000
       3          1          0       -1.823571    6.020442   -0.000000
       4          6          0       -1.313775    3.930271   -0.000000
       5          1          0       -2.351696    3.603154   -0.000000
       6          6          0        1.336660    4.774543    0.000000
       7          1          0        2.375280    5.100704    0.000000
       8          6          0       -0.286065    2.975143    0.000000
       9          6          0        1.050585    3.413881    0.000000
      10          1          0        1.845782    2.674329    0.000000
      11          6          0       -0.630101    1.556892   -0.000000
      12          6          0        0.313221    5.738893    0.000000
      13          7          0       -0.286065   -0.636754   -0.000000
      14          6          0        1.011005   -5.290875    0.000000
      15          1          0        1.820506   -6.018477    0.000000
      16          6          0        1.310037   -3.929752    0.000000
      17          1          0        2.347854   -3.602168    0.000000
      18          6          0       -1.340535   -4.775544   -0.000000
      19          1          0       -2.378780   -5.101049   -0.000000
      20          6          0        0.280654   -2.973899   -0.000000
      21          6          0       -1.054033   -3.412800   -0.000000
      22          1          0       -1.849543   -2.673585   -0.000000
      23          6          0        0.624595   -1.555398    0.000000
      24          6          0       -0.318404   -5.737848   -0.000000
      25          6          0        0.650262    7.206082    0.000000
      26          1          0        1.240310    7.472567    0.881544
      27          1          0        1.240310    7.472567   -0.881544
      28          1          0       -0.252028    7.820902    0.000000
      29          6          0       -0.628712   -7.211302   -0.000000
      30          1          0       -0.206084   -7.701260   -0.881775
      31          1          0       -0.206084   -7.701260    0.881775
```

```
     32           1           0        -1.705832   -7.389600   -0.000000
     33           1           0        -1.687377    1.271740   -0.000000
     34           1           0         1.681826   -1.270051    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):              2.4190742               0.1072134
 0.1027942
 Standard basis: 6-311G(d) (5D, 7F)
```

8~apa~(H, Me, Me), C_i at MP2(full)6-311G*

8_{apa}(H, Me, Me), _C__i at MP2(full)6-311G*

```
                          Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number      Type          X           Y           Z
 ---------------------------------------------------------------------
     1           7           0        -0.263788    0.001125    0.645871
     2           6           0         1.172386    0.009084    5.259160
     3           1           0         2.003584    0.015593    5.961299
     4           6           0         1.430373    0.005320    3.888222
     5           1           0         2.457934    0.005385    3.529786
     6           6           0        -1.193425    0.010016    4.812948
     7           1           0        -2.221375    0.017070    5.170527
     8           6           0         0.373637   -0.000183    2.964530
     9           6           0        -0.948522    0.005752    3.443555
    10           1           0        -1.765673    0.006120    2.728355
    11           6           0         0.674441   -0.000604    1.536406
    12           6           0        -0.141609    0.014663    5.745055
    13           7           0         0.263788   -0.001125   -0.645871
    14           6           0        -1.172386   -0.009084   -5.259160
    15           1           0        -2.003584   -0.015593   -5.961299
    16           6           0        -1.430373   -0.005320   -3.888222
    17           1           0        -2.457934   -0.005385   -3.529786
    18           6           0         1.193425   -0.010016   -4.812948
    19           1           0         2.221375   -0.017070   -5.170527
    20           6           0        -0.373637    0.000183   -2.964530
    21           6           0         0.948522   -0.005752   -3.443555
    22           1           0         1.765673   -0.006120   -2.728355
    23           6           0        -0.674441    0.000604   -1.536406
    24           6           0         0.141609   -0.014663   -5.745055
    25           6           0        -0.424218   -0.018718    7.223228
    26           1           0        -1.318015    0.560012    7.467923
    27           1           0        -0.592376   -1.045355    7.563741
    28           1           0         0.411772    0.388242    7.796264
    29           6           0         0.424218    0.018718   -7.223228
    30           1           0         0.592376    1.045355   -7.563741
    31           1           0         1.318015   -0.560012   -7.467923
    32           1           0        -0.411772   -0.388242   -7.796264
    33           1           0         1.722548   -0.003446    1.219206
    34           1           0        -1.722548    0.003446   -1.219206
 ---------------------------------------------------------------------
 Rotational constants (GHZ):              2.4174736               0.1072345
 0.1028118
```

8~pa~(H, Me, Me), C_1 at MP2(full)6-311G*

8_{pa}(H, Me, Me), _C_₁ at MP2(full)6-311G*

```
                          Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number      Type          X           Y           Z
 ---------------------------------------------------------------------
     1           7           0        -0.645870   -0.263793   -0.000927
     2           6           0        -5.259181    1.172315   -0.009102
     3           1           0        -5.961334    2.003489   -0.016995
     4           6           0        -3.888244    1.430324   -0.006870
     5           1           0        -3.529820    2.457886   -0.009530
```

```
     6         6          0        -4.812943   -1.193487   -0.004999
     7         1          0        -5.170514   -2.221454   -0.009484
     8         6          0        -2.964535    0.373613    0.000352
     9         6          0        -3.443550   -0.948561   -0.002242
    10         1          0        -2.728341   -1.765705   -0.001277
    11         6          0        -1.536414    0.674430   -0.000897
    12         6          0        -5.745065   -0.141694   -0.011362
    13         7          0         0.645870    0.263793   -0.000928
    14         6          0         5.259181   -1.172315   -0.009103
    15         1          0         5.961334   -2.003489   -0.016997
    16         6          0         3.888244   -1.430324   -0.006870
    17         1          0         3.529820   -2.457885   -0.009530
    18         6          0         4.812943    1.193487   -0.004998
    19         1          0         5.170514    2.221454   -0.009483
    20         6          0         2.964535   -0.373612    0.000353
    21         6          0         3.443550    0.948562   -0.002240
    22         1          0         2.728341    1.765705   -0.001274
    23         6          0         1.536414   -0.674430   -0.000894
    24         6          0         5.745065    0.141694   -0.011362
    25         6          0        -7.223211   -0.424243    0.023674
    26         1          0        -7.468297   -1.319320   -0.552907
    27         1          0        -7.563009   -0.590133    1.050916
    28         1          0        -7.796539    0.410839   -0.384739
    29         6          0         7.223211    0.424242    0.023673
    30         1          0         7.563016    0.590099    1.050918
    31         1          0         7.796536   -0.410827   -0.384769
    32         1          0         7.468294    1.319337   -0.552881
    33         1          0        -1.219225    1.722544   -0.000829
    34         1          0         1.219225   -1.722544   -0.000823
 ---------------------------------------------------------------------
 Rotational constants (GHZ):       2.4174603            0.1072344
0.1028118
```

8$_{pats}$(H, Me, Me), C_1 at MP2(full)6-311G*

