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Electronic Supplementary Information

Establishing the Mechanisms of Guest Responsive Binding via Twisted Capsules, a Computational Approach

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Computational Details:

Transition state optimizations. DFT calculations were performed to evaluate the proposed mechanism for the basket flipping from **B(+)** to **B(–)** diastereomers with a guest molecule (CX_4) inside. All ground state geometry optimizations were performed with Gaussian 16.[1] Ground state geometry optimizations were carried out with the restricted B3LYP functional.[2–4] The 6-31+G(d) basis set was used for all atoms[5–10] except Br with the 6-311+G(2d) basis set.[11–15] Note that because the default for a general basis set in Gaussian 16 is 5d spherical orbitals, 5d spherical orbitals were used for the CBr_4⊂**B** potential energy surface (PES). Optimized stationary points were confirmed to be local minima (all real vibrational frequencies) or transition states (one imaginary vibrational frequency) on the PES using vibrational frequency analysis. To generate the starting structures along the PES with a CCl_4 guest, all the previously optimized transition states from our previous work were aligned with a CCl_4 guest added into each structure.[16] Each intermediate (I1, I2, I3, etc.) was optimized with a two-step process: (1) the host frozen and the guest allowed to move freely and (2) the whole system allowed to move freely followed by a frequency analysis to confirm that each intermediate as a stationary point. For each transition state (TS1, TS2, TS3, etc.), the two-step optimization procedure was repeated for CCl_4 as a guest with the transition state Berny Algorithm[17] in step (2) and each structure was confirmed to have one correct imaginary frequency motion corresponding to the previously derived transition states from the empty basket transition states. The PES calculation for CBr_4 as a guest was calculated using the same protocol as CCl_4. H(T) and G(T) were calculated at T=298.15 and T=178 K and are reported in the supplemental information, but only G(T) at T=178 K is reported in the main manuscript (Tables S1 – S6). Single point corrections with the B3LYP-D3 functional were performed to address possible dispersion interactions and found $\leq$ 0.1 kcal/mol difference in energy for each structure along the host interconversion PESs (Tables S9 – S10).

Molecular dynamics (MD) of host guest complexes. To observe the stabilized interactions of the guest molecules, we first turned to conventional MD simulations at 300 K on the empty and CX_4 bound **B(+)** and **B(–)** diastereomers. Starting points for each MD simulation were taken from previously optimized geometries of the **B(+)**, **B(–)**, CCl_4⊂**B(+)**, CCl_4⊂**B(–)**, CBr_4⊂**B(+)**, and CBr_4⊂**B(–)** diastereomers at the B3LYP/6-31+G(d) level of theory. In preparation for MD simulations, Merz-Kollman single-point electrostatic potential (ESP) calculations[18] were performed to determine the charges of all atoms at the HF/6-31G(d)[19] level of theory on the MD starting points. Partial atomic charges and force field parameters for the MD starting points were calculated using the RESP protocol for the GAFF2 forcefield implemented in the Antechamber module in the AMBER 18 package.[20,21] The HF/6-31G(d) method correlates with the charge calculations of the standard residues in the AMBER ff14SB force field.[22]

The optimized **B(+)**, **B(–)**, CCl_4⊂**B(+)**, CCl_4⊂**B(–)**, CBr_4⊂**B(+)**, and CBr_4⊂**B(–)** diastereomers were solvated in a square box of $CHCl_3$ molecules[23] until about 20 Å of the basket with the tleap module in AMBER 18.[24–26] Realistically, it would be better to use DCM (CH_2Cl_2) as the solvent to probe for MD simulations; however, DCM is not a built-in solvent model in AMBER 18. DCM parameters have been published, but as a united atom forcefield without hydrogens, so they were not included in this work.[27] The MD protocol involved a two-step minimization, a heating step, a density equilibration, a set of four equilibrations slowly removing restraints on the basket, a production simulation where all restraints were removed, followed by a longer production simulation. In the minimization procedures, the solvent was first optimized followed by the entire system for 2500 steps. The temperature was raised from 0 to 300 K with a small force constant of 20 $\frac{\text{kcal}}{\text{mol}*\text{Å}^2}$ on the basket to resist any drastic changes over 500 ps. A density equilibration step was then performed in the NPT ensemble with the force constant 20 $\frac{\text{kcal}}{\text{mol}*\text{Å}^2}$ still imposed on the basket over 500 ps. The next three equilibration steps were performed in the NPT ensemble over 200 ns and decreased the force constant on the basket from 10, 5, and 1 $\frac{\text{kcal}}{\text{mol}*\text{Å}^2}$. The last equilibration step was performed in the NPT ensemble over 2 ns without any force constant on the basket final densities of those simulations were 1.4640 $\pm$ 0.0033, 1.4634 $\pm$ 0.0035, 1.4638 $\pm$ 0.0036, 1.4639 $\pm$ 0.0035, 1.4653 $\pm$ 0.0038, and 1.4655 $\pm$ 0.0033 $\frac{\text{g}}{\text{cm}^3}$ for **B(+)**, **B(–)**, CCl_4⊂**B(+)**, CCl_4⊂**B(–)**, CBr_4⊂**B(+)**, and CBr_4⊂**B(–)** diastereomers, respectively. The first production simulation was performed in the NPT ensemble with the Langevin piston and periodic boundary conditions over 200 ns and the results were evaluated.[28] For each MD simulation, a non-bonded cutoff of 10.0 Å was used. This process was done separately for **B(+)**, **B(–)**, CCl_4⊂**B(+)**, CCl_4⊂**B(–)**, CBr_4⊂**B(+)**, and CBr_4⊂**B(–)** diastereomers (Figures S2 – S6). Root mean square deviation (RMSD) and arm angle analysis coupled with visual analysis of the trajectory were used to distinguish the diastereomers along each trajectory. To measure the appearance of one basket **B(+)** versus **B(–)** diastereomers along each frame of a trajectory a clustering analysis was implemented using AMBER's CPPTRAJ module.[29]

Adaptive steered molecular dynamics (ASMD) simulations. To observe the dynamics of guest exiting for CCl_4⊂**B(+)**, CCl_4⊂**B(–)**, CBr_4⊂**B(+)**, and CBr_4⊂**B(–)** diastereomers we turned to ASMD simulations.[30–35] ASMD is an advanced interpolation scheme based on steered molecular dynamics (SMD) for the generation of guest exiting pathways that works as follows: SMD utilizes a pseudo

particle to apply a steering force to traverse the reaction coordinate at a specific velocity using an artificial bias potential in the form of a spring constant. The underlying drawback to SMD is that many simulations must be run to converge the potential mean force (PMF) along the designated reaction coordinate. ASMD divides the reaction coordinate into stages where many SMD simulations are performed, and one path is calculated to be the Jarzynski average (JA). In our case, for each ASMD simulation performed, the stage lengths were divided into 1 Å steps with 30 trajectories per stage over 15 stages and a spring constant of 5 $\frac{\text{kcal}}{\text{mol}*\text{Å}^2}$ with various pulling speeds. The reaction coordinate was chosen to be the distance between (1) the centroid of the aryl moiety (shown in magenta in Figure S1a) on one basket arm to (2) the center of mass of the guest molecule (shown in red in Figure S1a), resulting in a guest exit out of gate 1. To test convergence of different pulling speeds for guest exiting, CCl_4⊂**B(–)** ASMD simulations were performed using the end of the fourth equilibration step from previously performed MD simulations at 300 K in the NPT ensemble. For CCl_4⊂**B(–)** pulling speeds of 25, 10, 1, and 0.1 $\frac{\text{Å}}{\text{ns}}$ were performed (Figure S1b) at 300 K, showing excellent convergence of the PMF at a pulling speed of 0.1 $\frac{\text{Å}}{\text{ns}}$ (Figure S1c) and ASMD simulations at this pulling speed were repeated 2 more times (Figure S7). The ASMD protocol for CCl_4⊂**B(–)** was then repeated for CCl_4⊂**B(+)**, CBr_4⊂**B(+)**, and CBr_4⊂**B(–)** diastereomers in triplicate with a pulling speed of 0.1 $\frac{\text{Å}}{\text{ns}}$ (Figures S14, S18 and S22).

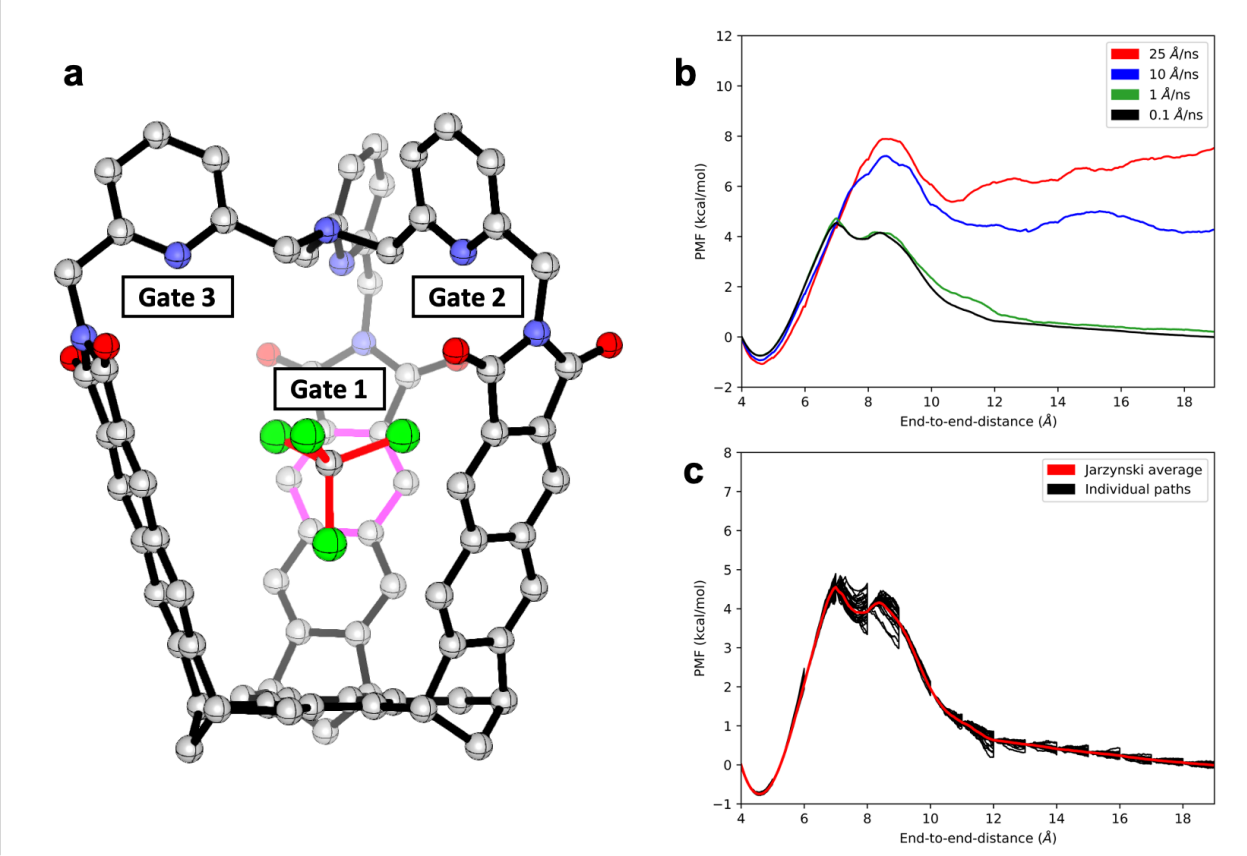

Figure S1. (a) Illustration of gates 1, 2, and 3 analyzed during the CCl_4⊂**B(–)** pulling simulations (hydrogens hidden for clarity), (b) pulling speed comparison or 25, 10, 1, and 0.1 $\frac{\text{Å}}{\text{ns}}$ for CCl_4⊂**B(–)** pulling simulations (c) Jarzynski PMF plots for every ASMD trajectory in the first run at a pulling speed of 0.1 $\frac{\text{Å}}{\text{ns}}$.

Voss Volume Voxelator (^{3}V) calculations.[36] To further analyze the change in volume over the course of each PES for CX_4⊂**B(+)** to CX_4⊂**B(–)**, ^{3}V was used to evaluate a possible volume component to the changes in energy. To measure the volume of each system, the "channel extractor" function was used with an outer probe radius of 10 Å and an inner probe radius of 0.3 Å. For the

CCl_4⊂**B(+)**, CCl_4⊂**B(–)**, CBr_4⊂**B(+)**, and CBr_4⊂**B(–)** diastereomers, the guests were removed, and the volumes of the empty complexes were measured along the different reaction coordinates (Table S7 – S8).

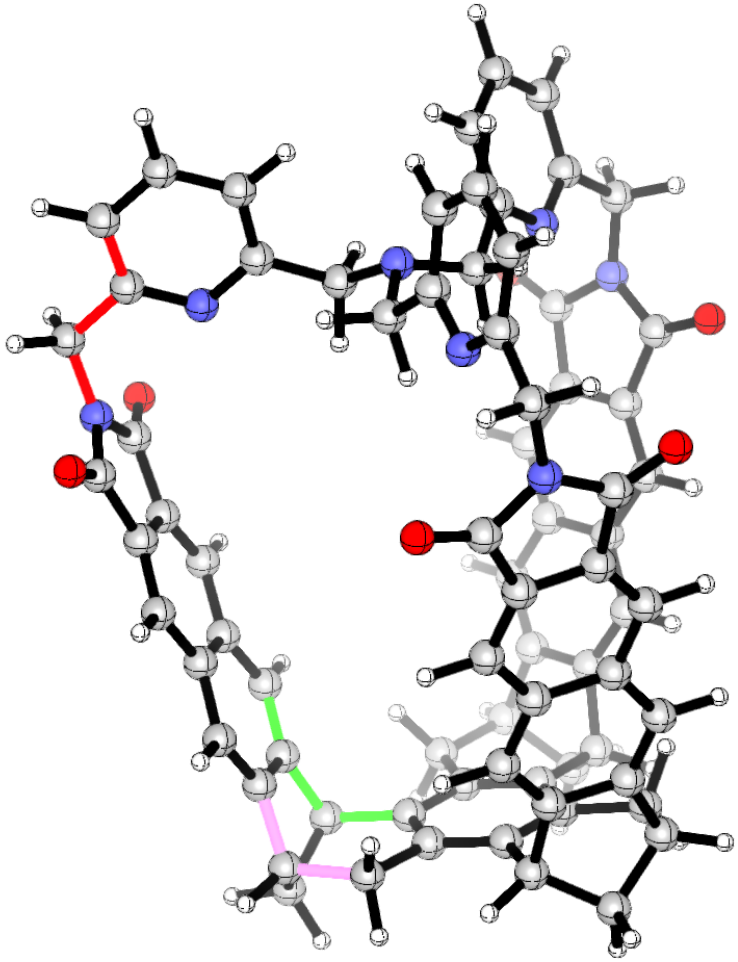

Figure S2. Arm angles measured during the conventional MD and NEB simulations shown on the **B(+)** diastereomer

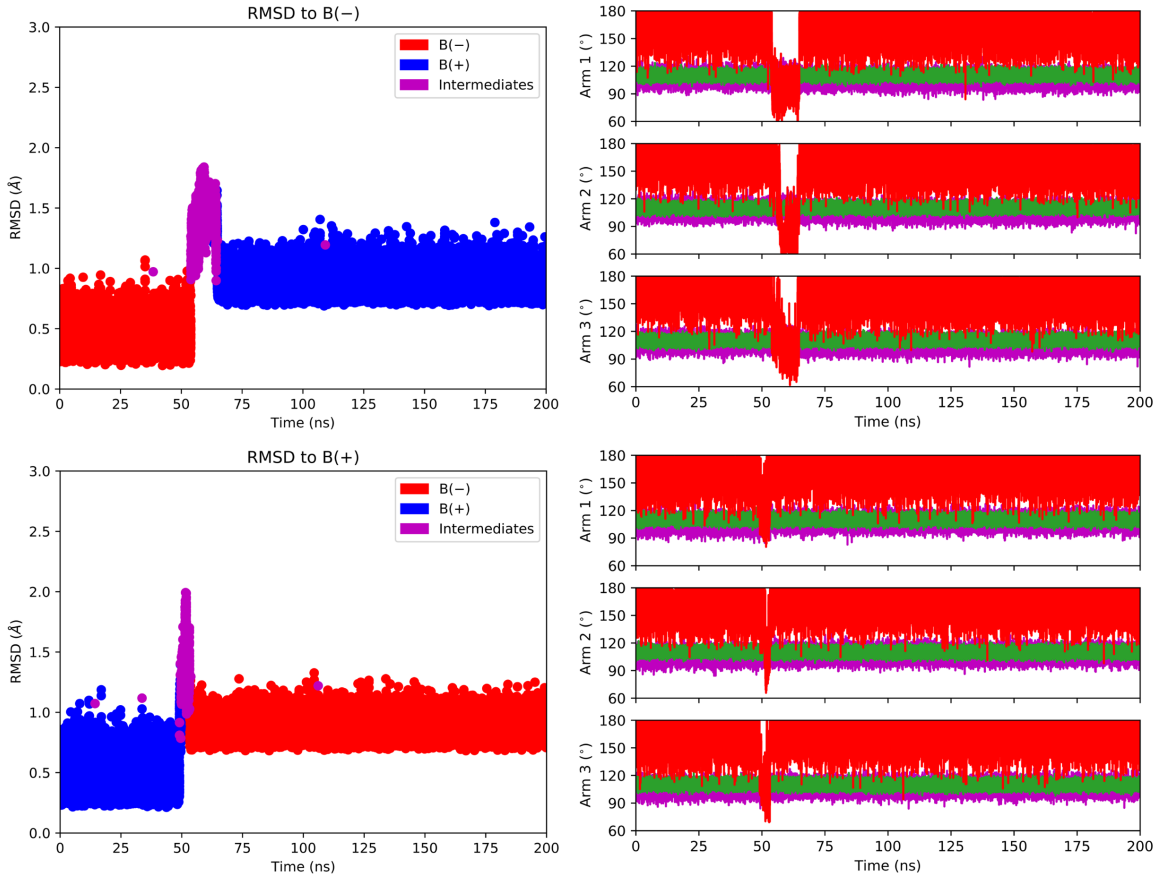

Figure S3. RMSD plot of the **B(–)** (top left) and **B(+)** (bottom left) diastereomers over 200 ns color-coded with the appearance of **B(–)** (red), **B(+)** (blue), and intermediate structures (purple). Plot of arm angles of the **B(–)** (top right) and **B(+)** (bottom right) diastereomers indicated in Figure S2. Note that in both cases we observed basket flipping mediated by correlated movements of arms 1, 2, and 3 near 50 ns.

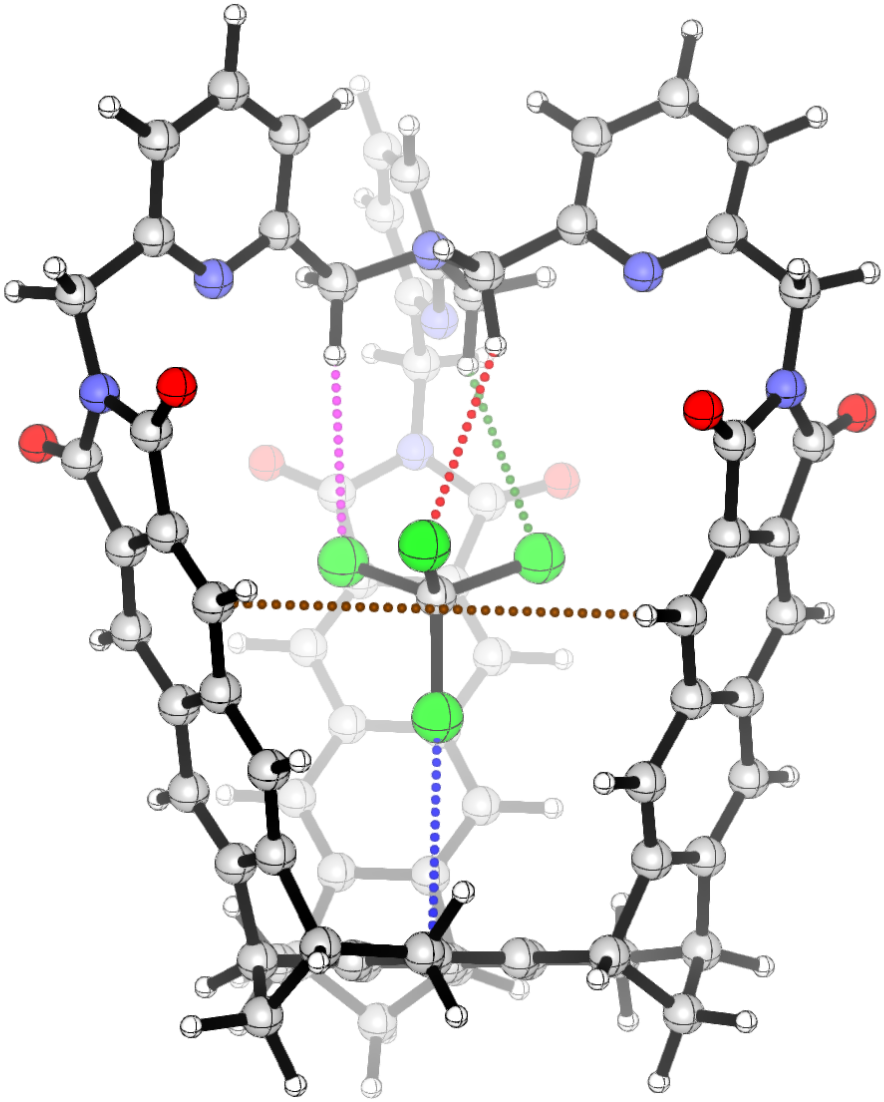

Figure S4. Distances measured during the conventional MD and ASMD simulations shown on the CCl_4⊂**B(+)** diastereomer.

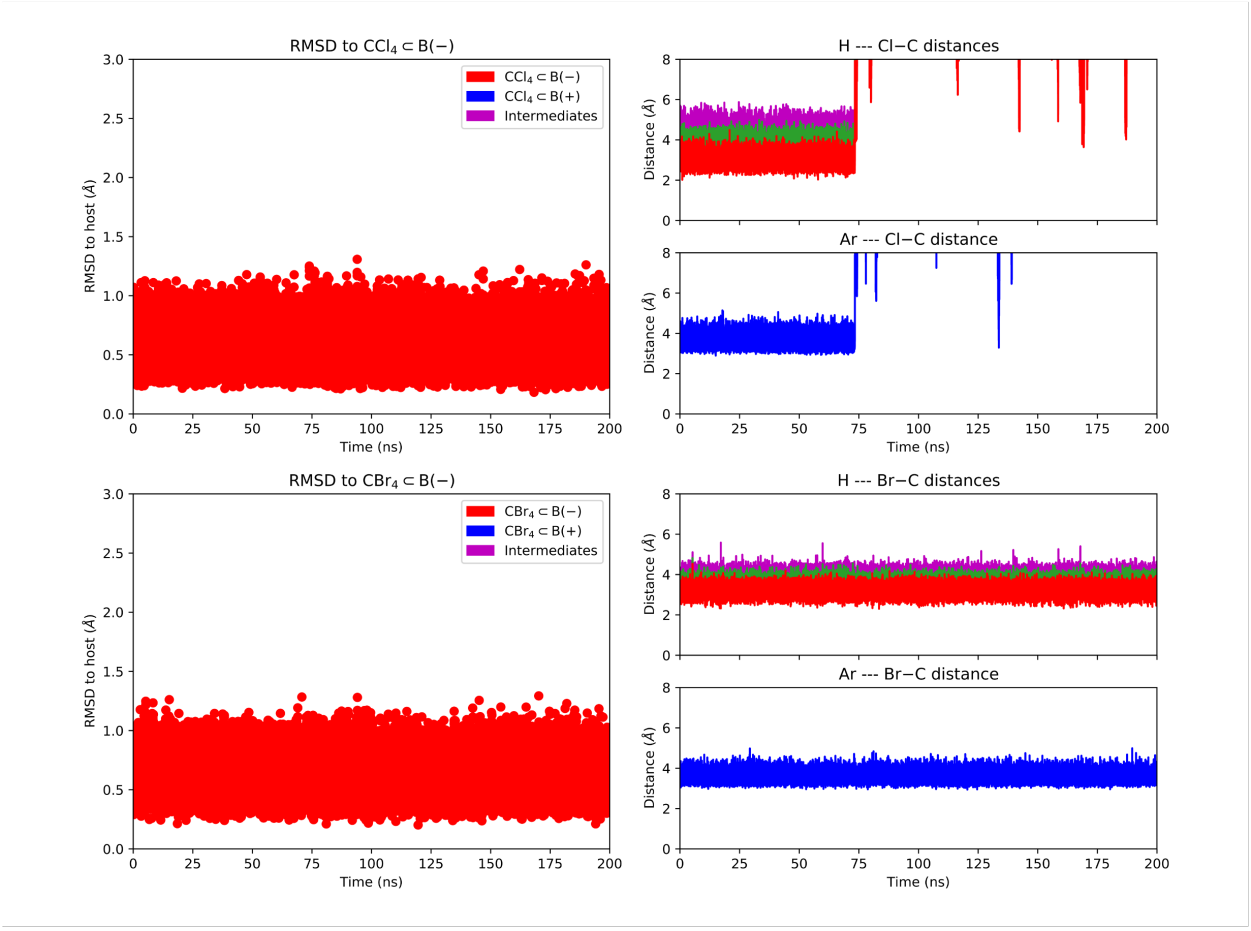

Figure S5. RMSD plot of the $CCl_4 \subset$**B(–)** (top left) and $CBr_4 \subset$**B(–)** (bottom left) diastereomers over 200 ns MD simulations color-coded with the appearance of $CX_4 \subset$**B(–)** (red), $CX_4 \subset$**B(+)** (blue), and intermediate host structures (purple). Plot of guest distances to important interactions in $CCl_4 \subset$**B(–)** (top right) and $CBr_4 \subset$**B(–)** (bottom right) diastereomers indicated in Figure S3. Note that in both cases we observed no basket flipping, but simultaneous guest exiting was observed near 75 ns in the $CCl_4 \subset$**B(–)** simulation.

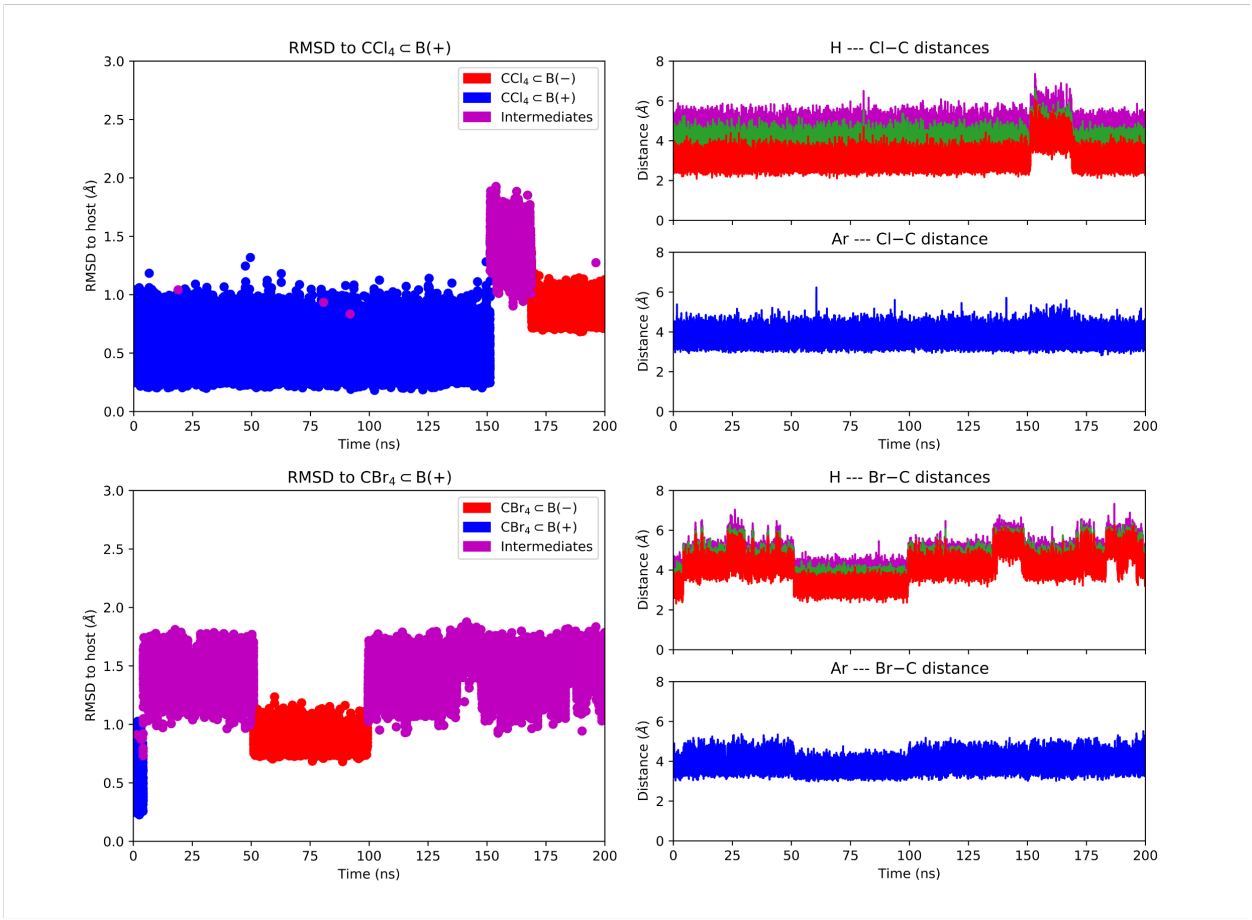

Figure S6. RMSD plot of the $CCl_4 \subset$**B(+)** (top left) and $CBr_4 \subset$**B(+)** (bottom left) diastereomers over 200 ns MD simulation color-coded with the appearance of $CX_4 \subset$**B(–)** (red), $CX_4 \subset$**B(+)** (blue), and intermediate host structures (purple). Plot of guest distances to important interactions in $CCl_4 \subset$**B(+)** (top right) and $CBr_4 \subset$**B(+)** (bottom right) diastereomers indicated in Figure S3. Note that in both cases we observed basket flipping near 160 ns ($CCl_4 \subset$**B(+)**) and 10 ns ($CBr_4 \subset$**B(+)**), but no guest exiting. Also, in the $CBr_4 \subset$**B(+)** simulation we observed an unusual number of intermediates correlating to the stability of the $CBr_4 \subset$**B(+)** intermediates along the PES of basket flipping.

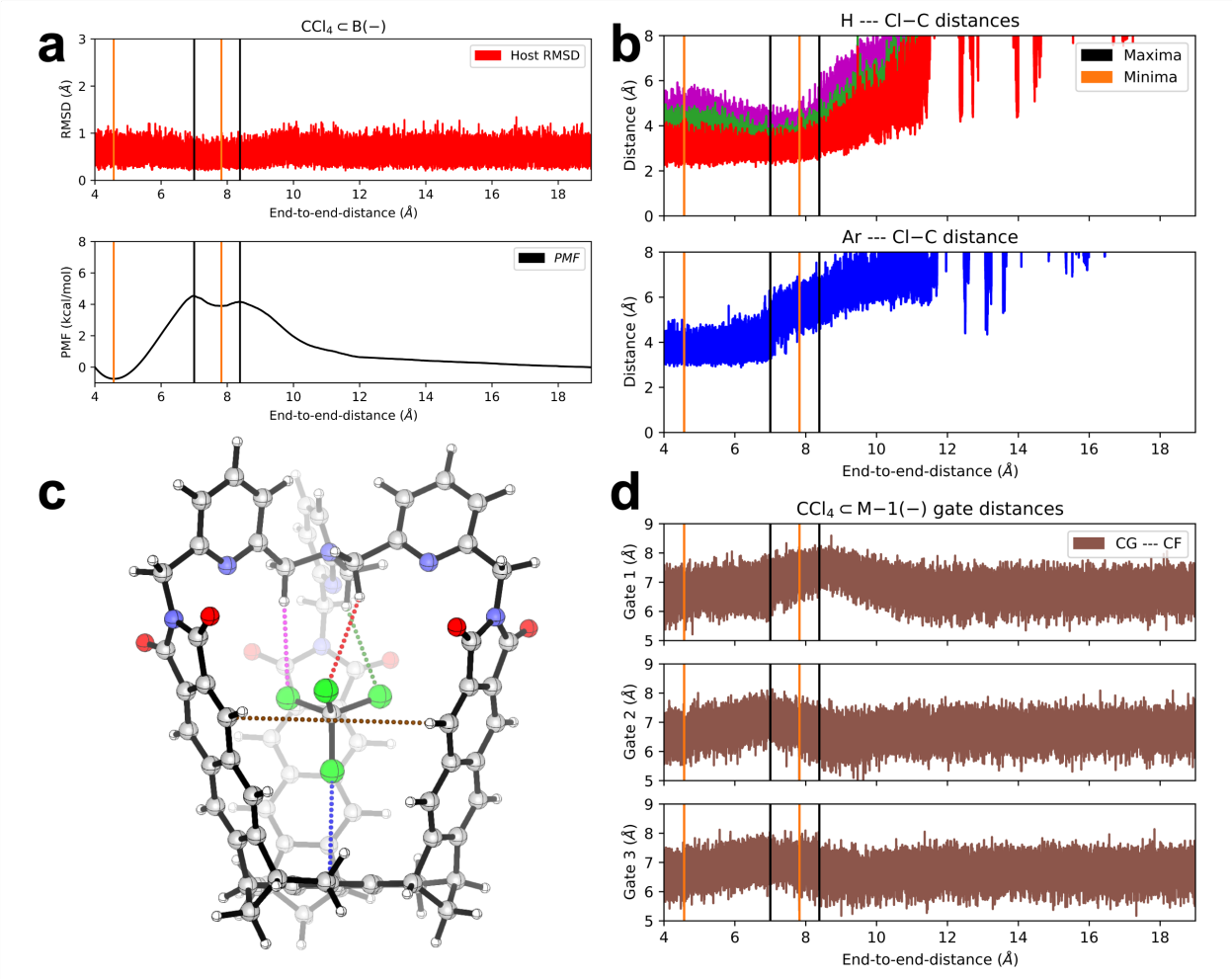

Figure S7. (a) RMSD analysis, (b-c) CCl_4 guest distances, and (d) gate distances for gates 1-3 along the second ASMD trajectory of CCl_4⊂**B(–)** guest exiting. Note that there was no significant deviation in the RMSD, suggesting that basket flipping, and guest exiting are decoupled processes.

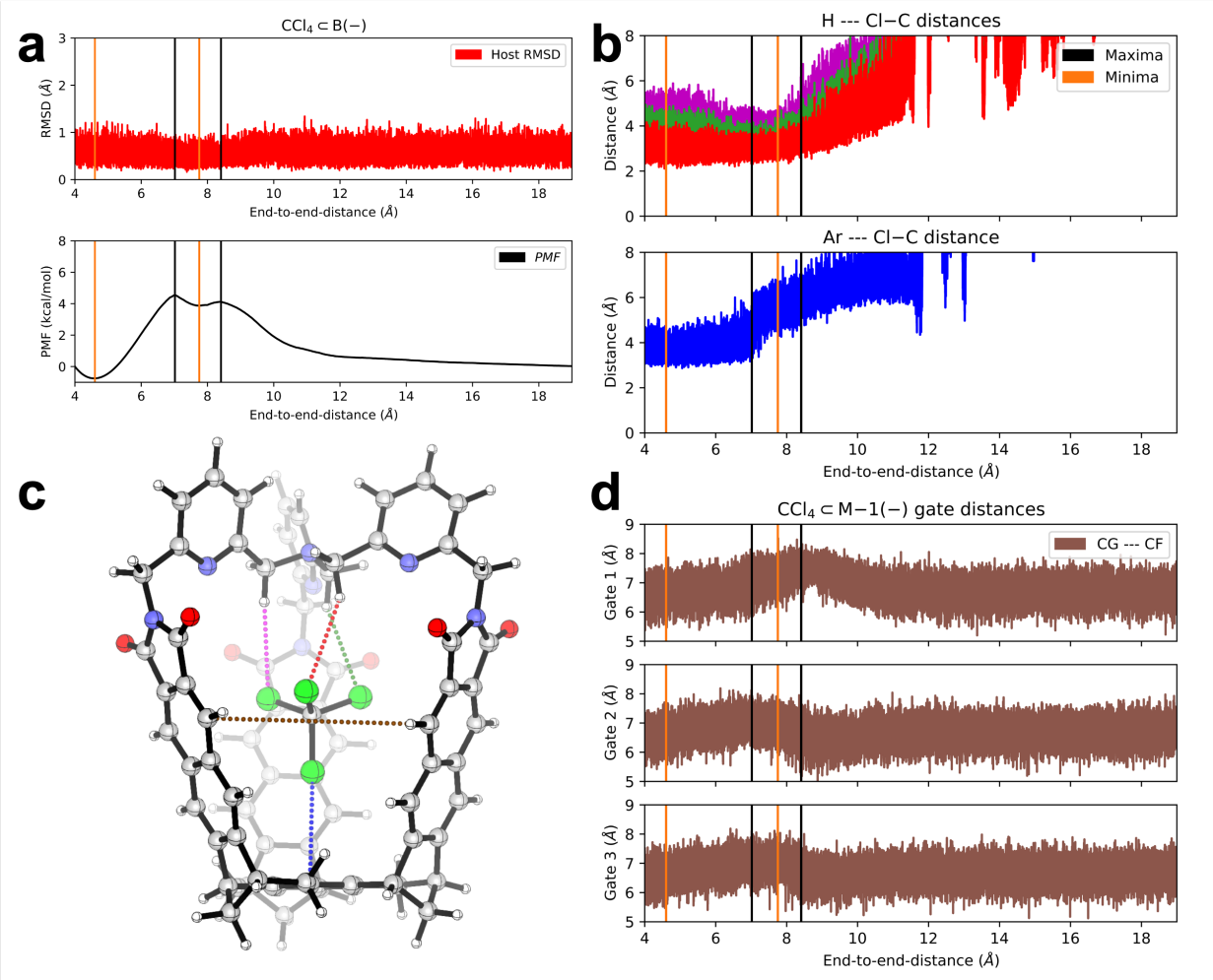

Figure S8. (a) RMSD analysis, (b-c) CCl_4 guest distances, and (d) gate distances for gates 1-3 along the second ASMD trajectory of CCl_4⊂**B(–)** guest exiting. Note that there was no significant deviation in the RMSD, suggesting that basket flipping, and guest exiting are decoupled processes.