```
                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic            Coordinates (Angstroms)
 Number     Number     Type           X           Y           Z
 ---------------------------------------------------------------------
     1         7          0        -0.645786   -0.264578   -0.001133
     2         6          0        -5.258606    1.173122   -0.008427
     3         1          0        -5.960470    2.004550   -0.015181
     4         6          0        -3.887580    1.430655   -0.005313
     5         1          0        -3.528803    2.458097   -0.006138
     6         6          0        -4.813182   -1.192836   -0.008096
     7         1          0        -5.171104   -2.220671   -0.014405
     8         6          0        -2.964237    0.373616    0.000482
     9         6          0        -3.443706   -0.948387   -0.004474
    10         1          0        -2.728778   -1.765776   -0.004616
    11         6          0        -1.536008    0.673942    0.000208
    12         6          0        -5.744942   -0.140713   -0.013034
    13         7          0         0.646151    0.262564    0.000239
    14         6          0         5.259408   -1.174259   -0.000716
    15         1          0         5.960962   -2.005760   -0.001884
    16         6          0         3.887607   -1.431999   -0.001592
    17         1          0         3.529103   -2.459530   -0.003452
    18         6          0         4.812648    1.191459    0.003121
    19         1          0         5.171001    2.219378    0.004970
    20         6          0         2.964500   -0.375634   -0.000131
    21         6          0         3.443936    0.947127    0.002263
    22         1          0         2.728779    1.764305    0.003398
    23         6          0         1.536369   -0.675996   -0.001099
    24         6          0         5.745218    0.138864    0.001661
```

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```
   25          6            0          -7.223196    -0.422811     0.021042
   26          1            0          -7.468400    -1.316836    -0.557121
   27          1            0          -7.563389    -0.590309     1.047893
   28          1            0          -7.796103     0.413151    -0.386156
   29          6            0           7.222124     0.430724     0.002628
   30          1            0           7.506274     1.010679     0.885339
   31          1            0           7.808995    -0.489982     0.001277
   32          1            0           7.506844     1.013628    -0.877954
   33          1            0          -1.218465     1.721948     0.002172
   34          1            0           1.218875    -1.724017    -0.003015
 ---------------------------------------------------------------------
 Rotational constants (GHZ):        2.4160258            0.1072449
 0.1028182
```

Stationary Structures of Acetophenone Azines Computed at MP2(full)6-311G* Level

1(Me, Cl, Cl), C_2 at MP2(full)/6-311G*

```
 Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic       Atomic              Coordinates (Angstroms)
 Number     Number        Type          X           Y            Z
 ---------------------------------------------------------------------
    1          17           0          -0.399949     7.344204    -0.240038
    2           7           0          -0.153031     0.669903    -0.391497
    3           6           0           0.797539     5.173690     0.856293
    4           1           0           1.252918     5.869696     1.554000
    5           6           0           1.066261     3.806564     0.934535
    6           1           0           1.731353     3.449487     1.715548
    7           6           0          -0.669785     4.763967    -1.033213
    8           1           0          -1.334937     5.148863    -1.800165
    9           6           0           0.472467     2.902856     0.038614
   10           6           0          -0.399949     3.401635    -0.944935
   11           1           0          -0.858196     2.705017    -1.639943
   12           6           0           0.740042     1.453579     0.133187
   13           6           0           1.984018     0.957809     0.814724
   14           1           0           2.243683    -0.024536     0.416578
   15           1           0           1.820248     0.842778     1.891804
   16           1           0           2.815826     1.648328     0.669359
   17           6           0          -0.068099     5.645336    -0.130215
   18          17           0           0.399949    -7.344204    -0.240038
   19           7           0           0.153031    -0.669903    -0.391497
   20           6           0          -0.797539    -5.173690     0.856293
   21           1           0          -1.252918    -5.869696     1.554000
   22           6           0          -1.066261    -3.806564     0.934535
   23           1           0          -1.731353    -3.449487     1.715548
   24           6           0           0.669785    -4.763967    -1.033213
   25           1           0           1.334937    -5.148863    -1.800165
   26           6           0          -0.472467    -2.902856     0.038614
   27           6           0           0.399949    -3.401635    -0.944935
   28           1           0           0.858196    -2.705017    -1.639943
   29           6           0          -0.740042    -1.453579     0.133187
   30           6           0          -1.984018    -0.957809     0.814724
   31           1           0          -2.243683     0.024536     0.416578
   32           1           0          -2.815826    -1.648328     0.669359
   33           1           0          -1.820248    -0.842778     1.891804
   34           6           0           0.068099    -5.645336    -0.130215
 ---------------------------------------------------------------------
 Rotational constants (GHZ):        1.3622078            0.0727417
 0.0718386
```

1(Me, Cl, Cl), C_i at MP2(full)/6-311G*

Standard orientation:

```
---------------------------------------------------------------------
Center     Atomic      Atomic           Coordinates (Angstroms)
Number     Number      Type          X            Y            Z
---------------------------------------------------------------------
    1         17          0       -0.520690     7.338931     0.065128
    2          7          0       -0.174235     0.670627     0.025802
    3          6          0        1.191153     5.241347     0.194418
    4          1          0        1.963564     5.979030     0.388834
    5          6          0        1.501724     3.882612     0.135468
    6          1          0        2.531655     3.578424     0.294789
    7          6          0       -1.136730     4.715472    -0.244952
    8          1          0       -2.157115     5.051641    -0.401890
    9          6          0        0.504367     2.922398    -0.106389
   10          6          0       -0.818556     3.361801    -0.296661
   11          1          0       -1.590766     2.625682    -0.493789
   12          6          0        0.830482     1.481706    -0.149519
   13          6          0        2.256186     1.064912    -0.379265
   14          1          0        2.301031     0.012040    -0.644922
   15          1          0        2.846481     1.213149     0.531300
   16          1          0        2.708010     1.668009    -1.169613
   17          6          0       -0.128235     5.651040     0.002528
   18         17          0        0.520690    -7.338931    -0.065128
   19          7          0        0.174235    -0.670627    -0.025802
   20          6          0       -1.191153    -5.241347    -0.194418
   21          1          0       -1.963564    -5.979030    -0.388834
   22          6          0       -1.501724    -3.882612    -0.135468
   23          1          0       -2.531655    -3.578424    -0.294789
   24          6          0        1.136730    -4.715472     0.244952
   25          1          0        2.157115    -5.051641     0.401890
   26          6          0       -0.504367    -2.922398     0.106389
   27          6          0        0.818556    -3.361801     0.296661
   28          1          0        1.590766    -2.625682     0.493789
   29          6          0       -0.830482    -1.481706     0.149519
   30          6          0       -2.256186    -1.064912     0.379265
   31          1          0       -2.301031    -0.012040     0.644922
   32          1          0       -2.846481    -1.213149    -0.531300
   33          1          0       -2.708010    -1.668009     1.169613
   34          6          0        0.128235    -5.651040    -0.002528
---------------------------------------------------------------------
 Rotational constants (GHZ):        1.2895287            0.0738460
0.0701347
```

1(Me, Cl, Cl), C_{2h} at MP2(full)/6-311G*

Standard orientation:

```
---------------------------------------------------------------------
Center     Atomic      Atomic           Coordinates (Angstroms)
Number     Number      Type          X            Y            Z
---------------------------------------------------------------------
    1         17          0        1.323066     7.250699     0.000000
    2          7          0       -0.002247     0.691637     0.000000
    3          6          0        2.481550     4.799955     0.000000
    4          1          0        3.429738     5.328687     0.000000
    5          6          0        2.444428     3.405215     0.000000
    6          1          0        3.386558     2.867184     0.000000
    7          6          0        0.057398     4.850998     0.000000
    8          1          0       -0.865729     5.422565     0.000000
    9          6          0        1.222063     2.710142     0.000000
   10          6          0        0.030364     3.460551     0.000000
   11          1          0       -0.917913     2.934659     0.000000
   12          6          0        1.185022     1.231055     0.000000
```

```
   13          6            0        2.481550    0.471346    0.000000
   14          1            0        2.289884   -0.597507    0.000000
   15          1            0        3.073951    0.729648    0.882285
   16          1            0        3.073951    0.729648   -0.882285
   17          6            0        1.286257    5.517375    0.000000
   18         17            0       -1.323066   -7.250699    0.000000
   19          7            0        0.002247   -0.691637    0.000000
   20          6            0       -2.481550   -4.799955    0.000000
   21          1            0       -3.429738   -5.328687    0.000000
   22          6            0       -2.444428   -3.405215    0.000000
   23          1            0       -3.386558   -2.867184    0.000000
   24          6            0       -0.057398   -4.850998    0.000000
   25          1            0        0.865729   -5.422565    0.000000
   26          6            0       -1.222063   -2.710142    0.000000
   27          6            0       -0.030364   -3.460551    0.000000
   28          1            0        0.917913   -2.934659    0.000000
   29          6            0       -1.185022   -1.231055    0.000000
   30          6            0       -2.481550   -0.471346    0.000000
   31          1            0       -2.289884    0.597507    0.000000
   32          1            0       -3.073951   -0.729648   -0.882285
   33          1            0       -3.073951   -0.729648    0.882285
   34          6            0       -1.286257   -5.517375    0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):        1.2960445              0.0736563
 0.0697558
```

2(Me, Br, Br), C_2 at MP2(full)6-311G*

```
                      Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic            Coordinates (Angstroms)
 Number     Number      Type         X           Y           Z
 ---------------------------------------------------------------------
    1          7            0       -0.135636    0.673555   -0.346072
    2          6            0        0.925050    5.151372    0.909164
    3          1            0        1.397126    5.830919    1.611931
    4          6            0        1.157987    3.776950    0.986067
    5          1            0        1.810303    3.402191    1.769766
    6          6            0       -0.545728    4.779751   -0.990192
    7          1            0       -1.198219    5.176820   -1.761740
    8          6            0        0.545728    2.889381    0.086460
    9          6            0       -0.309364    3.410571   -0.900649
   10          1            0       -0.781633    2.725896   -1.598357
   11          6            0        0.776070    1.433758    0.181169
   12          6            0        2.005217    0.905926    0.865457
   13          1            0        2.242126   -0.081378    0.465278
   14          1            0        1.835173    0.791727    1.941649
   15          1            0        2.854101    1.576340    0.724794
   16          6            0        0.075091    5.644299   -0.082175
   17          7            0        0.135636   -0.673555   -0.346072
   18          6            0       -0.925050   -5.151372    0.909164
   19          1            0       -1.397126   -5.830919    1.611931
   20          6            0       -1.157987   -3.776950    0.986067
   21          1            0       -1.810303   -3.402191    1.769766
   22          6            0        0.545728   -4.779751   -0.990192
   23          1            0        1.198219   -5.176820   -1.761740
   24          6            0       -0.545728   -2.889381    0.086460
   25          6            0        0.309364   -3.410571   -0.900649
   26          1            0        0.781633   -2.725896   -1.598357
   27          6            0       -0.776070   -1.433758    0.181169
   28          6            0       -2.005217   -0.905926    0.865457
   29          1            0       -2.242126    0.081378    0.465278
   30          1            0       -2.854101   -1.576340    0.724794
   31          1            0       -1.835173   -0.791727    1.941649
```

```
   32          6          0      -0.075091   -5.644299   -0.082175
   33         35          0       0.239216   -7.506933   -0.201789
   34         35          0      -0.239216    7.506933   -0.201789
 ---------------------------------------------------------------------
 Rotational constants (GHZ):         1.3133356              0.0418978
 0.0415838
```

2(Me, Br, Br), C_i at MP2(full)6-311G*

```
                        Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic            Coordinates (Angstroms)
 Number     Number      Type         X           Y           Z
 ---------------------------------------------------------------------
    1          7          0      -0.153452    0.675818    0.021611
    2          6          0       1.352419    5.202338    0.200852
    3          1          0       2.147643    5.911804    0.407743
    4          6          0       1.619725    3.833465    0.149014
    5          1          0       2.636896    3.497134    0.325739
    6          6          0      -0.986709    4.747923   -0.277059
    7          1          0      -1.995102    5.110316   -0.451850
    8          6          0       0.596894    2.904607   -0.108338
    9          6          0      -0.708415    3.384468   -0.320913
   10          1          0      -1.499677    2.672078   -0.530081
   11          6          0       0.878466    1.454361   -0.143536
   12          6          0       2.293122    0.992499   -0.354458
   13          1          0       2.307995   -0.061060   -0.620865
   14          1          0       2.875255    1.120711    0.564386
   15          1          0       2.774762    1.581671   -1.137633
   16          6          0       0.048154    5.651381   -0.013410
   17          7          0       0.153452   -0.675818   -0.021611
   18          6          0      -1.352419   -5.202338   -0.200852
   19          1          0      -2.147643   -5.911804   -0.407743
   20          6          0      -1.619725   -3.833465   -0.149014
   21          1          0      -2.636896   -3.497134   -0.325739
   22          6          0       0.986709   -4.747923    0.277059
   23          1          0       1.995102   -5.110316    0.451850
   24          6          0      -0.596894   -2.904607    0.108338
   25          6          0       0.708415   -3.384468    0.320913
   26          1          0       1.499677   -2.672078    0.530081
   27          6          0      -0.878466   -1.454361    0.143536
   28          6          0      -2.293122   -0.992499    0.354458
   29          1          0      -2.307995    0.061060    0.620865
   30          1          0      -2.875255   -1.120711   -0.564386
   31          1          0      -2.774762   -1.581671    1.137633
   32          6          0      -0.048154   -5.651381    0.013410
   33         35          0      -0.322890    7.506129    0.044440
   34         35          0       0.322890   -7.506129   -0.044440
 ---------------------------------------------------------------------
 Rotational constants (GHZ):         1.2431831              0.0422810
 0.0409930
 Standard basis: 6-311G(d) (5D, 7F)
```