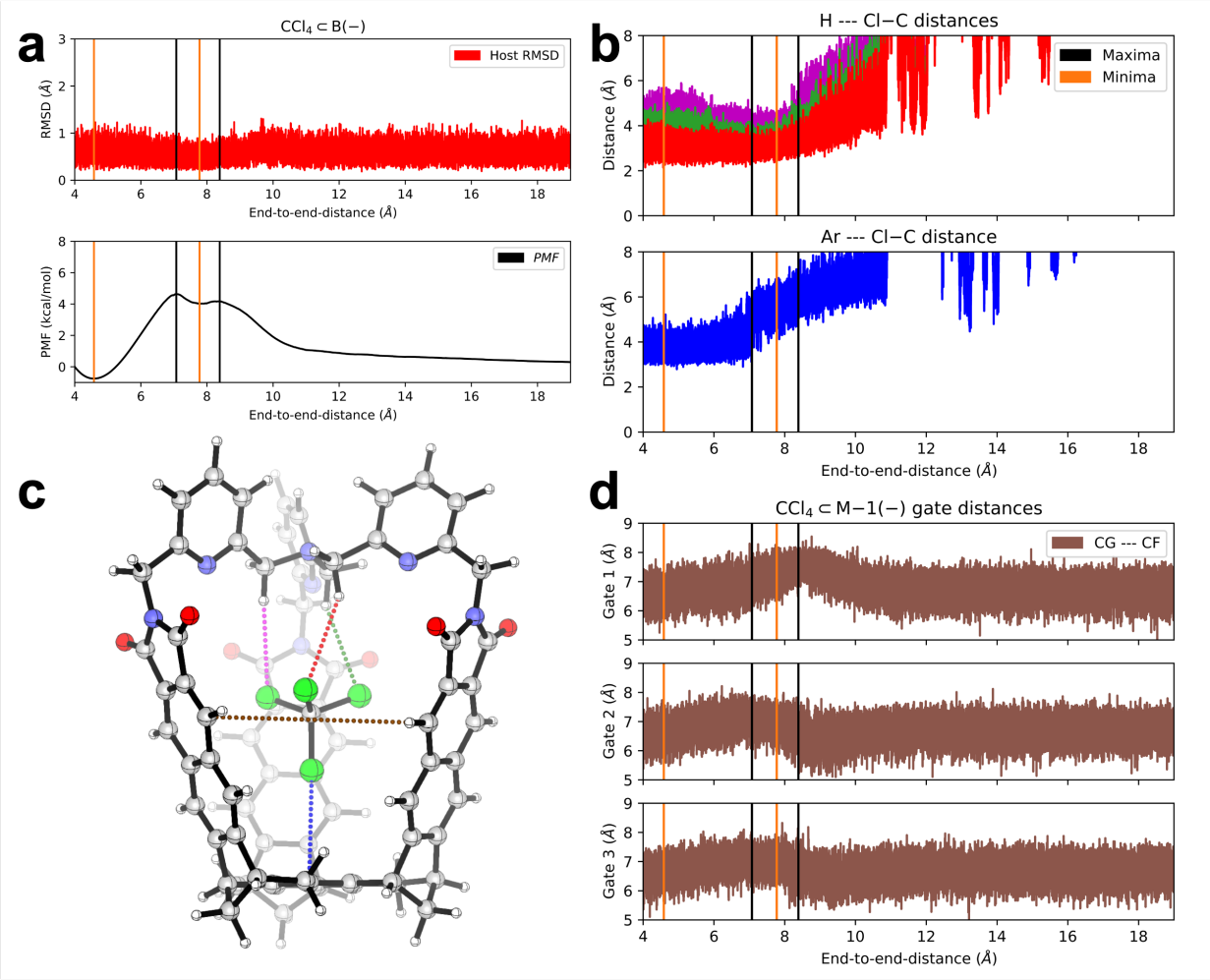

Figure S9. (a) RMSD analysis, (b-c) CCl_4 guest distances, and (d) gate distances for gates 1-3 along the third ASMD trajectory of $CCl_4 \subset$**B(–)** guest exiting. Note that there was no significant deviation in the RMSD, suggesting that basket flipping, and guest exiting are decoupled processes.

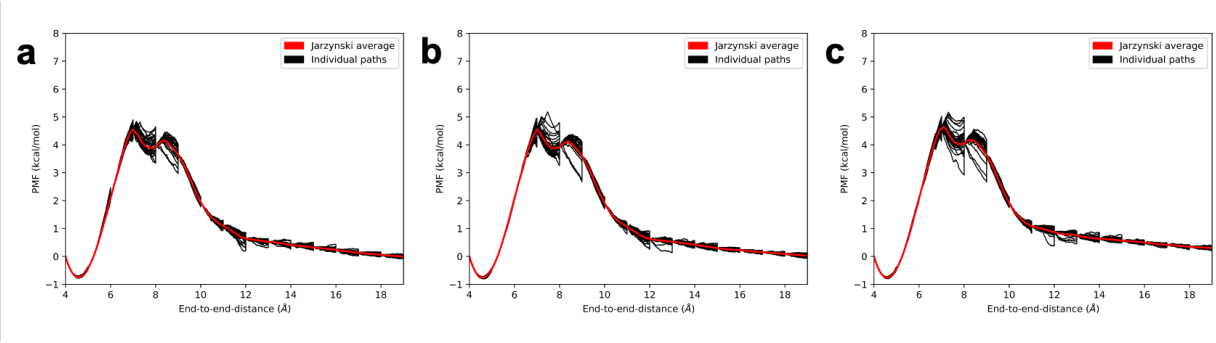

Figure S10. Jarzynski PMF plots for every ASMD trajectory in the (a) first run, (b) second run, and (c) third runs of the $CCl_4 \subset$**B(–)** pulling simulations.

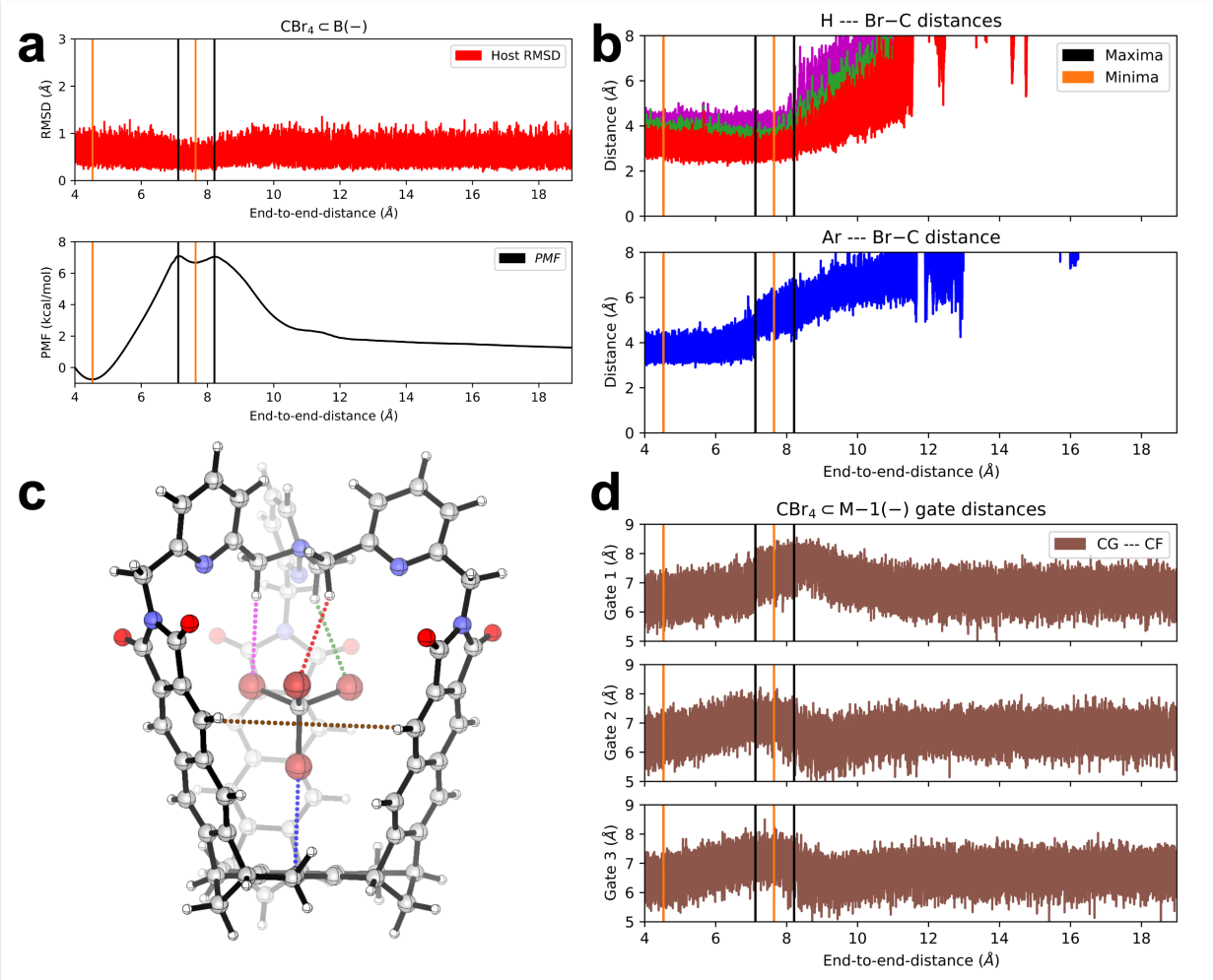

Figure S11. (a) RMSD analysis, (b-c) CBr_4 guest distances, and (d) gate distances for gates 1-3 along the first ASMD trajectory of CBr_4⊂**B(–)** guest exiting. Note that there was no significant deviation in the RMSD, suggesting that basket flipping, and guest exiting are decoupled processes.

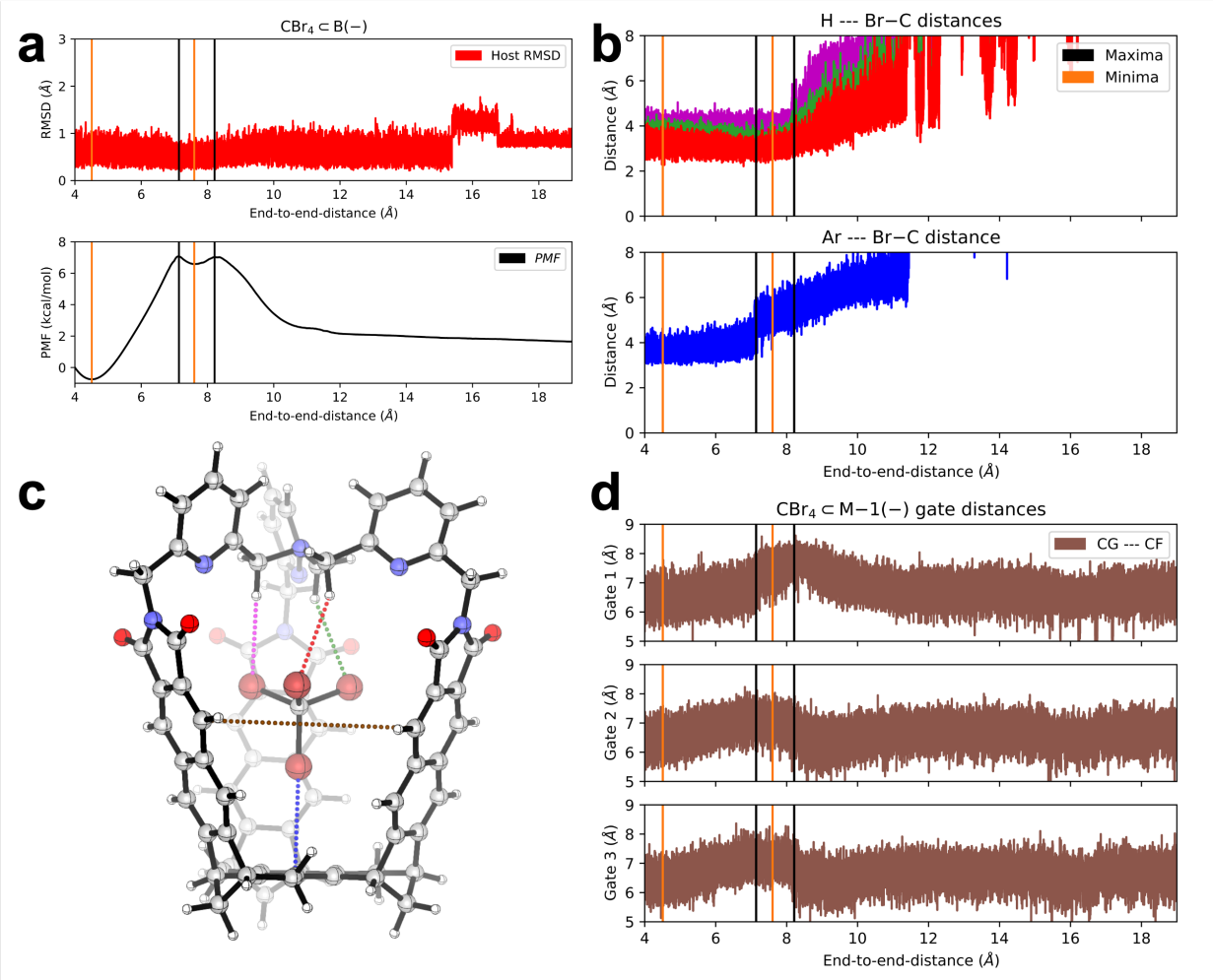

Figure S12. (a) RMSD analysis, (b-c) CBr_4 guest distances, and (d) gate distances for gates 1-3 along the second ASMD trajectory of CBr_4⊂**B(–)** guest exiting. Note that there was no significant deviation in the RMSD until ~15.5 Å, where the basket flipped to CBr_4⊂**B(+)**, when the guest had already left. Suggesting that basket flipping, and guest exiting are decoupled processes.

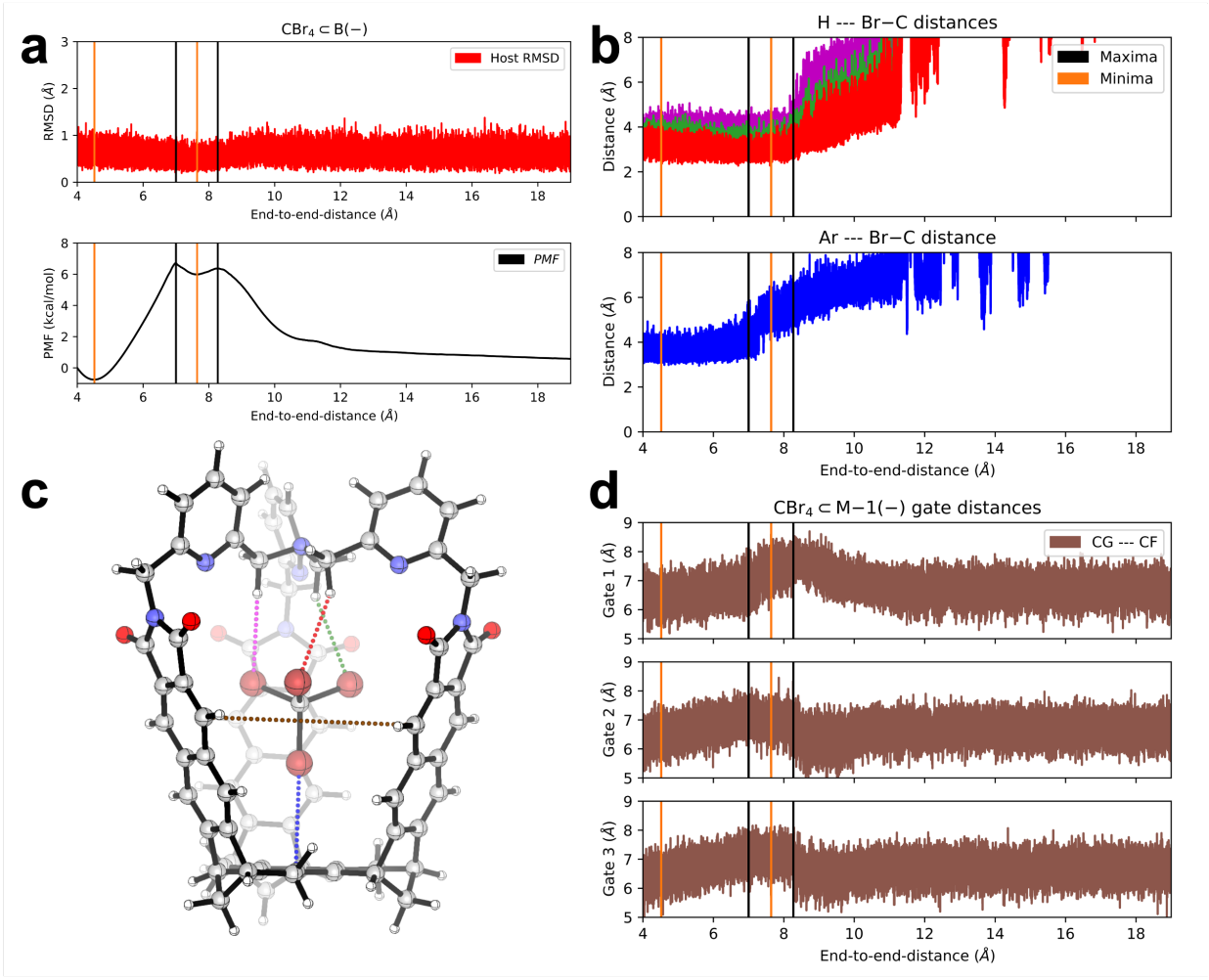

Figure S13. (a) RMSD analysis, (b-c) CBr_4 guest distances, and (d) gate distances for gates 1-3 along the third ASMD trajectory of CBr_4⊂**B(–)** guest exiting. Note that there was no significant deviation in the RMSD, suggesting that basket flipping, and guest exiting are decoupled processes.

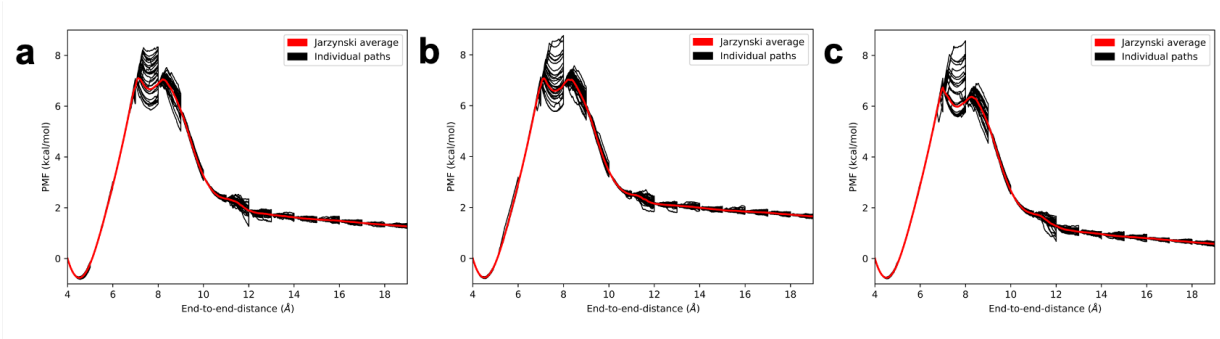

Figure S14. Jarzynski PMF plots for every ASMD trajectory in the (a) first run, (b) second run, and (c) third runs of the CBr_4⊂**B(–)** pulling simulations.