2(Me, Br, Br), C_{2h} at MP2(full)/6-311G*

```
                        Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic            Coordinates (Angstroms)
 Number     Number      Type         X           Y           Z
 ---------------------------------------------------------------------
    1          7          0      -0.002345    0.691572    0.000000
    2          6          0       2.481651    4.801067    0.000000
    3          1          0       3.432233    5.325434    0.000000
    4          6          0       2.443498    3.405720    0.000000
```

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```
     5          1          0        3.385882    2.867889    0.000000
     6          6          0        0.053897    4.851098    0.000000
     7          1          0       -0.872373    5.417503    0.000000
     8          6          0        1.221379    2.710183    0.000000
     9          6          0        0.029289    3.459909    0.000000
    10          1          0       -0.918735    2.933286    0.000000
    11          6          0        1.184989    1.231084    0.000000
    12          6          0        2.481651    0.471676    0.000000
    13          1          0        2.290218   -0.597226    0.000000
    14          1          0        3.073988    0.730103    0.882293
    15          1          0        3.073988    0.730103   -0.882293
    16          6          0        1.284210    5.517136    0.000000
    17          7          0        0.002345   -0.691572    0.000000
    18          6          0       -2.481651   -4.801067    0.000000
    19          1          0       -3.432233   -5.325434    0.000000
    20          6          0       -2.443498   -3.405720    0.000000
    21          1          0       -3.385882   -2.867889    0.000000
    22          6          0       -0.053897   -4.851098    0.000000
    23          1          0        0.872373   -5.417503    0.000000
    24          6          0       -1.221379   -2.710183    0.000000
    25          6          0       -0.029289   -3.459909    0.000000
    26          1          0        0.918735   -2.933286    0.000000
    27          6          0       -1.184989   -1.231084    0.000000
    28          6          0       -2.481651   -0.471676    0.000000
    29          1          0       -2.290218    0.597226    0.000000
    30          1          0       -3.073988   -0.730103   -0.882293
    31          1          0       -3.073988   -0.730103    0.882293
    32          6          0       -1.284210   -5.517136    0.000000
    33         35          0        1.324050    7.408658    0.000000
    34         35          0       -1.324050   -7.408658    0.000000
 ----------------------------------------------------------------------
 Rotational constants (GHZ):      1.2490063              0.0421596
 0.0408037
```

8_{ig}(Me, Me, Me), C_2 at MP2(full)6-311G*

```
                        Standard orientation:
 ----------------------------------------------------------------------
 Center     Atomic     Atomic            Coordinates (Angstroms)
 Number     Number     Type         X           Y           Z
 ----------------------------------------------------------------------
     1          7          0        0.166400    0.667327   -0.430500
     2          7          0       -0.166400   -0.667327   -0.430500
     3          6          0       -0.710064    1.467273    0.097578
     4          6          0       -0.418427    2.912378    0.007894
     5          6          0       -0.987830    3.822569    0.912378
     6          6          0       -0.691670    5.184703    0.829827
     7          6          0        0.166400    5.681883   -0.158462
     8          6          0        0.731035    4.765667   -1.060349
     9          6          0        0.447571    3.404971   -0.984054
    10          6          0       -1.961450    0.990108    0.780318
    11          6          0        0.710064   -1.467273    0.097578
    12          6          0        0.418427   -2.912378    0.007894
    13          6          0       -0.447571   -3.404971   -0.984054
    14          6          0       -0.731035   -4.765667   -1.060349
    15          6          0       -0.166400   -5.681883   -0.158462
    16          6          0        0.691670   -5.184703    0.829827
    17          6          0        0.987830   -3.822569    0.912378
    18          6          0        1.961450   -0.990108    0.780318
    19          1          0       -1.650695    3.471768    1.698761
    20          1          0       -1.141664    5.872146    1.543615
    21          1          0        1.393339    5.128343   -1.844444
    22          1          0        0.884672    2.705011   -1.689699
    23          1          0       -2.777837    1.701350    0.648510
```

```
24         1         0      -2.243796    0.018252    0.371618
25         1         0      -1.794396    0.857793    1.854935
26         1         0      -0.884672   -2.705011   -1.689699
27         1         0      -1.393339   -5.128343   -1.844444
28         1         0       1.141664   -5.872146    1.543615
29         1         0       1.650695   -3.471768    1.698761
30         1         0       2.777837   -1.701350    0.648510
31         1         0       2.243796   -0.018252    0.371618
32         1         0       1.794396   -0.857793    1.854935
33         6         0      -0.507953   -7.146439   -0.229943
34         1         0       0.274641   -7.759063    0.223154
35         1         0      -1.442350   -7.355042    0.300737
36         1         0      -0.637422   -7.472123   -1.264808
37         6         0       0.507953    7.146439   -0.229943
38         1         0      -0.274641    7.759063    0.223154
39         1         0       1.442350    7.355042    0.300737
40         1         0       0.637422    7.472123   -1.264808
---------------------------------------------------------------------
 Rotational constants (GHZ):        1.3927795           0.1060291
0.1043631
```

8_{og}(Me, Me, Me), C_2 at MP2(full)6-311G*

```
                         Standard orientation:
---------------------------------------------------------------------
Center     Atomic    Atomic          Coordinates (Angstroms)
Number     Number    Type         X            Y            Z
---------------------------------------------------------------------
   1         7         0       0.165029    0.667642   -0.432349
   2         7         0      -0.165029   -0.667642   -0.432349
   3         6         0      -0.711542    1.465293    0.098903
   4         6         0      -0.424844    2.911318    0.008663
   5         6         0      -0.987035    3.817645    0.921545
   6         6         0      -0.692434    5.180232    0.841634
   7         6         0       0.165029    5.680208   -0.145843
   8         6         0       0.723560    4.767675   -1.055176
   9         6         0       0.440644    3.406674   -0.982294
  10         6         0      -1.960086    0.984533    0.784381
  11         6         0       0.711542   -1.465293    0.098903
  12         6         0       0.424844   -2.911318    0.008663
  13         6         0      -0.440644   -3.406674   -0.982294
  14         6         0      -0.723560   -4.767675   -1.055176
  15         6         0      -0.165029   -5.680208   -0.145843
  16         6         0       0.692434   -5.180232    0.841634
  17         6         0       0.987035   -3.817645    0.921545
  18         6         0       1.960086   -0.984533    0.784381
  19         1         0      -1.642194    3.463090    1.712717
  20         1         0      -1.132477    5.864103    1.564997
  21         1         0       1.389928    5.132018   -1.835051
  22         1         0       0.879094    2.708241   -1.688641
  23         1         0      -2.776862    1.696704    0.660390
  24         1         0      -2.244442    0.015120    0.371147
  25         1         0      -1.788386    0.845386    1.857402
  26         1         0      -0.879094   -2.708241   -1.688641
  27         1         0      -1.389928   -5.132018   -1.835051
  28         1         0       1.132477   -5.864103    1.564997
  29         1         0       1.642194   -3.463090    1.712717
  30         1         0       2.776862   -1.696704    0.660390
  31         1         0       2.244442   -0.015120    0.371147
  32         1         0       1.788386   -0.845386    1.857402
  33         6         0      -0.446045   -7.154775   -0.260676
  34         1         0      -1.469061   -7.336997   -0.598389
  35         1         0       0.228533   -7.625322   -0.982991
  36         1         0      -0.309854   -7.660212    0.698043
```

```
      37          6          0         0.446045      7.154775     -0.260676
      38          1          0         1.469061      7.336997     -0.598389
      39          1          0        -0.228533      7.625322     -0.982991
      40          1          0         0.309854      7.660212      0.698043
 ---------------------------------------------------------------------
 Rotational constants (GHZ):         1.3984294                0.1059616
 0.1043878
```

8_{mg}(Me, Me, Me), C_1 at MP2(full)/6-311G*

```
                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number      Type         X            Y            Z
 ---------------------------------------------------------------------
      1          7          0        -0.666259      0.174022     -0.430812
      2          7          0         0.666111     -0.167759     -0.431978
      3          6          0        -1.471335     -0.697097      0.098236
      4          6          0        -2.914828     -0.397618      0.009101
      5          6          0        -3.825843     -0.954570      0.920520
      6          6          0        -5.185847     -0.647948      0.841714
      7          6          0        -5.678534      0.216648     -0.143190
      8          6          0        -4.761337      0.769868     -1.051094
      9          6          0        -3.402836      0.474950     -0.979301
     10          6          0        -1.001398     -1.951616      0.780288
     11          6          0         1.472172      0.701761      0.098215
     12          6          0         2.915255      0.400440      0.007484
     13          6          0         3.401669     -0.466255     -0.986903
     14          6          0         4.760374     -0.758852     -1.064239
     15          6          0         5.680610     -0.202978     -0.160992
     16          6          0         5.189529      0.655778      0.829739
     17          6          0         3.829465      0.961078      0.913373
     18          6          0         1.003708      1.954652      0.784241
     19          1          0        -3.476875     -1.615079      1.709723
     20          1          0        -5.873373     -1.084162      1.563931
     21          1          0        -5.120040      1.441569     -1.829006
     22          1          0        -2.700743      0.909359     -1.684515
     23          1          0        -1.720234     -2.762083      0.653323
     24          1          0        -0.034059     -2.242708      0.366917
     25          1          0        -0.861738     -1.784268      1.853930
     26          1          0         2.698552     -0.896619     -1.693548
     27          1          0         5.118364     -1.421511     -1.850188
     28          1          0         5.880176      1.099024      1.544654
     29          1          0         3.483342      1.624180      1.701625
     30          1          0         1.720677      2.766369      0.654683
     31          1          0         0.033925      2.244954      0.376169
     32          1          0         0.870029      1.785692      1.858390
     33          6          0         7.142785     -0.554347     -0.233839
     34          1          0         7.760718      0.221831      0.223079
     35          1          0         7.344779     -1.492707      0.292394
     36          1          0         7.467751     -0.681119     -1.269278
     37          6          0        -7.150618      0.510823     -0.256936
     38          1          0        -7.323958      1.536429     -0.591452
     39          1          0        -7.627124     -0.157391     -0.981253
     40          1          0        -7.657094      0.376088      0.701441
 ---------------------------------------------------------------------
 Rotational constants (GHZ):         1.3955542                0.1059961
 0.1043752
```

8_{mgts}(Me, Me, Me), C_1 at MP2(full)/6-311G*

```
                         Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
```

```
Number      Number      Type          X           Y           Z
-------------------------------------------------------------------------
    1          7          0       -0.666576    0.171378   -0.429834
    2          7          0        0.666095   -0.169179   -0.431131
    3          6          0       -1.471357   -0.701395    0.097032
    4          6          0       -2.914795   -0.401543    0.008597
    5          6          0       -3.827013   -0.965997    0.913104
    6          6          0       -5.188041   -0.660513    0.833145
    7          6          0       -5.679885    0.205927   -0.149322
    8          6          0       -4.760562    0.766752   -1.051763
    9          6          0       -3.402513    0.473742   -0.978590
   10          6          0       -1.001162   -1.957033    0.776796
   11          6          0        1.471337    0.700919    0.099380
   12          6          0        2.914699    0.401010    0.008473
   13          6          0        3.401908   -0.464814   -0.986287
   14          6          0        4.760891   -0.756067   -1.063801
   15          6          0        5.680634   -0.199647   -0.160388
   16          6          0        5.188771    0.658246    0.830702
   17          6          0        3.828416    0.962192    0.914527
   18          6          0        1.001763    1.953053    0.786017
   19          1          0       -3.479604   -1.632571    1.697849
   20          1          0       -5.876759   -1.105662    1.548494
   21          1          0       -5.119658    1.437740   -1.830379
   22          1          0       -2.699979    0.910173   -1.682082
   23          1          0       -1.717343   -2.768874    0.643677
   24          1          0       -0.031250   -2.244271    0.366885
   25          1          0       -0.867216   -1.793045    1.851679
   26          1          0        2.699174   -0.895593   -1.693061
   27          1          0        5.119482   -1.418073   -1.850026
   28          1          0        5.879024    1.101886    1.545753
   29          1          0        3.481691    1.624649    1.703056
   30          1          0        1.717758    2.765621    0.656380
   31          1          0        0.031454    2.242367    0.378514
   32          1          0        0.868829    1.783574    1.860177
   33          6          0        7.143144   -0.549575   -0.233442
   34          1          0        7.760348    0.227009    0.223772
   35          1          0        7.346064   -1.487957    0.292395
   36          1          0        7.468189   -0.675608   -1.268946
   37          6          0       -7.145182    0.539012   -0.244422
   38          1          0       -7.727680   -0.018942    0.491635
   39          1          0       -7.316693    1.605399   -0.070930
   40          1          0       -7.538774    0.301167   -1.236621
-------------------------------------------------------------------------
Rotational constants (GHZ):        1.3932749           0.1060298
0.1043712
```

8cc(Me, Me, Me), C_{2h} at MP2(full)/6-311G*