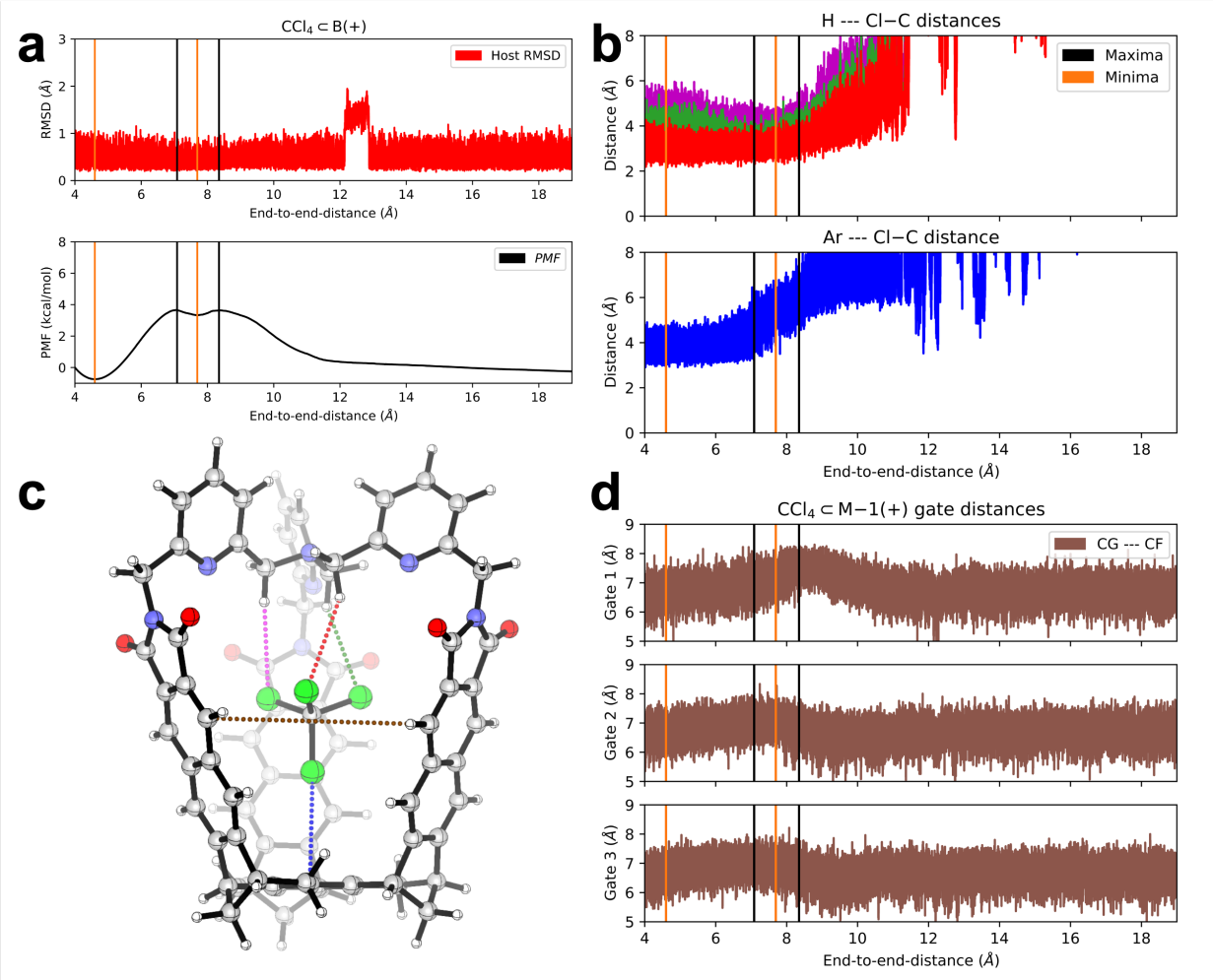

Figure S15. (a) RMSD analysis, (b-c) CCl_4 guest distances, and (d) gate distances for gates 1-3 along the first ASMD trajectory of $CCl_4 \subset$**B(+)** guest exiting. Note that there was no significant deviation in the RMSD until ~12 Å, when the guest had already left. Suggesting that basket flipping, and guest exiting are decoupled processes.

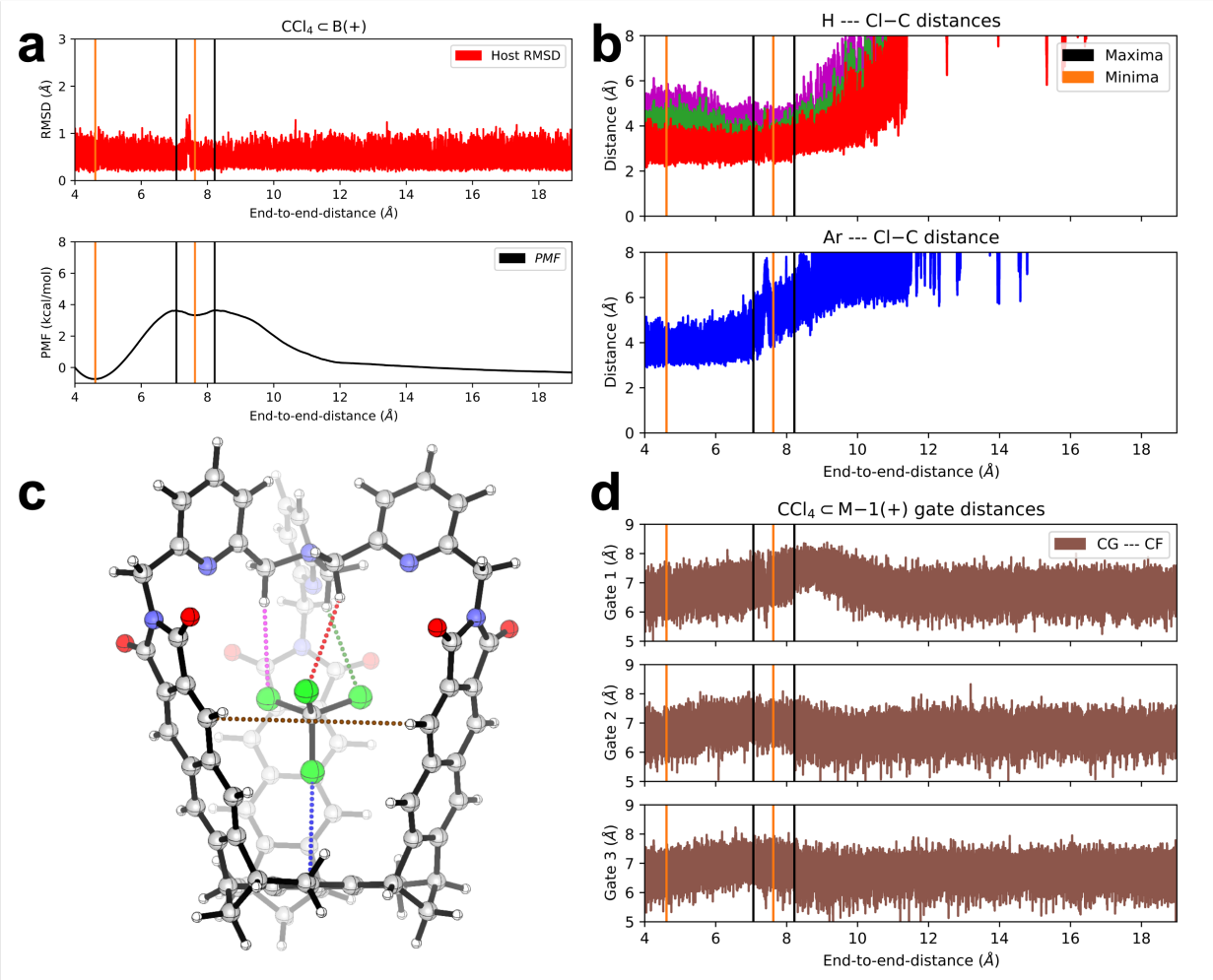

Figure S16. (a) RMSD analysis, (b-c) CCl_4 guest distances, and (d) gate distances for gates 1-3 along the third ASMD trajectory of $CCl_4 \subset$**B(+)** guest exiting. Note that there was no significant deviation in the RMSD, suggesting that basket flipping, and guest exiting are decoupled processes.

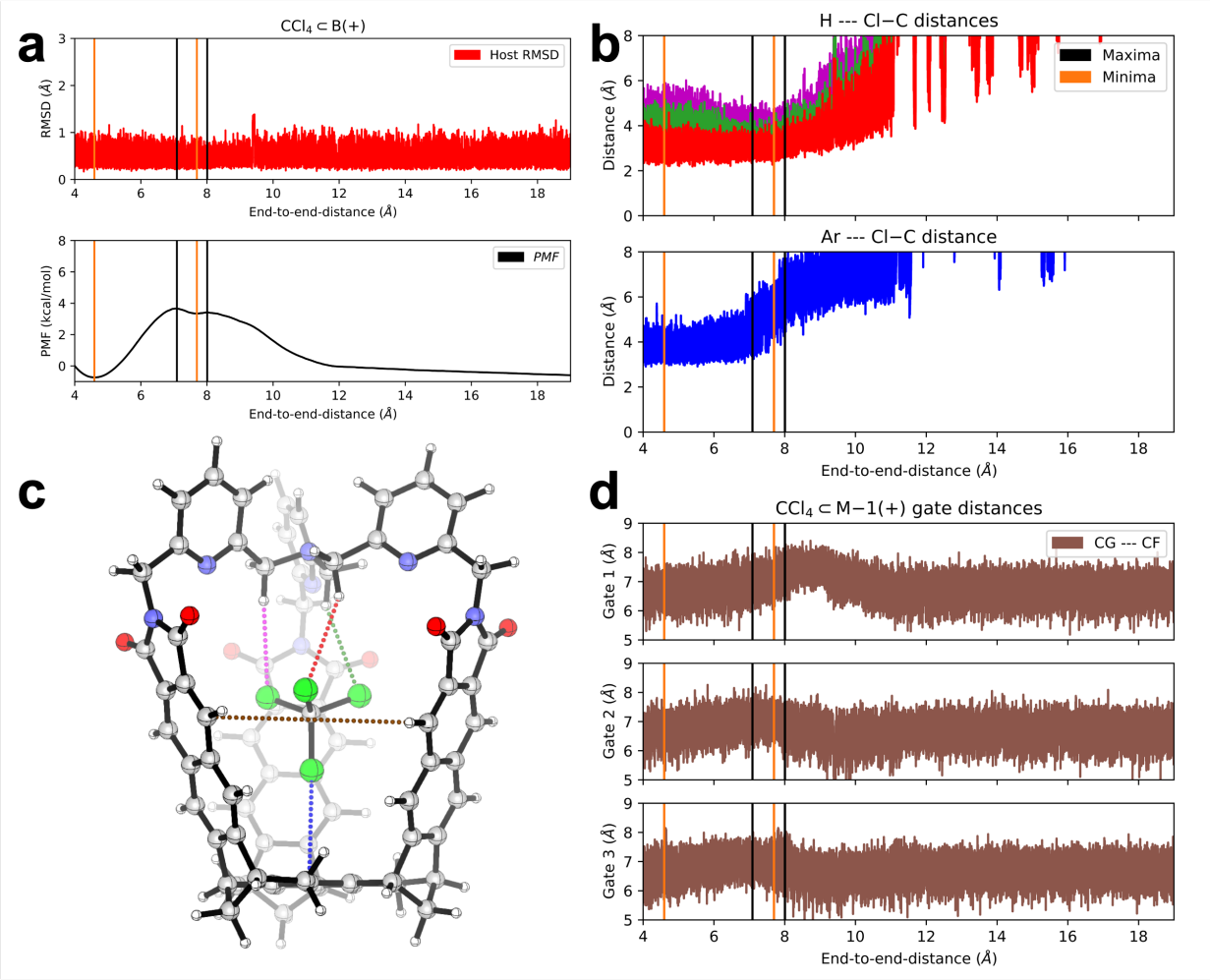

Figure S17. (a) RMSD analysis, (b-c) CCl_4 guest distances, and (d) gate distances for gates 1-3 along the second ASMD trajectory of CCl_4⊂**B(+)** guest exiting. Note that there was no significant deviation in the RMSD, suggesting that basket flipping, and guest exiting are decoupled processes.

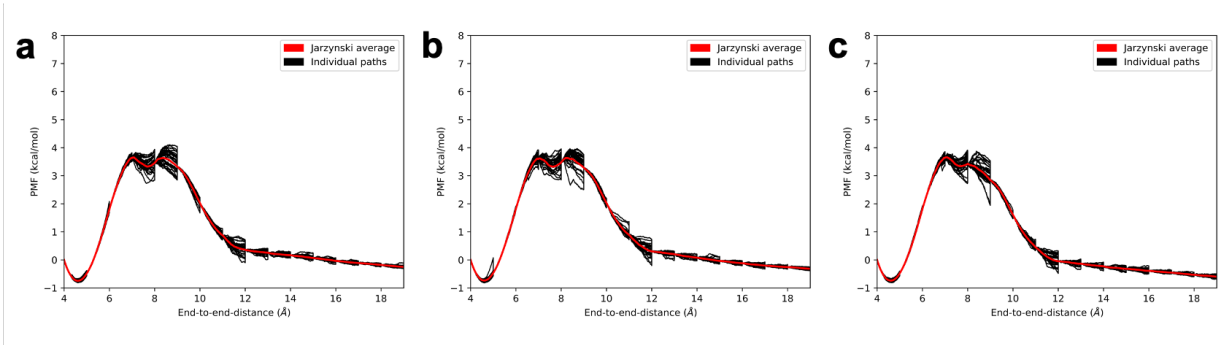

Figure S18. Jarzynski PMF plots for every ASMD trajectory in the (a) first run, (b) second run, and (c) third runs of the CCl_4⊂**B(+)** pulling simulations.

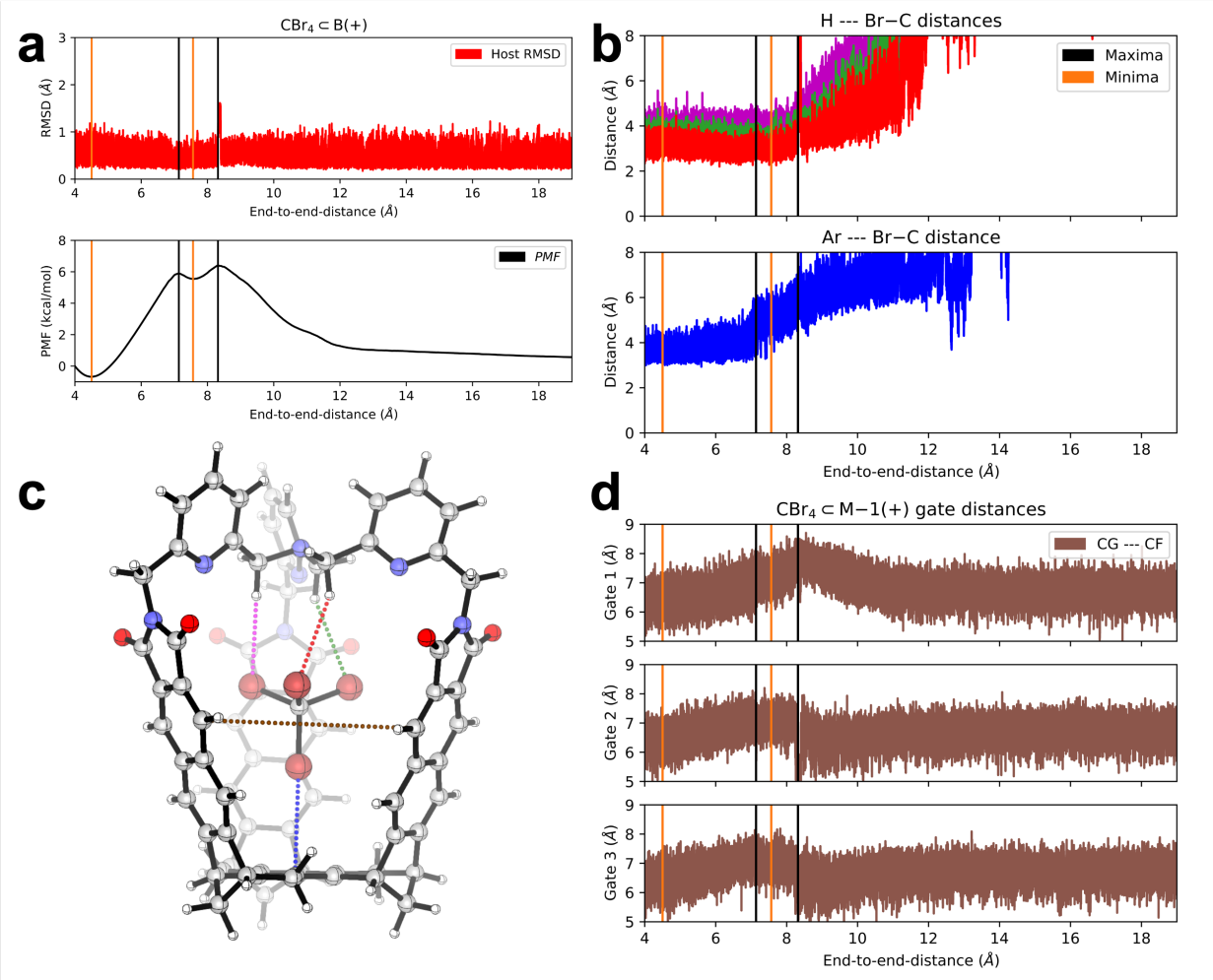

Figure S19. (a) RMSD analysis, (b-c) CBr_4 guest distances, and (d) gate distances for gates 1-3 along the first ASMD trajectory of CBr_4⊂**B(+)** guest exiting. Note that there was no significant deviation in the RMSD, suggesting that basket flipping, and guest exiting are decoupled processes.

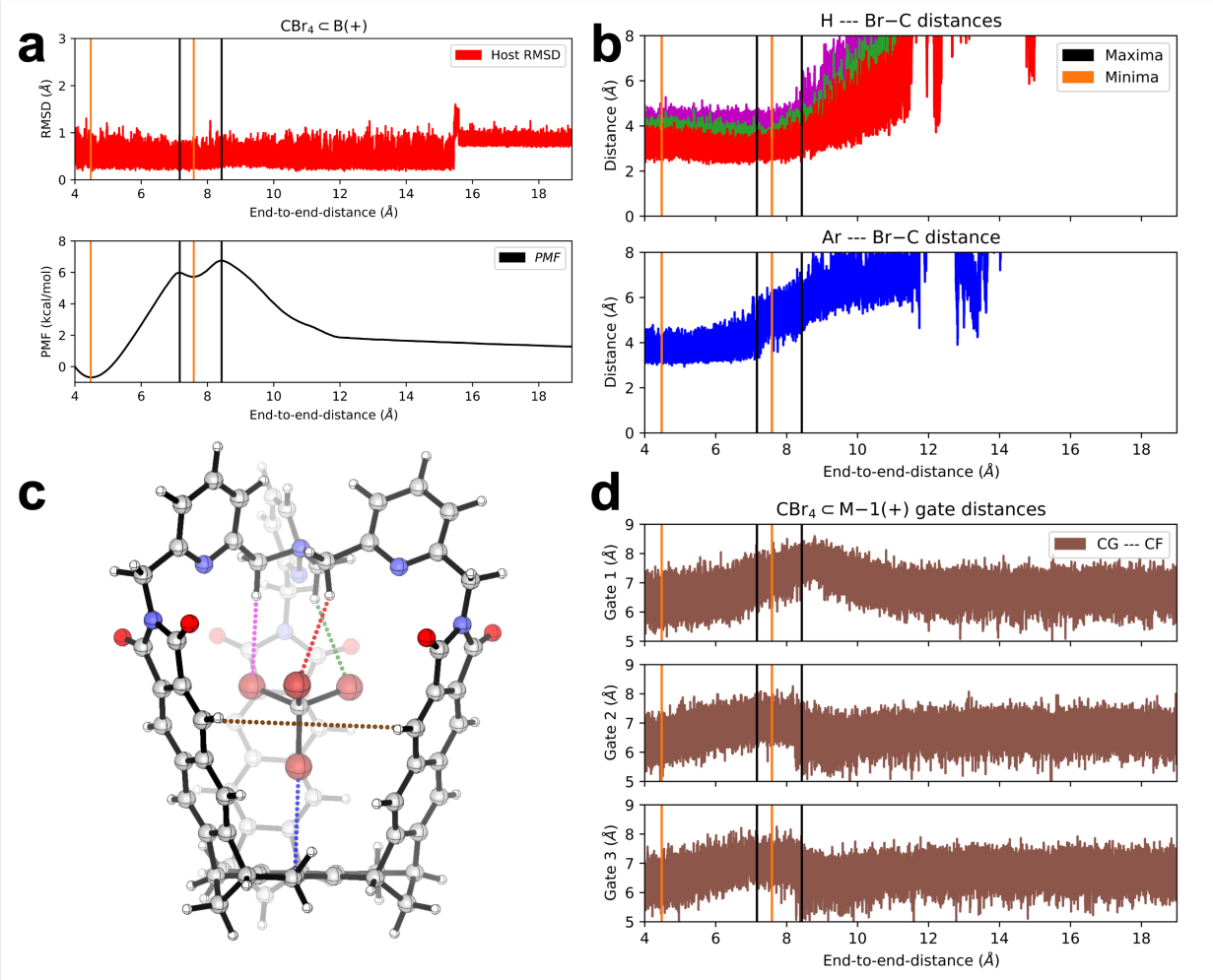

Figure S20. (a) RMSD analysis, (b-c) CBr_4 guest distances, and (d) gate distances for gates 1-3 along the second ASMD trajectory of CBr_4⊂**B(+)** guest exiting. Note that there was no significant deviation in the RMSD until ~15.5 Å, where the basket flipped to CBr_4⊂**B(–)**, when the guest had already left. Suggesting that basket flipping, and guest exiting are decoupled processes.

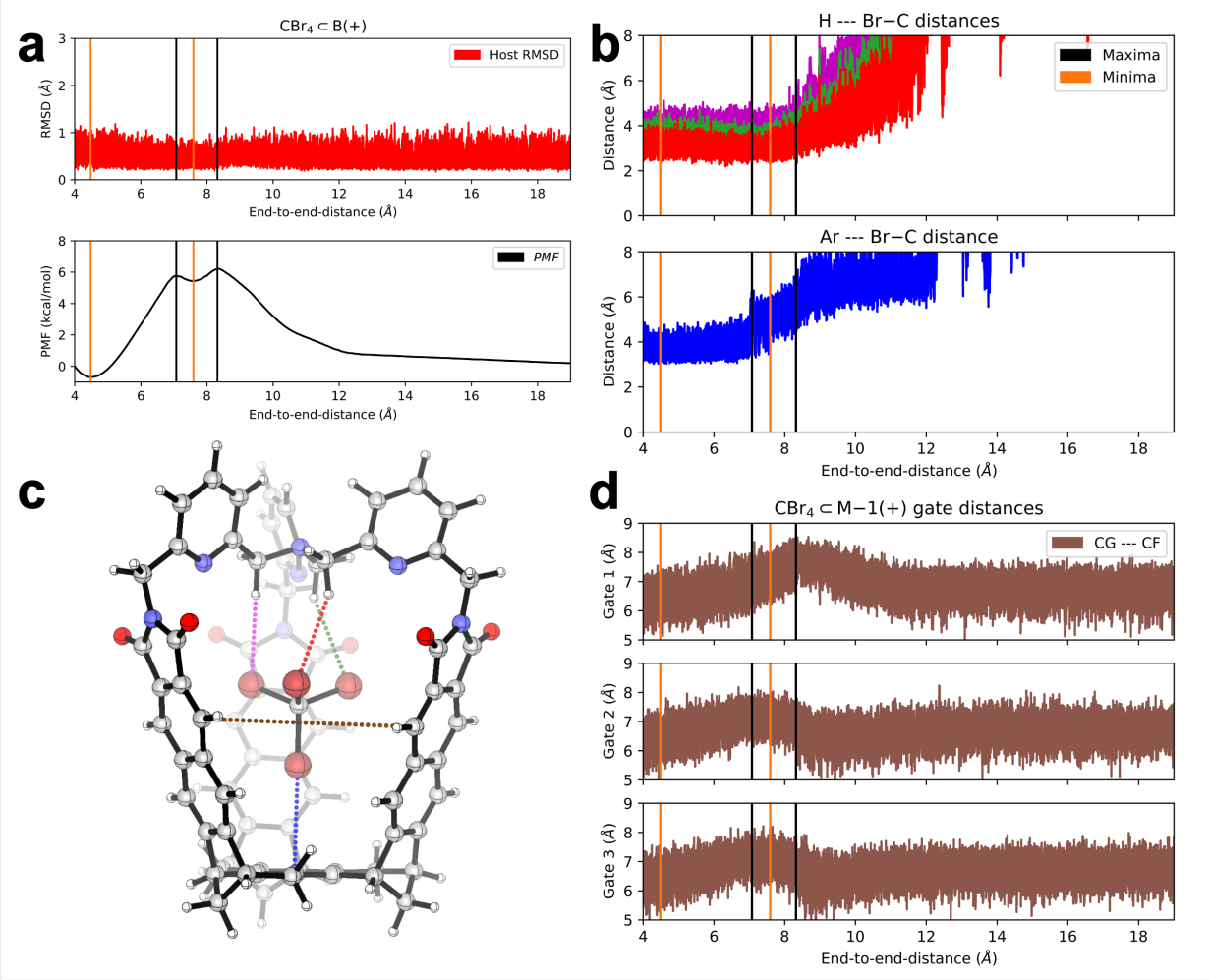

Figure S21. (a) RMSD analysis, (b-c) CBr_4 guest distances, and (d) gate distances for gates 1-3 along the first ASMD trajectory of CBr_4⊂**B(+)** guest exiting. Note that there was no significant deviation in the RMSD, suggesting that basket flipping, and guest exiting are decoupled processes.

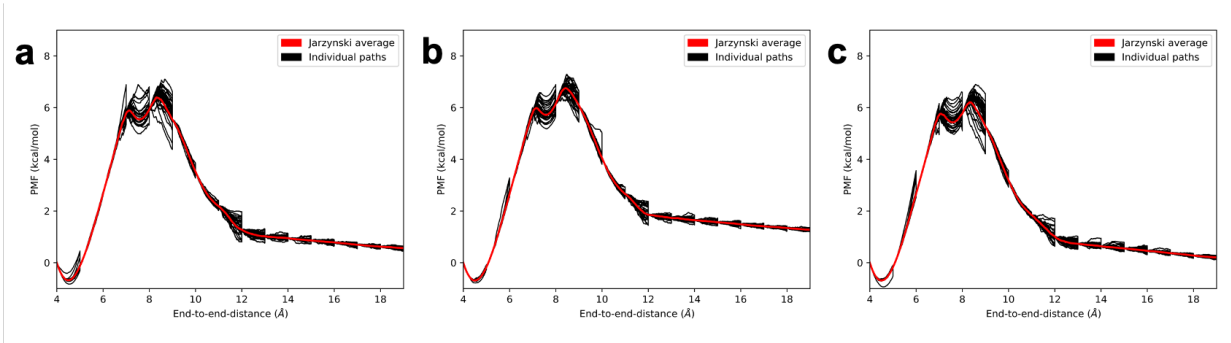

Figure S22. Jarzynski PMF plots for every ASMD trajectory in the (a) first run, (b) second run, and (c) third runs of the CBr_4⊂**B(+)** pulling simulations.

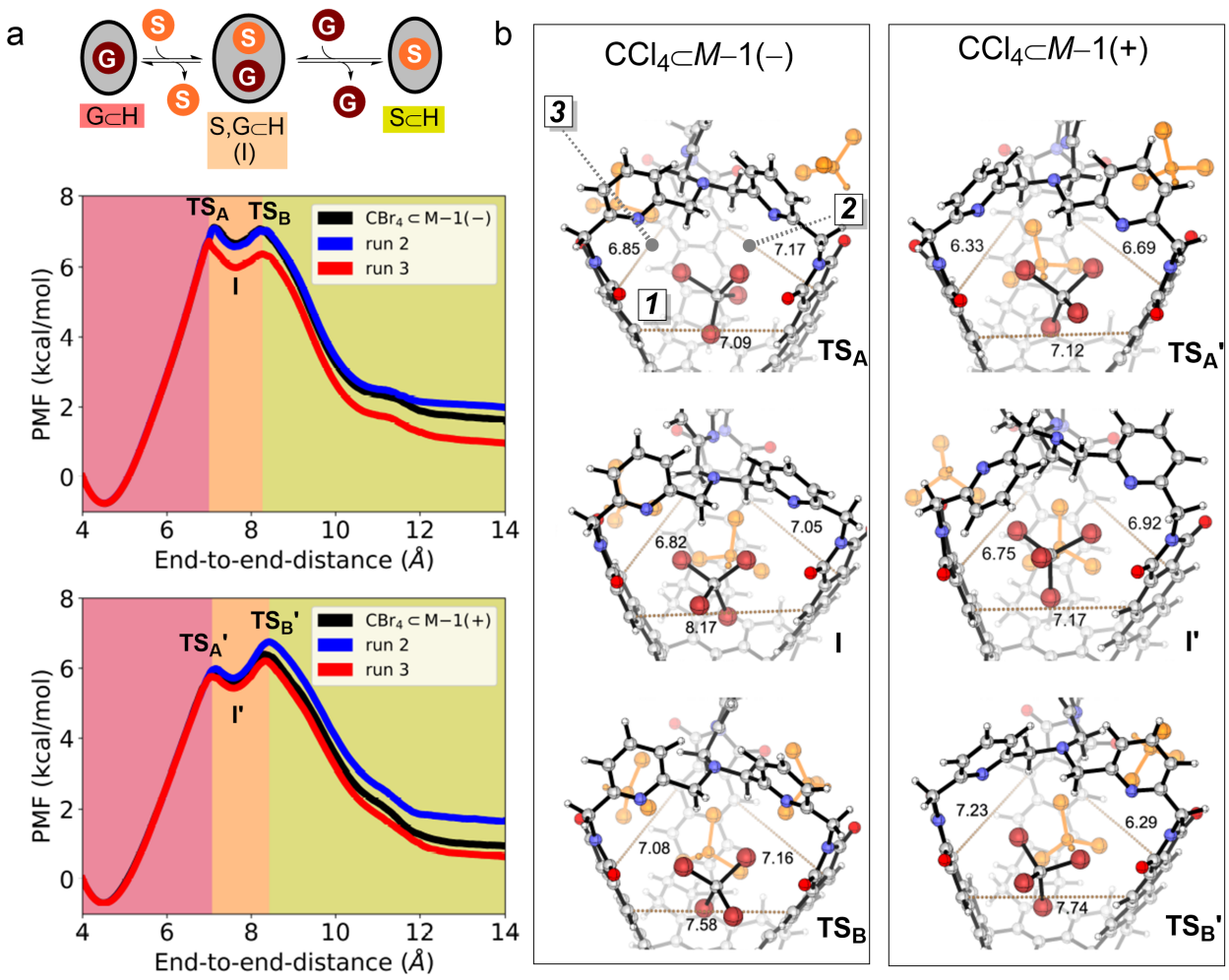

Figure S23. Calculated change in potential mean force (PMF) for the guest exiting of CBr_4⊂**B(–)** and CBr_4⊂**B(+)** diastereomers in the ff14SB forcefield at 300 K highlighting several important structures in the guest exiting mechanism (TS_A, $TS_{A'}$, I, I', TS_B, and $TS_{B'}$)

Table S1. Relative energy and imaginary frequency comparison for the empty basket flipping mechanism calculated at the B3LYP/6-31+G(d) level of theory in the gas phase at 298.15 K

Structure	Relative bottom of well energy (kcal/mol)	Relative enthalpy at 0 K (kcal/mol)	Relative enthalpy at 298.15 K (kcal/mol)	Relative free energy at 298.15 K (kcal/mol)	$\tilde{\nu}_{imaginary}$ (cm^{-1})
B(+)	0.0	0.0	0.0	0.0	N/A
TS1	8.7	8.5	8.1	9.3	44i
I1	7.1	7.1	7.2	7.2	N/A
TS2	8.4	8.7	8.2	10.3	22i
I2	6.1	6.7	6.5	7.7	N/A
TS3	7.5	7.8	7.2	9.2	33i
I3	4.9	5.3	5.3	5.0	N/A
TS4	5.7	5.8	5.3	6.7	16i
I4	5.3	5.4	5.5	5.1	N/A
TS5	9.7	9.4	9.1	9.9	23i
I5	8.8	8.8	8.9	8.9	N/A
TS6	9.3	9.2	8.7	10.6	24i
I6	6.1	6.5	6.5	6.6	N/A

TS7	7.0	7.1	6.6	7.9	18i
I7	6.2	6.3	6.4	6.1	N/A
TS8	7.8	7.7	7.3	8.7	25i
I8	7.4	7.5	7.6	7.6	N/A
TS9	8.6	8.4	8.1	9.2	39i
B(–)	-0.9	-0.9	-0.9	-1.4	N/A

Table S2. Relative energy comparison for the empty basket flipping mechanism calculated at the B3LYP/6-31+G(d) level of theory in the gas phase at 178 K

Structure	Relative bottom of well energy (kcal/mol)	Relative enthalpy at 0 K (kcal/mol)	Relative enthalpy at 178 K (kcal/mol)	Relative free energy at 178 K (kcal/mol)	$\tilde{\nu}_{imaginary}$ (cm^{-1})
B(+)	0.0	0.0	0.0	0.0	N/A
TS1	8.7	8.5	8.3	8.9	44i
I1	7.1	7.1	7.2	7.2	N/A
TS2	8.4	8.7	8.4	9.5	22i
I2	6.1	6.7	6.6	7.2	N/A
TS3	7.5	7.8	7.5	8.5	33i
I3	4.9	5.3	5.3	5.1	N/A
TS4	5.7	5.8	5.5	6.2	16i
I4	5.3	5.4	5.5	5.2	N/A
TS5	9.7	9.4	9.3	9.6	23i
I5	8.8	8.8	8.9	8.9	N/A
TS6	9.3	9.2	8.9	9.9	24i
I6	6.1	6.5	6.5	6.5	N/A
TS7	7.0	7.1	6.8	7.4	18i
I7	6.2	6.3	6.4	6.2	N/A
TS8	7.8	7.7	7.5	8.2	25i
I8	7.4	7.5	7.5	7.6	N/A
TS9	8.6	8.4	8.2	8.8	39i
B(–)	-0.9	-0.9	-0.9	-1.2	N/A

Table S3. Relative energy and imaginary frequency comparison for the CCl_4⊂**B** basket flipping mechanism calculated at the B3LYP/6-31+G(d) level of theory in the gas phase at 298.15 K

Structure	Relative bottom of well energy (kcal/mol)	Relative enthalpy at 0 K (kcal/mol)	Relative enthalpy at 298.15 K (kcal/mol)	Relative free energy at 298.15 K (kcal/mol)	$\tilde{\nu}_{imaginary}$ (cm^{-1})
B(+)	0.0	0.0	0.0	0.0	N/A
TS1	8.0	7.9	7.5	8.4	46i
I1	6.0	6.1	6.2	6.1	N/A
TS2	7.5	7.7	7.2	9.3	23i
I2	5.2	5.9	5.7	6.7	N/A
TS3	7.3	7.6	7.0	8.6	31i
I3	4.8	5.1	5.1	5.0	N/A
TS4	5.2	5.4	4.9	6.5	16i
I4	4.5	4.7	4.7	4.7	N/A
TS5	10.0	9.9	9.5	11.3	21i
I5	9.6	9.6	9.7	9.7	N/A
TS6	10.5	10.4	9.9	12.2	27i
I6	6.8	7.1	7.0	7.0	N/A
TS7	7.0	7.1	6.6	8.1	17i
I7	5.6	5.6	5.7	5.1	N/A
TS8	7.1	7.0	6.6	7.9	25i

I8	6.5	6.5	6.6	6.6	N/A
TS9	8.0	7.8	7.4	8.5	42i
B(–)	-0.7	-0.6	-0.7	-0.6	N/A

Table S4. Relative energy comparison for the CCl_4⊂**B** basket flipping mechanism calculated at the B3LYP/6-31+G(d) level of theory in the gas phase at 178 K

Structure	Relative bottom of well energy (kcal/mol)	Relative enthalpy at 0 K (kcal/mol)	Relative enthalpy at 178 K (kcal/mol)	Relative free energy at 178 K (kcal/mol)	$\tilde{\nu}_{imaginary}$ (cm^{-1})
B(+)	0.0	0.0	0.0	0.0	N/A
TS1	8.0	7.9	7.7	8.1	46i
I1	6.0	6.1	6.1	6.1	N/A
TS2	7.5	7.7	7.4	8.5	23i
I2	5.2	5.9	5.7	6.3	N/A
TS3	7.3	7.6	7.3	8.0	31i
I3	4.8	5.1	5.1	5.0	N/A
TS4	5.2	5.4	5.1	5.9	16i
I4	4.5	4.7	4.7	4.7	N/A
TS5	10.0	9.9	9.6	10.6	21i
I5	9.6	9.6	9.7	9.7	N/A
TS6	10.5	10.4	10.1	11.3	27i
I6	6.8	7.1	7.0	7.0	N/A
TS7	7.0	7.1	6.8	7.5	17i
I7	5.6	5.6	5.7	5.3	N/A
TS8	7.1	7.0	6.8	7.4	25i
I8	6.5	6.5	6.6	6.6	N/A
TS9	8.0	7.8	7.6	8.1	42i
B(–)	-0.7	-0.6	-0.6	-0.6	N/A

Table S5. Relative energy and imaginary frequency comparison for the CBr_4⊂**B** basket flipping mechanism calculated at the B3LYP/6-31+G(d) (6-311+G(2d) for Br) level of theory in the gas phase at 298.15 K

Structure	Relative bottom of well energy (kcal/mol)	Relative enthalpy at 0 K (kcal/mol)	Relative enthalpy at 298.15 K (kcal/mol)	Relative free energy at 298.15 K (kcal/mol)	$\tilde{\nu}_{imaginary}$ (cm^{-1})
B(+)	0.0	0.0	0.0	0.0	N/A
TS1	7.4	7.3	6.9	8.2	46i
I1	5.3	5.2	5.3	5.3	N/A
TS2	6.8	7.0	6.5	8.8	24i
I2	4.6	5.1	5.0	5.9	N/A
TS3	7.0	7.3	6.7	8.9	30i
I3	4.4	4.7	4.7	4.8	N/A
TS4	4.6	4.8	4.3	6.4	16i
I4	3.9	4.0	4.0	3.8	N/A
TS5	10.0	9.9	9.4	11.1	19i
I5	9.8	9.8	9.9	9.5	N/A
TS6	11.0	10.8	10.3	12.4	27i
I6	6.8	7.0	7.0	6.7	N/A
TS7	6.9	6.9	6.4	7.6	14i
I7	4.9	4.9	5.0	4.5	N/A
TS8	6.7	6.5	6.1	7.3	30i
I8	5.9	5.8	5.9	5.6	N/A
TS9	7.5	7.3	6.9	8.1	43i
B(–)	-0.4	-0.4	-0.4	-0.4	N/A

Table S6. Relative energy comparison for the CBr_4⊂**B** basket flipping mechanism calculated at the B3LYP/6-31+G(d) (6-311+G(2d) for Br) level of theory in the gas phase at 178 K

Structure	Relative bottom of well energy (kcal/mol)	Relative enthalpy at 0 K (kcal/mol)	Relative enthalpy at 178 K (kcal/mol)	Relative free energy at 178 K (kcal/mol)	$\tilde{\nu}_{imaginary}$ (cm^{-1})
B(+)	0.0	0.0	0.0	0.0	N/A
TS1	7.4	7.3	7.1	7.7	46i
I1	5.3	5.2	5.3	5.3	N/A
TS2	6.8	7.0	6.7	7.9	24i
I2	4.6	5.1	5.0	5.5	N/A
TS3	7.0	7.3	6.9	8.0	30i
I3	4.4	4.7	4.7	4.7	N/A
TS4	4.6	4.8	4.5	5.6	16i
I4	3.9	4.0	4.0	3.9	N/A
TS5	10.0	9.9	9.6	10.5	19i
I5	9.8	9.8	9.8	9.6	N/A
TS6	11.0	10.8	10.5	11.6	27i
I6	6.8	7.0	7.0	6.8	N/A
TS7	6.9	6.9	6.6	7.2	14i
I7	4.9	4.9	5.0	4.7	N/A
TS8	6.7	6.5	6.3	6.9	30i
I8	5.9	5.8	5.9	5.8	N/A
TS9	7.5	7.3	7.1	7.7	43i
B(–)	-0.4	-0.4	-0.4	-0.4	N/A