```
                    Standard orientation:
-------------------------------------------------------------------------
Center      Atomic      Atomic          Coordinates (Angstroms)
Number      Number      Type          X           Y           Z
-------------------------------------------------------------------------
    1          7          0       -0.002274    0.691858   -0.000000
    2          6          0        2.479987    4.799650   -0.000000
    3          1          0        3.441433    5.310538   -0.000000
    4          6          0        2.449144    3.405219   -0.000000
    5          1          0        3.389863    2.863958   -0.000000
    6          6          0        0.081091    4.859112   -0.000000
    7          1          0       -0.852568    5.418417   -0.000000
    8          6          0        1.225138    2.711383   -0.000000
    9          6          0        0.038608    3.467308   -0.000000
   10          1          0       -0.912003    2.944997   -0.000000
   11          6          0        1.184468    1.232017   -0.000000
```

```
12              6              0          2.479987      0.469069     -0.000000
13              1              0          2.285442     -0.599379     -0.000000
14              1              0          3.073093      0.727018      0.881933
15              1              0          3.073093      0.727018     -0.881933
16              6              0          1.299440      5.554093     -0.000000
17              7              0          0.002274     -0.691858      0.000000
18              6              0         -2.479987     -4.799650     -0.000000
19              1              0         -3.441433     -5.310538     -0.000000
20              6              0         -2.449144     -3.405219     -0.000000
21              1              0         -3.389863     -2.863958     -0.000000
22              6              0         -0.081091     -4.859112      0.000000
23              1              0          0.852568     -5.418417      0.000000
24              6              0         -1.225138     -2.711383     -0.000000
25              6              0         -0.038608     -3.467308      0.000000
26              1              0          0.912003     -2.944997      0.000000
27              6              0         -1.184468     -1.232017     -0.000000
28              6              0         -2.479987     -0.469069     -0.000000
29              1              0         -2.285442      0.599379     -0.000000
30              1              0         -3.073093     -0.727018     -0.881933
31              1              0         -3.073093     -0.727018      0.881933
32              6              0         -1.299440     -5.554093     -0.000000
33              6              0          1.348926      7.058896     -0.000000
34              1              0          1.875749      7.434902      0.881713
35              1              0          1.875749      7.434902     -0.881713
36              1              0          0.345004      7.488278     -0.000000
37              6              0         -1.348926     -7.058896     -0.000000
38              1              0         -1.875749     -7.434902      0.881713
39              1              0         -1.875749     -7.434902     -0.881713
40              1              0         -0.345004     -7.488278      0.000000
 ----------------------------------------------------------------------
 Rotational constants (GHZ):            1.3356177              0.1079059
 0.1000877
```

8_{tt}(Me, Me, Me), C_i at MP2(full)/6-311G*

```
                       Standard orientation:
 ----------------------------------------------------------------------
 Center     Atomic      Atomic            Coordinates (Angstroms)
 Number     Number      Type          X            Y            Z
 ----------------------------------------------------------------------
    1          7           0       -0.001289      0.692091      0.000000
    2          6           0        2.481355      4.799834      0.000000
    3          1           0        3.442848      5.309518     -0.000000
    4          6           0        2.449691      3.403256     -0.000000
    5          1           0        3.390457      2.862029     -0.000000
    6          6           0        0.082124      4.857012      0.000000
    7          1           0       -0.851278      5.417667      0.000000
    8          6           0        1.227270      2.710435      0.000000
    9          6           0        0.039054      3.467342      0.000000
   10          1           0       -0.911604      2.945122      0.000000
   11          6           0        1.185948      1.231388     -0.000000
   12          6           0        2.481355      0.468298     -0.000000
   13          1           0        2.286870     -0.600125     -0.000000
   14          1           0        3.074457      0.726341      0.881899
   15          1           0        3.074457      0.726341     -0.881899
   16          6           0        1.302787      5.552856      0.000000
   17          7           0        0.001289     -0.692091      0.000000
   18          6           0       -2.481355     -4.799834      0.000000
   19          1           0       -3.442848     -5.309518      0.000000
   20          6           0       -2.449691     -3.403256     -0.000000
   21          1           0       -3.390457     -2.862029     -0.000000
   22          6           0       -0.082124     -4.857012      0.000000
   23          1           0        0.851278     -5.417667      0.000000
   24          6           0       -1.227270     -2.710435      0.000000
```

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```
25          6          0      -0.039054    -3.467342     0.000000
26          1          0       0.911604    -2.945122     0.000000
27          6          0      -1.185948    -1.231388    -0.000000
28          6          0      -2.481355    -0.468298    -0.000000
29          1          0      -2.286870     0.600125    -0.000000
30          1          0      -3.074457    -0.726341    -0.881899
31          1          0      -3.074457    -0.726341     0.881899
32          6          0      -1.302787    -5.552856     0.000000
33          6          0       1.326390     7.057908     0.000000
34          1          0       0.817438     7.458112    -0.881597
35          1          0       0.817438     7.458112     0.881597
36          1          0       2.349658     7.439110     0.000000
37          6          0      -1.326390    -7.057908     0.000000
38          1          0      -0.817438    -7.458112    -0.881597
39          1          0      -0.817438    -7.458112     0.881597
40          1          0      -2.349658    -7.439110     0.000000
 ---------------------------------------------------------------
 Rotational constants (GHZ):        1.3310855            0.1080027
0.1001454
```