Table S7. Volume measurements ($Å^3$) of the empty, CCl_4⊂**B**, and CBr_4⊂**B** basket flipping mechanisms calculated at the B3LYP/6-31+G(d) (6-311+G(2d) for Br) level of theory in the gas phase

Structure	Empty	CCl_4⊂B	CBr_4⊂B
B(+)	251	263	268
TS1	258	274	279
I1	259	270	276
TS2	257	270	275
I2	252	264	270
TS3	257	271	276
I3	235	245	248
TS4	240	250	250
I4	245	265	271
TS5	242	254	262
I5	232	251	259
TS6	229	247	255
I6	260	270	263
TS7	257	269	268
I7	262	272	279
TS8	270	278	284
I8	269	278	281
TS9	267	280	286
B(–)	238	262	265

Table S8. Calculated change in potential mean force (PMF) for the guest exiting of CCl_4⊂**B** and CBr_4⊂**B** compared to the change in volume of each basket cavity averaged over the three ASMD simulations in the ff14SB forcefield at 300 K

ΔG [kcal/mol] / Volume [$Å^3$]	**Structures**			
	CCl_4⊂**B(–)**	**TS$^{(I)}$ (RLS)**	**I**	**TS$^{(II)}$**
CCl_4⊂B(–)	0.0 / 201 ± 11	5.3 ± 0.0 / 230 ± 10	4.7 ± 0.1 / 230 ± 10	4.9 ± 0.0 / 229 ± 14
	CCl_4⊂**B(+)**	**TS$^{(I)'}$ (RLS)**	**I'**	**TS$^{(II)'}$**
CCl_4⊂B(+)	0.0 / 209 ± 14	4.4 ± 0.0 / 236 ± 15	4.1 ± 0.0 / 237 ± 7	4.3 ± 0.1 / 229 ± 7
	CBr_4⊂**B(–)**	**TS$^{(I)}$ (RLS)**	**I**	**TS$^{(II)}$**
CBr_4⊂B(–)	0.0 / 180 ± 13	7.7 ± 0.2 / 241 ± 11	7.1 ± 0.4 / 231 ± 28	7.6 ± 0.4 / 221 ± 11
	CBr_4⊂**B(+)**	**TS$^{(I)'}$**	**I'**	**TS$^{(II)'}$ (RLS)**
CBr_4⊂B(+)	0.0 / 208 ± 24	6.6 ± 0.1 / 235 ± 5	6.3 ± 0.1 / 238 ± 4	7.1 ± 0.3 / 242 ± 9

Table S9. Relative free energy comparison for the basket flipping mechanism calculated at the B3LYP-D3//B3LYP/6-31+G(d)(6-311+G(2d) for Br) level of theory in the gas phase at 298 K

Structure	**Empty (kcal/mol)**	**CCl_4⊂B (kcal/mol)**	**CBr_4⊂B (kcal/mol)**
B(+)	0.0	0.0	0.0
TS1	9.3	8.4	8.2
I1	7.2	6.1	5.3
TS2	10.3	9.3	8.8
I2	7.7	6.7	5.9
TS3	9.3	8.7	8.9
I3	5.0	5.0	4.8
TS4	6.7	6.5	6.4
I4	5.1	4.7	3.8
TS5	9.9	11.3	11.2
I5	8.9	9.7	9.5
TS6	10.6	12.3	12.4
I6	6.6	7.0	6.7
TS7	8.0	8.1	7.6
I7	6.1	5.1	4.5
TS8	8.7	7.9	7.3
I8	7.6	6.6	5.7
TS9	9.3	8.6	8.2
B(–)	-1.4	-0.6	-0.4

Table S10. Relative free energy comparison for the basket flipping mechanism calculated at the B3LYP/6-31+G(d)(6-311+G(2d) for Br) level of theory in the gas phase at 178 K.

Structure	**Empty (kcal/mol)**	**CCl_4⊂B (kcal/mol)**	**CBr_4⊂B (kcal/mol)**
B(+)	0.0	0.0	0.0
TS1	8.9	8.1	7.7
I1	7.2	6.1	5.3
TS2	9.5	8.5	7.9
I2	7.2	6.3	5.5
TS3	8.5	8.1	8.1
I3	5.1	5.0	4.7

TS4	6.2	5.9	5.6
I4	5.3	4.7	3.9
TS5	9.6	10.6	10.5
I5	8.9	9.7	9.6
TS6	9.9	11.4	11.6
I6	6.6	7.0	6.8
TS7	7.5	7.6	7.2
I7	6.2	5.3	4.7
TS8	8.2	7.5	6.9
I8	7.6	6.6	5.8
TS9	8.8	8.2	7.7
B(–)	-1.2	-0.6	-0.4

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Structural coordinates

B(+)

E(RB3LYP) = -3723.61376169

E(RB3LYP-D3) = -3723.80197905

H - Sum of electronic and thermal Enthalpies= -3722.451061

G - Sum of electronic and thermal Free Energies= -3722.610951

Number of imaginary frequencies: 0

Cartesian Coordinates

C	-5.65950	-1.34092	-0.43453
C	-5.67254	-0.29306	-1.37400
C	-5.65934	1.05027	-0.94512
C	-5.67011	1.33987	0.43234
C	-5.65782	0.29665	1.38102
C	-5.67096	-1.04066	0.94306
C	-5.62959	-2.79246	-0.91675
C	-5.52757	-3.83401	0.22224
C	-6.47809	-3.38392	1.35415
C	-5.66585	-2.20556	1.94186
C	-5.62688	0.60437	2.87936
C	-5.52456	2.11124	3.21148
C	-5.66451	2.78731	0.94160
C	-5.62836	2.19336	-1.96173
C	-5.52732	1.72618	-3.43234
C	-5.66811	-0.57714	-2.88206
C	-6.47905	0.52199	-3.60889
C	-6.47572	2.86709	2.25672
C	-1.87978	0.79030	-4.42859
C	-3.01335	1.62656	-4.20201
C	-4.18199	1.08285	-3.72756
C	-4.27264	-0.30927	-3.43518
C	-3.20820	-1.14837	-3.65217
C	-1.98583	-0.62455	-4.16458
C	-1.98176	3.91884	1.54241
C	-1.87654	3.44184	2.90033
C	-3.01070	2.82856	3.51136
C	-4.17887	2.68825	2.80259
C	-4.26898	3.13071	1.45053
C	-3.20398	3.73707	0.83247
C	-1.98408	-3.29371	2.62177
C	-1.88026	-4.23364	1.53158
C	-3.01450	-4.45586	0.69493
C	-4.18178	-3.76993	0.92651
C	-4.27062	-2.81874	1.98440
C	-3.20530	-2.58586	2.81799
C	-0.87064	-3.09100	3.48831
C	0.28605	-3.78480	3.24656
C	0.39762	-4.68762	2.16259
C	-0.65396	-4.92855	1.31577
C	-0.65234	1.32493	-4.91907
C	0.39830	0.47052	-5.13572
C	0.28477	-0.92038	-4.90115
C	-0.87312	-1.47686	-4.42413
C	-0.64943	3.60057	3.60898
C	0.40172	4.21402	2.97674
C	0.28919	4.70340	1.65373
C	-0.86853	4.56796	0.93322
C	1.58763	5.32936	1.27813
O	1.89950	5.89683	0.24823
N	2.41997	5.17207	2.40104
C	1.78506	4.49348	3.45372
O	2.30400	4.22273	4.52203
C	1.78211	0.74440	-5.61437
O	2.30199	1.80558	-5.91021
C	1.58306	-1.55848	-5.25661
O	1.89447	-2.73431	-5.23565
C	1.58478	-3.77202	3.97584
O	1.89721	-3.16300	4.98154
C	1.78095	-5.24065	2.16597
O	2.29938	-6.03140	1.39796
N	2.41668	-4.66663	3.27866
N	2.41615	-0.50674	-5.67906
C	3.82920	5.50253	2.40231
C	3.82538	-0.67090	-5.96604
C	3.82599	-4.83274	3.56437
C	6.27811	-2.08137	1.42454
C	6.85465	-3.26906	1.87378
C	6.06565	-4.19050	2.56094
C	4.71705	-3.88236	2.77050
N	4.15837	-2.75239	2.32610
C	4.91785	-1.86011	1.67072
C	6.27746	-0.19773	-2.51283
C	6.85467	0.00604	-3.76586
C	6.06571	-0.12697	-4.90760
C	4.71650	-0.46029	-4.74581
N	4.15715	-0.63917	-3.54519
C	4.91663	-0.51906	-2.44458
C	6.27953	2.27562	1.08127
C	6.85872	3.26082	1.88051
C	6.07051	4.31634	2.33687
C	4.71989	4.34092	1.97227
N	4.15883	3.38910	1.22028
C	4.91775	2.37589	0.77277
C	4.21706	1.38643	-0.14000
C	4.21763	-0.81700	-1.13085
C	4.21939	-0.57279	1.27320
N	4.67910	-0.00106	0.00040
H	-6.54497	-3.00713	-1.48790
H	-4.79432	-2.93624	-1.61338
H	-5.74901	-4.83109	-0.17377
H	-6.60377	-4.17388	2.10390
H	-7.46689	-3.08121	0.99133
H	-6.54181	0.21680	3.35143
H	-6.03022	-1.58308	-3.09966
H	-6.54234	2.79735	-1.86161

H	-4.79122	2.86674	-1.73979
H	-7.46784	0.68582	-3.16568
H	-6.60470	0.26790	-4.66795
H	-4.79103	0.07341	3.35159
H	-5.74489	2.26709	4.27317
H	-7.46461	2.40164	2.17643
H	-6.60112	3.91125	2.56649
H	-2.93453	2.68837	-4.42899
H	-3.27433	-2.21515	-3.44901
H	-5.74728	2.56730	-4.09882
H	-2.93262	2.49562	4.54492
H	-3.26962	4.09428	-0.19295
H	-6.02529	3.47963	0.17942
H	-2.93702	-5.18562	-0.10920
H	-3.26997	-1.87389	3.63806
H	-6.02636	-1.89182	2.92267
H	-0.55961	-5.62998	0.49059
H	-0.94246	-2.39378	4.31922
H	-0.94639	-2.54561	-4.23952
H	-0.55642	2.39081	-5.11016
H	-0.94139	4.94092	-0.08525
H	-0.55401	3.23490	4.62829
H	4.10333	5.83680	3.40695
H	3.96165	6.34007	1.70828
H	4.09928	0.03040	-6.75936
H	3.95759	-1.69146	-6.34242
H	3.95826	-4.64661	4.63608
H	4.09989	-5.87072	3.35525
H	6.85551	-1.33903	0.88382
H	7.90548	-3.47644	1.68703
H	6.48074	-5.12993	2.91691
H	6.85485	-0.10186	-1.59944
H	7.90599	0.26959	-3.85181
H	6.48126	0.03379	-5.89907
H	6.85628	1.43646	0.70713
H	7.91103	3.20484	2.14819
H	6.48768	5.09621	2.96878
H	4.40594	0.16960	2.05951
H	3.13194	-0.76177	1.27370
H	4.40236	-1.86952	-0.88137
H	3.13031	-0.72093	-1.29442
H	4.39935	1.69602	-1.17684
H	3.13010	1.47976	0.02738

Frequencies

12.0975	15.7538	15.9296
25.4409	27.2040	27.2971
28.7245	33.9921	34.2194
46.7194	47.0422	51.9146
52.6425	61.5312	61.6013
86.4644	91.7037	91.8153
105.8504	118.5908	118.6705
119.0559	127.6624	127.7632
138.9815	139.1661	147.4315
151.2463	159.7667	159.9909
167.1673	170.9777	171.0127
175.6292	175.6900	178.1648
195.0541	195.1190	208.6935
221.7085	221.8023	232.5609
236.2115	242.7872	242.8569
253.6503	253.7779	253.8696
257.9033	258.0344	268.3068
274.9207	276.3218	276.3486
300.4829	300.5849	307.6159
319.4483	319.4789	321.9980
327.8415	327.9011	332.4811
343.2726	347.2070	347.4267
373.4889	373.6164	379.2795
388.8737	398.1684	399.8250
399.9600	405.7273	405.8367
419.3700	429.3720	429.4289
436.5164	436.6243	439.9382
459.2209	459.2603	468.0138
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484.3518	484.9878	501.2035
503.2798	503.3937	530.1994
531.6834	548.7612	548.8501
553.7151	553.7581	568.9048
571.5459	571.5771	574.9721
576.6789	576.8212	578.8827
594.9578	594.9831	605.6208
606.2660	606.2944	623.5910
630.4928	645.6449	645.7101
652.9178	652.9231	653.5058
656.6510	659.0305	659.1102
660.3022	660.6308	660.7948
715.7394	715.8050	719.1610
723.2179	723.2317	726.7521
734.5277	734.5575	736.3960
740.3168	744.8767	744.9160
750.3249	752.5862	752.6442
762.7560	763.8891	763.9054
767.7251	768.4133	774.6615
774.7306	779.4433	779.5122
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798.3495	799.1356	799.2239
811.9077	811.9788	816.5715
825.4895	825.5680	827.6059
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884.6154	888.2340	888.2950
894.2682	896.3671	896.5900
899.6549	911.0711	913.1609
913.3052	913.8784	919.5466
919.8168	935.1987	935.2340
935.2478	936.0439	936.2783
941.0207	941.1793	941.4788
955.9558	957.0609	957.1164

963.6694 963.7290 967.5581
967.6015 970.7441 973.5617
988.7372 1004.4931 1005.5668
1005.6396 1011.0531 1011.0926
1012.5229 1014.7285 1014.7805
1015.2000 1015.2828 1026.0795
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1066.6363 1075.2654 1077.8077
1077.9247 1106.9194 1107.0202
1107.8453 1108.0490 1111.1160
1117.8970 1117.9207 1118.1421
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1192.1034 1192.1804 1226.9666
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1390.9049 1400.6568 1407.8738
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1483.4664 1484.8759 1484.8923
1484.8994 1491.9642 1492.0020
1495.4489 1501.2066 1501.8138
1501.9903 1509.5416 1509.6685
1509.9948 1521.2432 1521.3835
1522.1871 1534.3248 1534.3877
1534.7187 1606.5351 1606.8117
1631.1408 1631.2048 1632.9458
1636.7869 1636.8276 1638.1544
1649.1127 1649.1376 1649.2475
1676.1172 1676.2432 1676.2617
1678.7791 1678.8891 1678.9111
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1822.3528 1822.3735 1824.2174
2982.3523 2982.4839 2987.0946
3016.8934 3017.1737 3017.2979
3057.2786 3057.2896 3057.3840
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3065.8534 3066.8135 3067.0298
3074.4818 3074.5519 3074.5745
3078.4084 3078.6760 3078.8001
3103.3010 3103.3266 3103.5978
3124.8800 3124.9429 3124.9976
3126.4409 3126.7556 3126.8299
3173.0371 3173.1047 3173.1475
3179.7780 3179.8583 3180.9252
3184.1275 3184.1598 3184.2554
3199.4661 3199.5225 3199.5335
3199.8209 3199.8651 3200.1003
3200.7631 3200.7930 3200.8240
3221.4048 3221.5079 3223.7116

TS1

E(RB3LYP) = -3723.59995113
E(RB3LYP-D3) = -3723.78650753
H - Sum of electronic and thermal Enthalpies= -3722.438080
G - Sum of electronic and thermal Free Energies= -3722.596165
Number of imaginary frequencies: 0

Cartesian Coordinates

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C	5.82584	-0.76707	1.19518
C	5.78980	0.63668	1.32476
C	5.79297	1.44005	0.16928
C	5.79920	0.84972	-1.11138
C	5.80939	-0.55237	-1.22884
C	5.79486	-2.89187	-0.19980
C	5.63130	-3.40700	-1.64914
C	6.54884	-2.55822	-2.55631
C	5.74753	-1.23642	-2.59996
C	5.79899	1.71762	-2.37212
C	5.68484	3.23515	-2.09616
C	5.74831	2.97034	0.26111
C	5.74341	1.29144	2.70737
C	5.63947	0.28595	3.87870
C	5.81884	-1.61617	2.47252
C	6.60661	-0.88141	3.58213
C	6.59000	3.57059	-0.89047
C	1.97954	-0.96854	4.32927
C	3.11463	-0.12100	4.49735
C	4.29977	-0.43195	3.87641
C	4.41114	-1.59318	3.05764
C	3.34490	-2.43946	2.88156

C	2.10068	-2.15235	3.51297
C	2.03456	4.14431	0.00980
C	1.99159	4.26472	-1.42770
C	3.16516	3.97619	-2.18455
C	4.31536	3.58763	-1.54289
C	4.35203	3.45208	-0.12474
C	3.24296	3.72298	0.63839
C	1.98781	-1.89940	-3.39541
C	1.91030	-3.20367	-2.78236
C	3.08067	-3.76222	-2.18813
C	4.26017	-3.05812	-2.20412
C	4.33060	-1.76551	-2.80040
C	3.22645	-1.19530	-3.38393
C	0.83106	-1.33858	-4.01114
C	-0.33513	-2.05796	-3.99797
C	-0.41459	-3.33448	-3.39194
C	0.67430	-3.91500	-2.79330
C	0.73221	-0.66704	4.95073
C	-0.32647	-1.51433	4.74666
C	-0.20377	-2.67919	3.95275
C	0.97710	-3.01285	3.34364
C	0.78703	4.68333	-2.06512
C	-0.30495	4.96751	-1.28668
C	-0.25903	4.86298	0.12375
C	0.87573	4.45991	0.77846
C	-1.58584	5.27767	0.66059
O	-1.95811	5.36286	1.81648
N	-2.36075	5.60953	-0.46256
C	-1.66594	5.43533	-1.67108
O	-2.11929	5.66155	-2.77819
C	-1.72852	-1.44492	5.24500
O	-2.25109	-0.61622	5.96937
C	-1.52024	-3.37706	3.94275
O	-1.82577	-4.43109	3.41863
C	-1.66230	-1.74229	-4.59553
O	-1.99659	-0.77895	-5.25784
C	-1.79928	-3.84891	-3.58595
O	-2.27995	-4.92048	-3.26179
N	-2.48805	-2.83918	-4.27819
N	-2.37698	-2.57207	4.71665
C	-3.74688	6.01202	-0.38816
C	-3.79245	-2.84463	4.90872
C	-3.85186	-2.98795	-4.76135
C	-6.97370	-2.39864	-1.94036
C	-6.90406	-3.62895	-2.58976
C	-5.86015	-3.85591	-3.48578
C	-4.92607	-2.83611	-3.69629
N	-4.97220	-1.66453	-3.04566
C	-5.97540	-1.44198	-2.18172
C	-6.29044	-0.32543	2.56013
C	-6.53899	-0.40099	3.92859
C	-5.72660	-1.21117	4.72233
C	-4.69071	-1.91690	4.10453
N	-4.44235	-1.83770	2.79013
C	-5.22614	-1.06332	2.02527
C	-6.48077	2.77608	0.06316
C	-6.97551	4.08179	0.09215
C	-6.09030	5.14443	-0.05312
C	-4.73008	4.85541	-0.23197
N	-4.25613	3.61023	-0.27457
C	-5.10972	2.58062	-0.12116
C	-4.46023	1.20468	-0.11924
C	-4.92821	-1.09832	0.52966
C	-6.03365	-0.07536	-1.52227
N	-5.38937	0.08160	-0.19501
H	6.73370	-3.30163	0.20210
H	4.99093	-3.30681	0.41977
H	5.84286	-4.48129	-1.68237
H	6.62601	-2.99291	-3.55988
H	7.55818	-2.43098	-2.14891
H	6.73035	1.54207	-2.93108
H	6.19260	-2.62402	2.28527
H	6.65224	1.89286	2.85800
H	4.90115	1.99250	2.75962
H	7.59661	-0.54709	3.25190
H	6.72715	-1.52876	4.45871
H	4.98196	1.41464	-3.03824
H	5.93172	3.79265	-3.00624
H	7.58890	3.12584	-0.96355
H	6.69476	4.65470	-0.76493
H	3.02070	0.76147	5.12793
H	3.42287	-3.33269	2.26573
H	5.84207	0.80252	4.82320
H	3.13119	4.08700	-3.26706
H	3.26267	3.63188	1.72235
H	6.06568	3.32185	1.24389
H	3.01897	-4.75227	-1.73958
H	3.27108	-0.21102	-3.84494
H	6.07571	-0.56935	-3.39821
H	0.60466	-4.89956	-2.33768
H	0.88064	-0.36083	-4.48346
H	1.05957	-3.90899	2.73395
H	0.62689	0.22338	5.56546
H	0.89925	4.38211	1.86248
H	0.74268	4.77502	-3.14744
H	-3.96870	6.56411	-1.30750
H	-3.85649	6.69718	0.45940
H	-4.02366	-2.76261	5.97485
H	-3.94758	-3.88015	4.59009
H	-3.98827	-2.21010	-5.51917
H	-3.94161	-3.96875	-5.23855
H	-7.78571	-2.17586	-1.25297
H	-7.65254	-4.39568	-2.40691
H	-5.76814	-4.80115	-4.01233
H	-6.89014	0.29733	1.90663
H	-7.34893	0.17128	4.37442
H	-5.87552	-1.27778	5.79612
H	-7.13708	1.92232	0.18485