8ct(Me, Me, Me), C_s at MP2(full)6-311G*

```
                       Standard orientation:
 ---------------------------------------------------------------
 Center     Atomic     Atomic          Coordinates (Angstroms)
 Number     Number     Type         X            Y            Z
 ---------------------------------------------------------------
    1          7          0      -0.000000    -0.691962     0.000000
    2          6          0      -2.510194    -4.782700     0.000000
    3          1          0      -3.475122    -5.286934     0.000000
    4          6          0      -2.469783    -3.388514     0.000000
    5          1          0      -3.406834    -2.840871     0.000000
    6          6          0      -0.111685    -4.858512     0.000000
    7          1          0       0.818111    -5.424174     0.000000
    8          6          0      -1.241092    -2.703027     0.000000
    9          6          0      -0.059760    -3.467012     0.000000
   10          1          0       0.894453    -2.951264     0.000000
   11          6          0      -1.190344    -1.223958     0.000000
   12          6          0      -2.480792    -0.452506     0.000000
   13          1          0      -2.279291     0.614645     0.000000
   14          1          0      -3.075595    -0.706596     0.881915
   15          1          0      -3.075595    -0.706596    -0.881915
   16          6          0      -1.334772    -5.545105     0.000000
   17          7          0       0.004941     0.692103     0.000000
   18          6          0       2.512978     4.784434     0.000000
   19          1          0       3.477675     5.288029     0.000000
   20          6          0       2.472679     3.388074     0.000000
   21          1          0       3.410106     2.841083     0.000000
   22          6          0       0.114138     4.856552     0.000000
   23          1          0      -0.815667     5.423146     0.000000
   24          6          0       1.245973     2.702877     0.000000
   25          6          0       0.062484     3.467177     0.000000
   26          1          0      -0.891315     2.950736     0.000000
   27          6          0       1.195402     1.224083     0.000000
   28          6          0       2.485867     0.452705     0.000000
   29          1          0       2.284484    -0.614462     0.000000
   30          1          0       3.080599     0.706910    -0.881911
   31          1          0       3.080599     0.706910     0.881911
   32          6          0       1.339059     5.544777     0.000000
   33          6          0      -1.394499    -7.049515     0.000000
   34          1          0      -1.923911    -7.421753     0.881754
   35          1          0      -1.923911    -7.421753    -0.881754
   36          1          0      -0.393474    -7.485606     0.000000
```

```
    37            6            0        1.372529      7.049672      0.000000
    38            1            0        0.866322      7.453277     -0.881629
    39            1            0        0.866322      7.453277      0.881629
    40            1            0        2.398325      7.423977      0.000000
 ---------------------------------------------------------------------
 Rotational constants (GHZ):               1.3335487                0.1079545
0.1001178
 Standard basis: 6-311G(d) (5D, 7F)
```

8apa(Me, Me, Me), C_i at MP2(full)6-311G*

```
                        Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic          Coordinates (Angstroms)
 Number     Number      Type          X           Y           Z
 ---------------------------------------------------------------------
     1           7           0       -0.263788     0.001125     0.645871
     2           6           0        1.172386     0.009084     5.259160
     3           1           0        2.003584     0.015593     5.961299
     4           6           0        1.430373     0.005320     3.888222
     5           1           0        2.457934     0.005385     3.529786
     6           6           0       -1.193425     0.010016     4.812948
     7           1           0       -2.221375     0.017070     5.170527
     8           6           0        0.373637    -0.000183     2.964530
     9           6           0       -0.948522     0.005752     3.443555
    10           1           0       -1.765673     0.006120     2.728355
    11           6           0        0.674441    -0.000604     1.536406
    12           6           0       -0.141609     0.014663     5.745055
    13           7           0        0.263788    -0.001125    -0.645871
    14           6           0       -1.172386    -0.009084    -5.259160
    15           1           0       -2.003584    -0.015593    -5.961299
    16           6           0       -1.430373    -0.005320    -3.888222
    17           1           0       -2.457934    -0.005385    -3.529786
    18           6           0        1.193425    -0.010016    -4.812948
    19           1           0        2.221375    -0.017070    -5.170527
    20           6           0       -0.373637     0.000183    -2.964530
    21           6           0        0.948522    -0.005752    -3.443555
    22           1           0        1.765673    -0.006120    -2.728355
    23           6           0       -0.674441     0.000604    -1.536406
    24           6           0        0.141609    -0.014663    -5.745055
    25           6           0       -0.424218    -0.018718     7.223228
    26           1           0       -1.318015     0.560012     7.467923
    27           1           0       -0.592376    -1.045355     7.563741
    28           1           0        0.411772     0.388242     7.796264
    29           6           0        0.424218     0.018718    -7.223228
    30           1           0        0.592376     1.045355    -7.563741
    31           1           0        1.318015    -0.560012    -7.467923
    32           1           0       -0.411772    -0.388242    -7.796264
    33           1           0        1.722548    -0.003446     1.219206
    34           1           0       -1.722548     0.003446    -1.219206
 ---------------------------------------------------------------------
 Rotational constants (GHZ):               2.4174736                0.1072345
0.1028118
```

8pa(Me, Me, Me), C_1 at MP2(full)6-311G*

```
                        Standard orientation:
 ---------------------------------------------------------------------
 Center     Atomic      Atomic          Coordinates (Angstroms)
 Number     Number      Type          X           Y           Z
 ---------------------------------------------------------------------
     1           7           0       -0.664900    -0.185730     0.056251
     2           6           0       -5.272937     1.058082     0.169354
     3           1           0       -6.018260     1.835923     0.324381
```

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```
    4              6              0         -3.923780      1.409260      0.098931
    5              1              0         -3.645838      2.453248      0.209605
    6              6              0         -4.695055     -1.249382     -0.162807
    7              1              0         -4.989118     -2.290809     -0.281127
    8              6              0         -2.936925      0.427901     -0.094554
    9              6              0         -3.346492     -0.911184     -0.229224
   10              1              0         -2.591824     -1.673298     -0.394303
   11              6              0         -1.504647      0.788310     -0.153420
   12              6              0         -1.125255      2.215283     -0.438364
   13              1              0         -0.068145      2.282197     -0.681307
   14              1              0         -1.316206      2.840471      0.440265
   15              1              0         -1.723785      2.611203     -1.261738
   16              6              0         -5.684518     -0.273714      0.036881
   17              7              0          0.666864      0.199074     -0.002033
   18              6              0          5.264873     -1.028302     -0.292473
   19              1              0          6.003756     -1.782450     -0.556826
   20              6              0          3.915962     -1.383079     -0.237073
   21              1              0          3.630018     -2.405844     -0.465278
   22              6              0          4.701046      1.229215      0.305118
   23              1              0          5.000383      2.252633      0.524371
   24              6              0          2.937587     -0.428677      0.088123
   25              6              0          3.352578      0.888024      0.357531
   26              1              0          2.602298      1.628816      0.614854
   27              6              0          1.505446     -0.789952      0.126978
   28              6              0          1.123249     -2.233933      0.300347
   29              1              0          0.083892     -2.310388      0.609813
   30              1              0          1.236450     -2.773308     -0.646271
   31              1              0          1.770506     -2.714747      1.036439
   32              6              0          5.682666      0.281010     -0.023965
   33              6              0         -7.136787     -0.655329      0.143305
   34              1              0         -7.374153     -1.495244     -0.513927
   35              1              0         -7.386163     -0.955876      1.165933
   36              1              0         -7.787407      0.180119     -0.124677
   37              6              0          7.141421      0.652350     -0.038917
   38              1              0          7.570678      0.587050      0.965936
   39              1              0          7.713609     -0.014538     -0.687743
   40              1              0          7.284959      1.676127     -0.392550
 ------------------------------------------------------------------
 Rotational constants (GHZ):         1.3259399           0.1082005
0.1007995
```

8pats(Me, Me, Me), C_1 at MP2(full)6-311G*