H	-8.03827	4.26470	0.23153
H	-6.43799	6.17438	-0.02860
H	-7.09451	0.20806	-1.44425
H	-5.56628	0.62970	-2.21787
H	-5.42564	-1.98614	0.12757
H	-3.84883	-1.28203	0.40497
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Frequencies

-44.2258	12.0609	15.8282
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27.9102	32.3141	38.2357
44.7906	46.5432	48.6844
50.6351	53.5530	60.6315
67.2910	91.3602	95.2648
101.1213	108.5295	116.5015
118.1710	120.3170	129.0624
138.3094	138.6815	148.5933
150.1954	159.8338	160.5436
167.3707	169.2950	173.1507
173.8369	179.0325	180.4301
189.1704	193.2153	202.5664
211.5417	224.3814	229.1779
234.3258	235.4718	242.0918
242.4473	248.2721	248.7392
257.5770	259.4622	267.6059
270.6305	278.0945	289.4494
292.6643	298.6122	300.7195
305.1870	306.3572	312.2654
319.3702	323.6550	330.3271
346.8874	348.5884	361.6898
370.8687	373.0226	379.0274
386.6650	396.4286	399.6784
400.0914	404.2329	405.3338
418.7885	419.5949	429.1038
429.8163	436.5858	438.7346
448.0266	459.8674	470.1909
476.7109	482.2028	483.9878
484.4229	485.1720	500.8447
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532.8896	542.8214	548.3796
548.8844	554.4951	568.9697
571.8947	573.8848	575.8378
576.0428	576.6142	578.3222
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606.8371	607.9323	612.7689
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1187.8535	1189.9160	1191.0039
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1273.8047	1277.6889	1278.0235
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1377.2572	1382.7475	1385.5717

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1636.4605	1637.4594	1639.2212
1648.7952	1649.3837	1649.7993
1675.3782	1676.6299	1676.9182
1678.2173	1679.0288	1679.4381
1771.4593	1774.4335	1774.7628
1821.6725	1822.0669	1823.9301
2977.8614	2996.1228	3000.4643
3015.4801	3015.6720	3016.5618
3057.2088	3057.2628	3057.4339
3065.0713	3066.7742	3068.6208
3070.7298	3071.3618	3076.4325
3078.9782	3079.1837	3079.3596
3080.0262	3086.0568	3099.9533
3103.2318	3103.3223	3103.5832
3115.5271	3126.0211	3126.1453
3127.9941	3128.1535	3129.8821
3172.5564	3172.9957	3173.1169
3179.9339	3180.9595	3181.5782
3182.5624	3186.1007	3186.8661
3197.3332	3199.4607	3199.5659
3199.9845	3200.0726	3200.6955
3201.0896	3201.7224	3207.3014
3212.6857	3230.8723	3235.7757

I1

E(RB3LYP) = -3723.60246114

E(RB3LYP-D3) = -3723.79055565

H - Sum of electronic and thermal Enthalpies= -3722.439516

G - Sum of electronic and thermal Free Energies= -3722.599492

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.82850	-1.40324	-0.10200
C	5.84432	-0.86095	1.19637
C	5.84524	0.53701	1.38775
C	5.85978	1.39078	0.26923
C	5.89598	0.85705	-1.03541
C	5.87825	-0.53767	-1.21368
C	5.75829	-2.92062	-0.29847
C	5.61259	-3.36495	-1.77546
C	6.57577	-2.50509	-2.62159
C	5.82075	-1.15607	-2.61379
C	5.96716	1.77819	-2.25623
C	5.81775	3.28081	-1.92410
C	5.77502	2.91459	0.42052
C	5.84974	1.13267	2.79807
C	5.76675	0.08214	3.93115
C	5.81702	-1.76116	2.43760
C	6.67255	-1.10928	3.55048
C	6.65412	3.58397	-0.66244
C	2.07621	-1.02534	4.46120
C	3.25767	-0.24677	4.63319
C	4.40146	-0.58010	3.95083
C	4.42829	-1.69809	3.06779
C	3.31301	-2.47810	2.88416
C	2.10627	-2.16390	3.57473
C	2.02049	3.91617	0.01171
C	2.05273	4.10850	-1.41842
C	3.28157	3.92655	-2.11671
C	4.41354	3.56827	-1.42749
C	4.38076	3.36396	-0.01779
C	3.21548	3.53358	0.69046
C	2.03783	-1.61725	-3.43572
C	1.92141	-2.97378	-2.95650
C	3.06785	-3.61472	-2.40001
C	4.26652	-2.94561	-2.34257
C	4.38690	-1.62009	-2.85185
C	3.30211	-0.96380	-3.37864
C	0.89084	-0.95043	-3.95700
C	-0.29873	-1.62893	-4.00355
C	-0.40530	-2.97177	-3.57113
C	0.66863	-3.64830	-3.05162
C	0.86886	-0.69194	5.14128
C	-0.24322	-1.46226	4.92126
C	-0.21309	-2.58220	4.05722
C	0.92910	-2.94798	3.39391
C	0.86400	4.48580	-2.10835
C	-0.28723	4.66188	-1.38641
C	-0.31865	4.48765	0.01753
C	0.79972	4.12090	0.72126
C	-1.69372	4.81897	0.49095
O	-2.13068	4.85284	1.62652
N	-2.42098	5.15361	-0.66312
C	-1.64219	5.08990	-1.83115
O	-2.03087	5.37402	-2.94923
C	-1.62637	-1.33091	5.45565
O	-2.07313	-0.51909	6.24778
C	-1.57448	-3.18975	4.03633
O	-1.95728	-4.19111	3.46342
C	-1.63220	-1.19449	-4.50367

O	-1.95785	-0.13196	-4.99651
C	-1.80016	-3.42608	-3.82774
O	-2.28498	-4.53562	-3.68774
N	-2.48525	-2.30448	-4.32334
N	-2.36505	-2.36711	4.86448
C	-3.79276	5.61022	-0.64797
C	-3.80201	-2.53823	5.06245
C	-3.86243	-2.33761	-4.81244
C	-6.88206	-3.02694	-1.90287
C	-6.44829	-4.11004	-2.66411
C	-5.44172	-3.90464	-3.60378
C	-4.90679	-2.61837	-3.74362
N	-5.31485	-1.57619	-3.00275
C	-6.28615	-1.77189	-2.09332
C	-6.03922	0.26387	2.76680
C	-5.93478	0.48066	4.13989
C	-5.21360	-0.42339	4.92023
C	-4.61574	-1.51588	4.28371
N	-4.70530	-1.72099	2.96250
C	-5.40513	-0.85541	2.21379
C	-6.76606	2.59708	-0.20179
C	-7.15013	3.93882	-0.15937
C	-6.17872	4.92225	-0.30145
C	-4.84870	4.52095	-0.49463
N	-4.47883	3.24111	-0.55364
C	-5.41749	2.28679	-0.39993
C	-4.90411	0.85080	-0.43714
C	-5.51236	-1.23014	0.74180
C	-6.76074	-0.57094	-1.28173
N	-5.93248	-0.14884	-0.14163
H	6.67164	-3.38387	0.10377
H	4.92512	-3.33353	0.28335
H	5.79193	-4.44281	-1.85238
H	6.65835	-2.89261	-3.64390
H	7.58054	-2.43228	-2.19031
H	6.93459	1.63033	-2.75990
H	6.13458	-2.77781	2.20085
H	6.77302	1.71402	2.93916
H	5.02149	1.84337	2.91086
H	7.66447	-0.80338	3.19936
H	6.79398	-1.79771	4.39511
H	5.19785	1.50213	-2.98678
H	6.09575	3.88059	-2.79757
H	7.66647	3.16650	-0.70493
H	6.72539	4.66395	-0.48716
H	3.23167	0.60346	5.31261
H	3.32320	-3.33681	2.21630
H	6.02673	0.55153	4.88615
H	3.30171	4.08605	-3.19352
H	3.17800	3.38178	1.76722
H	6.03115	3.23570	1.43079
H	2.97114	-4.63457	-2.03163
H	3.37984	0.05426	-3.75351
H	6.18425	-0.46583	-3.37597
H	0.57368	-4.67819	-2.71679
H	0.96490	0.07590	-4.30716
H	0.94013	-3.80864	2.73000
H	0.83400	0.16558	5.80852
H	0.76515	3.99217	1.80015
H	0.87804	4.63435	-3.18517
H	-3.95185	6.14215	-1.59226
H	-3.90331	6.32929	0.17158
H	-4.00985	-2.45981	6.13345
H	-4.04297	-3.54547	4.71458
H	-4.04521	-1.35356	-5.25016
H	-3.92916	-3.09773	-5.59901
H	-7.67802	-3.14632	-1.17249
H	-6.88820	-5.09494	-2.52998
H	-5.06230	-4.72016	-4.21018
H	-6.59021	0.94221	2.12584
H	-6.40475	1.34822	4.59651
H	-5.09068	-0.27553	5.98854
H	-7.48940	1.80102	-0.06860
H	-8.19250	4.20913	-0.00791
H	-6.43556	5.97799	-0.25925
H	-7.76664	-0.80108	-0.90209
H	-6.85679	0.28425	-1.95746
H	-6.25980	-2.03065	0.67504
H	-4.55775	-1.69288	0.44127
H	-4.11255	0.77249	0.31660
H	-4.41725	0.67382	-1.40889

Frequencies

12.3502	17.3566	19.3198
20.3566	25.8536	27.0502
36.4263	38.3319	42.4982
43.9916	47.0041	51.6601
53.1752	58.2805	61.8813
70.5335	94.9373	98.4682
99.7987	115.1871	115.6992
120.6307	121.3686	134.0560
137.2783	138.6482	148.7640
149.2948	158.4560	161.4098
164.7422	167.7718	174.6057
177.6357	181.2466	184.9487
189.4393	197.5057	202.0639
207.3484	224.4050	228.0276
230.8307	236.2635	240.4055
240.6868	243.4065	246.6719
255.5832	260.5325	265.8512
266.7261	271.1759	286.5430
288.5607	297.2093	299.2689
303.6372	304.9699	317.5165
324.0740	329.0764	343.0340
347.5793	348.9069	371.1554
372.3038	382.1668	385.5665
393.4278	393.8355	399.2997
401.7705	403.7707	405.4357

419.6561	426.2898	427.9930	1178.8228	1179.1348	1185.9318
429.5355	436.2172	437.4398	1187.9065	1189.8338	1190.6849
445.9085	460.0347	470.1140	1191.0926	1192.9372	1222.4284
478.1098	482.7681	483.4569	1228.3686	1230.6432	1231.1277
485.0406	486.0710	498.5362	1237.1614	1243.1453	1243.6906
500.8632	505.5187	528.1139	1244.7201	1248.6125	1249.5057
534.6250	538.5699	543.1276	1254.0052	1254.2030	1254.2322
549.4659	550.2210	567.8896	1257.0285	1259.8995	1269.7640
571.4414	574.4903	575.0246	1276.2496	1276.6330	1277.3801
576.8118	577.1252	579.4048	1278.3830	1278.4340	1289.6408
592.3328	594.7891	601.9464	1290.6428	1298.6919	1300.6543
606.4309	607.5389	608.9989	1300.9563	1301.9900	1303.9551
622.8288	626.3759	634.1420	1314.0142	1316.2437	1318.6984
648.0838	652.2908	653.3618	1320.0910	1322.5526	1324.2772
655.7126	659.5790	660.3948	1326.7815	1339.3222	1339.8611
660.8591	664.5063	703.2857	1341.5218	1344.9974	1345.8987
714.9123	716.8529	720.7876	1346.7558	1355.3989	1365.3454
721.4111	723.5012	726.0314	1366.2137	1373.9584	1376.4766
733.5290	735.8414	739.0399	1376.9287	1378.3845	1379.6058
741.1050	741.9914	742.7068	1386.2495	1400.9252	1402.0693
746.9883	750.7822	757.5645	1405.5733	1410.8822	1412.0152
762.2841	763.9139	764.0369	1412.4753	1412.7140	1415.9600
765.3525	768.6302	770.5831	1419.7281	1421.6419	1452.1953
775.8969	779.0038	779.6156	1452.6574	1468.6123	1472.5614
781.7786	782.3147	785.3059	1473.1880	1474.0116	1474.4405
787.9901	802.5469	805.2026	1474.8301	1475.4611	1475.5557
813.5327	819.3209	824.8822	1476.2172	1479.0195	1484.0612
825.6227	833.3729	837.8169	1484.4173	1484.5879	1487.4972
839.2414	841.9422	852.1682	1489.5244	1490.7238	1491.4903
863.8778	869.0611	869.4177	1496.8192	1498.1937	1501.2159
876.6494	887.7656	888.2498	1502.4119	1503.2196	1503.8869
894.7903	895.9533	896.9374	1510.1535	1520.9503	1521.1322
899.9603	909.4861	912.3753	1521.9062	1534.3025	1534.6779
915.7525	919.0134	920.1973	1535.2800	1606.7572	1607.4557
922.6821	928.5464	934.9134	1628.5091	1629.1148	1633.9150
935.5646	936.2916	936.9942	1636.7290	1636.9694	1638.8560
940.5492	940.8193	941.6402	1648.6920	1649.0551	1649.9353
944.3327	955.2857	958.3629	1675.0505	1676.2703	1676.8621
960.0916	963.0218	965.8444	1677.9137	1678.7479	1679.4216
966.5603	968.1685	969.8051	1770.2089	1772.6667	1774.9047
986.7734	988.4820	995.3945	1820.9132	1821.5815	1823.9563
1005.6070	1006.4489	1007.0501	2992.8412	3013.6094	3014.0457
1009.5645	1010.1408	1011.0835	3016.1689	3016.8443	3021.8202
1013.1081	1014.9528	1015.0584	3056.8184	3057.3317	3057.4959
1017.2685	1018.1599	1030.4687	3062.8997	3064.8018	3066.0276
1040.1271	1043.9518	1045.0121	3066.9201	3068.4809	3071.6462
1066.9533	1074.9938	1077.5136	3079.3769	3079.5548	3080.0517
1078.4696	1098.6208	1104.9025	3087.5422	3089.2344	3102.7936
1108.0417	1108.8655	1117.3798	3103.3727	3103.9370	3107.1634
1117.7342	1120.3628	1127.8814	3109.4259	3126.6089	3131.9994
1138.5504	1140.3599	1153.5697	3132.8023	3141.8752	3146.6742
1155.8912	1156.5623	1166.6427	3171.7098	3172.9272	3173.4566
1167.0483	1171.4285	1176.3818	3179.4661	3179.7562	3181.0162
1176.8972	1177.1105	1178.4973	3183.2813	3185.9853	3190.3313

3196.3077	3199.3660	3199.5427
3199.9155	3200.5876	3200.9349
3201.7449	3202.2525	3216.7966
3224.8094	3230.7156	3236.4604

TS2

E(RB3LYP) = -3723.60030463

E(RB3LYP-D3) = -3723.78902754

H - Sum of electronic and thermal Enthalpies= -3722.438048

G - Sum of electronic and thermal Free Energies= -3722.594592

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.78993	-1.38050	-0.22452
C	5.87740	-0.90300	1.09647
C	5.92879	0.48360	1.35257
C	5.88203	1.38998	0.27806
C	5.79927	0.92340	-1.04978
C	5.76485	-0.46113	-1.29393
C	5.74407	-2.88826	-0.49155
C	5.57761	-3.27001	-1.98399
C	6.46267	-2.32380	-2.82329
C	5.64412	-1.01476	-2.71658
C	5.76299	1.90758	-2.22307
C	5.66060	3.39436	-1.80338
C	5.83715	2.90368	0.51127
C	6.05548	1.01089	2.78454
C	5.96704	-0.08461	3.87256
C	5.85929	-1.85707	2.29770
C	6.79061	-1.30269	3.40172
C	6.61672	3.62366	-0.61379
C	2.22227	-0.95744	4.44416
C	3.46203	-0.27984	4.62966
C	4.56688	-0.66691	3.91235
C	4.49749	-1.74314	2.98138
C	3.32567	-2.43449	2.79139
C	2.15580	-2.06076	3.51588
C	2.05704	3.87355	0.50803
C	1.96370	4.19446	-0.89612
C	3.12516	4.07661	-1.71398
C	4.31348	3.66740	-1.16012
C	4.41104	3.37460	0.23077
C	3.31227	3.47026	1.04952
C	1.86544	-1.65184	-3.45824
C	1.84463	-3.03812	-3.05662
C	3.03885	-3.63520	-2.55686
C	4.19484	-2.89713	-2.48641
C	4.22476	-1.54019	-2.92040
C	3.08843	-0.92322	-3.38396
C	0.66851	-1.03619	-3.92984
C	-0.47380	-1.79055	-4.00556
C	-0.48394	-3.15918	-3.64731
C	0.63879	-3.78889	-3.17586
C	1.04789	-0.54700	5.14015
C	-0.12600	-1.21072	4.89594
C	-0.18863	-2.30351	3.99978
C	0.91805	-2.74153	3.31986
C	0.71531	4.61284	-1.44329
C	-0.37721	4.67313	-0.61789
C	-0.29117	4.33559	0.75365
C	0.89278	3.95219	1.32776
C	-1.64444	4.49771	1.35567
O	-1.99674	4.33318	2.50879
N	-2.47634	4.92523	0.30491
C	-1.78202	5.07788	-0.90523
O	-2.27032	5.48628	-1.94343
C	-1.49696	-0.97082	5.42574
O	-1.87528	-0.14127	6.23490
C	-1.59665	-2.79355	3.96329
O	-2.05742	-3.74920	3.37048
C	-1.84214	-1.42228	-4.46617
O	-2.24846	-0.35806	-4.89089
C	-1.84797	-3.69301	-3.90997
O	-2.25618	-4.83813	-3.81666
N	-2.61381	-2.59809	-4.34138
N	-2.31994	-1.92212	4.80365
C	-3.89053	5.21531	0.46639
C	-3.76811	-1.97970	5.00172
C	-4.00493	-2.70267	-4.78272
C	-6.83674	-3.35102	-1.67541
C	-6.30890	-4.46752	-2.32075
C	-5.36937	-4.27702	-3.33147
C	-4.99376	-2.96798	-3.65739
N	-5.50120	-1.89172	-3.03677
C	-6.40528	-2.07300	-2.05663
C	-5.85749	0.72858	2.45923
C	-5.57307	1.14228	3.76062
C	-4.89190	0.27992	4.62049
C	-4.51624	-0.97774	4.13421
N	-4.77631	-1.37200	2.88118
C	-5.43205	-0.54138	2.05603
C	-6.48650	2.61194	-1.66470
C	-6.73840	3.97930	-1.71464
C	-5.88305	4.84948	-1.03984
C	-4.80756	4.30488	-0.33559
N	-4.56204	2.98737	-0.28673
C	-5.38048	2.14385	-0.93700
C	-5.02758	0.66207	-0.85230
C	-5.72228	-1.13587	0.68784
C	-6.96520	-0.82520	-1.38051
N	-6.13008	-0.18734	-0.34701
H	6.67631	-3.34549	-0.12808
H	4.93328	-3.34933	0.08620
H	5.80871	-4.33235	-2.11767
H	6.51973	-2.65902	-3.86564
H	7.48018	-2.22037	-2.42998