```
                         Standard orientation:
 ----------------------------------------------------------------------
 Center     Atomic     Atomic              Coordinates (Angstroms)
 Number     Number     Type            X              Y              Z
 ----------------------------------------------------------------------
    1          7          0         -0.665626      0.187070     -0.045687
    2          6          0         -5.272634     -1.053151     -0.188309
    3          1          0         -6.017486     -1.827565     -0.361673
    4          6          0         -3.923647     -1.405671     -0.121451
    5          1          0         -3.644958     -2.447022     -0.253425
    6          6          0         -4.695880      1.247015      0.193449
    7          1          0         -4.990439      2.285709      0.332700
    8          6          0         -2.937572     -0.428408      0.095113
    9          6          0         -3.347423      0.907619      0.256257
   10          1          0         -2.593133      1.666071      0.439148
   11          6          0         -1.505484     -0.789760      0.150287
   12          6          0         -1.126292     -2.220532      0.415683
   13          1          0         -0.071805     -2.288876      0.669637
   14          1          0         -1.304757     -2.831272     -0.475702
   15          1          0         -1.733507     -2.631639      1.225033
   16          6          0         -5.684650      0.275616     -0.029197
```

```
17          7           0       0.666081    -0.198306    0.012656
18          6           0       5.265673     1.032211    0.269547
19          1           0       6.006839     1.790992    0.514945
20          6           0       3.918073     1.386498    0.213387
21          1           0       3.633366     2.413243    0.424555
22          6           0       4.700946    -1.233934   -0.292558
23          1           0       4.998775    -2.259374   -0.502741
24          6           0       2.937154     0.426113   -0.091011
25          6           0       3.351084    -0.892616   -0.345150
26          1           0       2.600314    -1.636722   -0.591227
27          6           0       1.505061     0.787927   -0.133558
28          6           0       1.124105     2.229383   -0.329502
29          1           0       0.081763     2.303269   -0.629127
30          1           0       1.249599     2.785792    0.605620
31          1           0       1.764643     2.694764   -1.081336
32          6           0       5.683234    -0.281780    0.016100
33          6           0      -7.136688     0.659272   -0.131495
34          1           0      -7.375828     1.485485    0.542252
35          1           0      -7.383466     0.980762   -1.148368
36          1           0      -7.787913    -0.181536    0.117584
37          6           0       7.142941    -0.646843    0.074263
38          1           0       7.554388    -0.461251    1.070585
39          1           0       7.296969    -1.701763   -0.161583
40          1           0       7.725448    -0.054166   -0.636799
 ---------------------------------------------------------------
 Rotational constants (GHZ):          1.3259993           0.1081822
 0.1007809
```

8_{apafp}(Me, Me, Me), C_i at MP2(full)6-311G*

Constraints: C=N-N=C = 180 deg.; N=C-C-C$_{ortho}$ = 0 deg. for both phenyls.

```
                         Standard orientation:
 ---------------------------------------------------------------
 Center     Atomic      Atomic           Coordinates (Angstroms)
 Number     Number      Type         X            Y            Z
 ---------------------------------------------------------------
     1          7           0      -0.339138    -0.108863    0.593340
     2          6           0      -0.468244     0.286726    5.374830
     3          1           0       0.005133     0.616848    6.297609
     4          6           0       0.189413     0.490799    4.160278
     5          1           0       1.163388     0.969593    4.170420
     6          6           0      -2.307403    -0.727066    4.213319
     7          1           0      -3.288529    -1.198719    4.222547
     8          6           0      -0.392126     0.079949    2.948180
     9          6           0      -1.660825    -0.529002    2.997667
    10          1           0      -2.122965    -0.846709    2.069248
    11          6           0       0.297474     0.295804    1.656860
    12          6           0       1.652617     0.946907    1.656530
    13          1           0       2.030115     1.025788    0.641306
    14          1           0       2.354926     0.362890    2.257942
    15          1           0       1.594429     1.946209    2.097220
    16          6           0      -1.728554    -0.319501    5.425972
    17          7           0       0.339138     0.108863   -0.593340
    18          6           0       0.468244    -0.286726   -5.374830
    19          1           0      -0.005133    -0.616848   -6.297609
    20          6           0      -0.189413    -0.490799   -4.160278
    21          1           0      -1.163388    -0.969593   -4.170420
    22          6           0       2.307403     0.727066   -4.213319
    23          1           0       3.288529     1.198719   -4.222547
    24          6           0       0.392126    -0.079949   -2.948180
    25          6           0       1.660825     0.529002   -2.997667
    26          1           0       2.122965     0.846709   -2.069248
    27          6           0      -0.297474    -0.295804   -1.656860
    28          6           0      -1.652617    -0.946907   -1.656530
```

29	1	0	-2.030115	-1.025788	-0.641306
30	1	0	-2.354926	-0.362890	-2.257942
31	1	0	-1.594429	-1.946209	-2.097220
32	6	0	1.728554	0.319501	-5.425972
33	6	0	-2.422100	-0.572163	6.737667
34	1	0	-3.504682	-0.460663	6.640204
35	1	0	-2.225984	-1.588996	7.092459
36	1	0	-2.077235	0.120487	7.508622
37	6	0	2.422100	0.572163	-6.737667
38	1	0	2.225984	1.588996	-7.092459
39	1	0	3.504682	0.460663	-6.640204
40	1	0	2.077235	-0.120487	-7.508622

 Rotational constants (GHZ):   1.3329051   0.1079796
0.1001370
 Standard basis: 6-311G(d) (5D, 7F)