H	6.67660	1.78488	-2.82422
H	6.10968	-2.87777	2.00557
H	7.02210	1.52591	2.89170
H	5.28446	1.76545	2.98140
H	7.78322	-1.03284	3.02389
H	6.90803	-2.03485	4.20941
H	4.92504	1.66994	-2.88944
H	5.86282	4.03501	-2.66858
H	7.61537	3.20216	-0.77482
H	6.71742	4.69208	-0.38903
H	3.50902	0.54381	5.34009
H	3.26034	-3.25909	2.08460
H	6.28949	0.32584	4.83562
H	3.04704	4.31345	-2.77373
H	3.37075	3.23291	2.10960
H	6.19154	3.17126	1.50724
H	3.01441	-4.67870	-2.24770
H	3.09614	0.11656	-3.70368
H	5.93593	-0.27388	-3.46196
H	0.61754	-4.83971	-2.89826
H	0.66907	0.01076	-4.22216
H	0.85552	-3.57758	2.62791
H	1.08558	0.28917	5.83386
H	0.94819	3.70285	2.38434
H	0.63682	4.86989	-2.49668
H	-4.07437	6.25842	0.18758
H	-4.09456	5.10290	1.53644
H	-3.96306	-1.79586	6.06185
H	-4.08075	-2.99192	4.73670
H	-4.24373	-1.74825	-5.25650
H	-4.06372	-3.50380	-5.52736
H	-7.57857	-3.46402	-0.88937
H	-6.62477	-5.46960	-2.04210
H	-4.91947	-5.11676	-3.84997
H	-6.38924	1.36645	1.76218
H	-5.87450	2.12974	4.10095
H	-4.63612	0.57610	5.63312
H	-7.13450	1.92213	-2.19251
H	-7.58150	4.36379	-2.28323
H	-6.03499	5.92468	-1.07232
H	-7.92437	-1.08295	-0.91310
H	-7.17194	-0.08905	-2.15989
H	-6.54557	-1.84939	0.82516
H	-4.84813	-1.74337	0.39950
H	-4.17881	0.58468	-0.16827
H	-4.68192	0.30847	-1.83440

Frequencies

-22.3635	17.0928	19.1225
21.9048	22.0408	25.9486
29.8768	37.9337	41.6542
45.0985	47.1455	51.8017
52.4635	59.6514	64.9283
70.7525	94.8257	96.2883
105.2906	111.3830	114.2646
120.9626	122.0470	128.1080
137.8350	138.5821	145.9584
150.4654	159.0452	160.4625
160.8932	167.4560	171.0440
174.8806	184.9166	186.6371
191.0160	198.0333	203.9187
209.6359	225.4995	230.3277
233.7688	236.7054	240.5878
242.5221	244.8670	250.1003
256.3437	260.5532	262.0125
270.3202	281.2331	289.9747
292.7280	296.8982	299.8929
302.9616	309.0583	317.0616
329.1875	338.7056	344.0143
348.1425	348.9970	371.6476
371.9212	384.7765	388.6726
392.2020	394.3518	399.2535
402.2661	403.6618	409.5319
419.8642	421.8739	427.5040
428.5463	435.5533	436.1436
442.9034	460.9725	470.2250
470.5385	483.0868	483.6626
484.4162	486.2725	498.2652
501.7022	502.0340	527.8632
530.6346	536.4552	543.2522
549.0405	550.6783	567.5232
572.2750	573.6320	575.2245
576.5213	577.3206	579.6178
592.1357	593.3251	600.3583
606.4954	607.4873	608.8033
617.1270	623.8646	636.5320
652.3992	653.2420	654.6460
658.8428	659.8369	661.7202
663.6588	667.8450	704.4670
714.8907	717.9784	721.7038
722.6078	724.0603	726.3465
733.4825	737.6840	739.7347
741.2519	742.3586	743.1436
748.3472	755.7663	760.5123
762.2204	764.2442	764.7929
768.5593	771.6156	777.2634
778.0098	778.8528	780.9621
781.6428	781.9656	784.1147
797.1245	801.5814	804.3228
813.0967	819.5745	824.0492
828.4507	833.7734	837.4948
840.1178	840.7219	850.3229
863.9399	868.9287	869.3276
876.5027	888.0777	888.1124
895.1641	896.3410	896.5916
899.9846	904.2266	911.6408
914.6564	917.9426	920.2655
922.6028	930.0616	934.7322

935.3512	935.9021	936.3100
939.9831	941.0352	941.4328
941.9150	948.3967	955.6833
959.3063	961.5837	965.8803
966.4642	968.3815	972.1480
984.9938	986.7214	988.3596
1000.8414	1006.2457	1007.1176
1008.7228	1010.5745	1010.8718
1013.4778	1014.6099	1015.6358
1016.7591	1019.2958	1024.0091
1039.9999	1043.7385	1044.7104
1066.8340	1075.1367	1077.8645
1078.0360	1095.2473	1101.8774
1107.9190	1108.1576	1114.1140
1118.4269	1120.4924	1124.6910
1133.3192	1138.7314	1144.0229
1148.6747	1152.6095	1156.5315
1166.6475	1166.8713	1175.5772
1176.4093	1176.8096	1177.6964
1178.6853	1178.9071	1186.9454
1189.3364	1190.2173	1190.4674
1192.1956	1195.1128	1227.5925
1230.2635	1230.3669	1233.6206
1237.0081	1244.1681	1245.7505
1247.8868	1248.9320	1249.4312
1253.7653	1253.9689	1254.4125
1259.8023	1267.2089	1273.1674
1277.1804	1277.8896	1277.9721
1278.2409	1280.0966	1289.9357
1290.5772	1298.9712	1300.0570
1300.9957	1301.7513	1303.9928
1313.4265	1314.3793	1318.8371
1319.6306	1322.2053	1324.6667
1327.5223	1339.4371	1339.7248
1341.5719	1345.3150	1346.0624
1349.1684	1355.8680	1358.8307
1365.5987	1372.6001	1375.2782
1376.7488	1377.0078	1378.3885
1387.1863	1390.8064	1400.3333
1400.8167	1407.4834	1411.2556
1412.1325	1412.5133	1414.4352
1418.0008	1423.7049	1452.1775
1452.4074	1471.1429	1472.1434
1472.7625	1474.6296	1474.7145
1474.8185	1474.9078	1476.1589
1477.2589	1483.5394	1483.9470
1484.2133	1486.2922	1487.5045
1490.6732	1493.2909	1494.3600
1495.4156	1498.1376	1501.7738
1502.6678	1503.0191	1507.0584
1514.9352	1520.8998	1521.0639
1521.8589	1534.5195	1534.7894
1535.1475	1606.7008	1607.5326
1628.0268	1628.5239	1630.4051
1636.2393	1638.6200	1640.9930
1649.0005	1649.2987	1649.4583
1674.5810	1676.4035	1676.6022
1677.8394	1678.8404	1678.9109
1769.4768	1771.8943	1774.1485
1820.1488	1821.1949	1822.9154
2988.1822	3014.5718	3014.6745
3017.3743	3030.6354	3046.3037
3055.1301	3056.9908	3057.0825
3057.5005	3063.5625	3066.9818
3068.1973	3068.4139	3075.1557
3079.5049	3079.7891	3080.2560
3093.3358	3102.9175	3103.2613
3103.9822	3113.9933	3122.0491
3130.0791	3130.5843	3132.1574
3133.5400	3148.3696	3152.4467
3172.0896	3172.4398	3173.7751
3179.7435	3180.9207	3181.5939
3186.7783	3187.3988	3191.6641
3199.3086	3199.3268	3200.2212
3200.8389	3201.3084	3201.9681
3203.0221	3204.2008	3216.4678
3228.3420	3231.4914	3232.7014

I2

E(RB3LYP) = -3723.60410532

E(RB3LYP-D3) = -3723.79575105

H - Sum of electronic and thermal Enthalpies= -3722.440639

G - Sum of electronic and thermal Free Energies= -3722.598754

Number of imaginary frequencies: 0

Cartesian Coordinates

C	-5.44481	-0.72960	-1.88155
C	-5.75316	0.53059	-1.33688
C	-5.95453	0.67846	0.05173
C	-5.87058	-0.44942	0.88756
C	-5.59687	-1.72393	0.34895
C	-5.36795	-1.85439	-1.03302
C	-5.23609	-0.87563	-3.39181
C	-4.84231	-2.30154	-3.84965
C	-5.68147	-3.31764	-3.04527
C	-4.99895	-3.20285	-1.66025
C	-5.59787	-2.96617	1.24677
C	-5.78188	-2.66871	2.75700
C	-6.03357	-0.33600	2.40626
C	-6.30143	2.04420	0.65121
C	-6.29717	3.20552	-0.37090
C	-5.84027	1.78458	-2.21597
C	-6.95926	2.70559	-1.67315
C	-6.83860	-1.55604	2.91634
C	-2.63775	4.38470	-0.94542
C	-3.92981	4.33821	-0.34624

C	-4.88402	3.48662	-0.84510
C	-4.60636	2.64762	-1.96252
C	-3.37924	2.67839	-2.57872
C	-2.35999	3.54481	-2.08595
C	-2.42776	-0.23077	3.90658
C	-2.31968	-1.64363	4.18245
C	-3.40898	-2.50193	3.85912
C	-4.54445	-1.97870	3.29328
C	-4.67385	-0.57910	3.06306
C	-3.64229	0.27987	3.35942
C	-1.11342	-3.43747	-2.01274
C	-1.03464	-2.91884	-3.35757
C	-2.23144	-2.51784	-4.01935
C	-3.44133	-2.64870	-3.38347
C	-3.52427	-3.18364	-2.06528
C	-2.38975	-3.55943	-1.38656
C	0.08169	-3.83365	-1.34099
C	1.27874	-3.72123	-2.00171
C	1.35034	-3.23350	-3.32840
C	0.23034	-2.83179	-4.00893
C	-1.61267	5.22325	-0.41882
C	-0.37428	5.19271	-1.00493
C	-0.10381	4.37814	-2.12918
C	-1.06472	3.57201	-2.68180
C	-1.11120	-2.16825	4.72394
C	-0.05486	-1.31728	4.91331
C	-0.14228	0.06114	4.60766
C	-1.30434	0.61890	4.13836
C	1.20573	0.66651	4.82210
O	1.55578	1.82279	4.68951
N	2.03780	-0.39818	5.23034
C	1.33528	-1.60657	5.35417
O	1.81266	-2.65851	5.74390
C	0.88688	5.88632	-0.62511
O	1.08326	6.68313	0.27682
C	1.33082	4.55468	-2.49541
O	1.94617	4.07289	-3.42603
C	2.65941	-4.07693	-1.56541
O	3.03248	-4.56222	-0.51415
C	2.77195	-3.29127	-3.76531
O	3.25687	-3.02758	-4.85196
N	3.49587	-3.76037	-2.65662
N	1.86022	5.43689	-1.53033
C	3.49900	-0.31692	5.31616
C	3.28264	5.76462	-1.40647
C	4.93172	-4.03556	-2.69164
C	7.37166	-0.55069	-2.62619
C	7.16732	-1.18116	-3.85158
C	6.35978	-2.31686	-3.89882
C	5.79601	-2.78382	-2.70708
N	5.99633	-2.18017	-1.52506
C	6.76151	-1.07353	-1.47645
C	5.13767	3.14172	1.39226
C	4.60091	4.33517	1.87291
C	4.01102	5.22916	0.97809
C	3.97304	4.88117	-0.37733
N	4.49135	3.73636	-0.84359
C	5.06466	2.88326	0.01858
C	4.99063	-2.30647	1.86785
C	5.02202	-2.99363	3.07978
C	4.59635	-2.34506	4.23864
C	4.13887	-1.02730	4.13151
N	4.14830	-0.34808	2.97515
C	4.57339	-0.96694	1.86104
C	4.54782	-0.14730	0.58396
C	5.67847	1.64756	-0.62094
C	6.92241	-0.39709	-0.11885
N	5.83727	0.51181	0.28766
H	-6.16729	-0.60054	-3.90896
H	-4.47403	-0.16692	-3.73920
H	-4.96365	-2.38394	-4.93516
H	-5.56686	-4.33011	-3.45012
H	-6.74825	-3.06931	-3.01318
H	-6.41513	-3.63012	0.92713
H	-5.97590	1.52924	-3.26774
H	-7.30250	1.99216	1.10454
H	-5.60921	2.28722	1.46701
H	-7.90189	2.17350	-1.50236
H	-7.14339	3.53585	-2.36516
H	-4.67083	-3.53686	1.11231
H	-6.02573	-3.59585	3.28689
H	-7.74933	-1.73464	2.33379
H	-7.11379	-1.42566	3.96970
H	-4.13631	4.98166	0.50730
H	-3.15609	2.04353	-3.43363
H	-6.78433	4.08295	0.06806
H	-3.31236	-3.56917	4.05094
H	-3.71824	1.34748	3.16367
H	-6.48144	0.61526	2.69487
H	-2.16511	-2.12645	-5.03297
H	-2.43915	-3.96120	-0.37665
H	-5.24519	-4.03438	-0.99899
H	0.29736	-2.45772	-5.02740
H	0.03670	-4.22012	-0.32595
H	-0.84262	2.94358	-3.54054
H	-1.80875	5.85211	0.44596
H	-1.36342	1.67945	3.90714
H	-1.02283	-3.22925	4.94351
H	3.81570	-0.76521	6.26219
H	3.75079	0.74539	5.30839
H	3.35427	6.82034	-1.13132
H	3.73284	5.60273	-2.38755
H	5.14962	-4.62007	-1.79487
H	5.13738	-4.64300	-3.57886
H	7.99728	0.33494	-2.55588
H	7.62582	-0.79240	-4.75725
H	6.15376	-2.82389	-4.83584
H	5.58708	2.40898	2.05368

H	4.63058	4.56155	2.93565
H	3.56210	6.15709	1.31832
H	5.26537	-2.79074	0.93600
H	5.34613	-4.03063	3.11569
H	4.56302	-2.86044	5.19294
H	7.84928	0.18904	-0.11870
H	7.02470	-1.16783	0.64948
H	6.67832	1.92950	-0.97817
H	5.08868	1.40944	-1.52215
H	3.80836	0.64465	0.72448
H	4.21555	-0.77740	-0.25661

Frequencies

16.4344	18.8109	21.1555
22.6106	24.8080	28.6657
36.1857	40.1709	42.5786
48.4681	52.1112	53.9913
58.7571	61.7185	68.9624
79.9327	89.3709	99.7597
105.1652	110.9027	116.2948
121.0540	121.6122	132.9892
138.3966	141.2100	145.6457
151.1706	158.2377	159.3965
162.0646	172.4463	173.8570
177.4177	185.0699	186.1716
196.2490	203.9011	205.9666
212.0450	225.8433	229.6979
236.6286	240.3262	243.6557
247.5601	249.3875	255.0059
258.8958	260.9349	269.9737
273.4502	289.9355	295.3058
296.5321	299.8586	306.5439
311.4171	317.0140	322.8189
332.6362	343.9417	347.1102
348.8420	370.5782	371.6593
372.6115	384.4976	390.6250
393.3374	394.6299	401.9454
402.6978	409.2574	415.3874
419.4116	424.6875	426.6188
427.1170	435.4220	438.4366
441.7686	460.8079	467.6833
471.8900	483.0631	484.2074
484.7731	489.6225	497.8892
500.4034	501.0587	527.4174
532.7305	537.5863	547.4444
550.4967	557.2863	566.2501
570.5088	573.0083	574.7932
577.2410	580.0953	583.8181
591.0259	592.2502	601.9778
605.2192	605.6830	608.8895
616.3835	624.0508	633.4897
652.7367	653.2181	654.2612
659.1614	660.7631	661.1851
665.2954	677.9040	705.0279
715.0213	717.3658	721.3711
722.5010	723.3121	726.9648
732.5834	736.9646	741.0939
741.7114	742.7498	742.9357
748.5306	761.2903	762.1339
764.2163	764.8748	768.9680
771.2201	773.3407	777.6685
777.9074	779.9310	781.6112
782.0386	783.5697	791.3387
801.3749	803.5708	811.0246
819.0233	819.8068	824.2195
831.7124	835.3376	837.0840
839.9500	842.1306	853.8793
868.2020	869.0294	869.6758
876.6053	887.7149	888.4230
894.9149	896.3610	896.9445
899.9008	911.4591	914.1402
917.1176	920.2819	922.0183
930.9660	935.5248	935.7223
936.1485	936.4953	936.6986
940.8158	941.0583	941.6740
942.8618	950.2142	953.5352
958.5731	959.9111	965.6129
966.5072	968.4577	969.3150
985.5767	989.5278	991.8598
1000.7765	1004.2924	1007.4280
1009.5999	1010.2899	1012.7479
1014.3743	1014.9682	1015.4388
1017.7290	1019.9835	1025.5913
1039.7600	1043.0516	1044.1969
1066.5727	1075.1159	1077.9666
1078.7177	1092.9809	1098.2531
1102.1691	1107.9602	1108.2196
1115.5759	1119.6546	1125.6251
1132.1968	1137.2344	1138.1160
1141.8081	1152.0090	1156.4726
1165.8691	1166.7534	1175.0587
1175.3519	1175.8935	1176.9932
1178.4038	1178.9177	1188.1277
1189.3228	1190.1775	1190.4966
1192.0202	1192.6996	1227.1737
1229.5386	1230.9522	1235.6142
1237.0292	1244.0715	1248.1450
1248.4757	1249.7534	1253.5477
1254.0318	1254.3725	1254.8208
1259.5244	1265.3696	1272.3816
1276.2264	1277.1567	1277.6919
1278.1349	1281.3953	1288.4788
1290.8370	1291.3286	1299.8619
1300.1573	1301.3427	1301.6174
1313.1975	1314.0598	1318.1343
1319.1951	1319.9545	1323.0553
1327.7739	1339.5889	1340.0860
1341.3610	1344.5923	1345.5053

1346.0943	1356.2893	1358.6860
1365.5844	1366.1319	1369.3169
1374.9571	1375.2667	1376.2630
1377.2662	1384.1056	1399.3505
1400.6387	1405.7157	1407.2019
1411.6082	1412.7451	1413.7998
1417.9334	1420.1330	1451.7132
1451.9993	1470.9936	1471.2180
1472.6767	1473.7438	1474.2930
1475.0461	1475.4455	1477.1121
1477.3075	1483.3315	1484.1037
1484.3458	1487.2900	1489.7466
1491.4621	1493.1467	1494.4336
1497.6415	1499.2025	1501.5626
1502.4257	1503.0817	1510.6091
1512.4178	1520.8736	1521.1198
1521.9027	1533.9388	1535.3472
1535.7344	1606.0013	1607.1186
1626.1602	1627.2844	1628.5254
1636.8729	1637.4152	1638.0511
1647.4074	1648.4800	1650.1054
1672.8692	1676.0396	1676.7858
1677.0581	1678.9847	1679.4374
1768.8261	1771.2047	1771.9077
1818.5897	1820.8127	1822.0524
2986.4274	3002.0353	3014.9875
3016.6981	3016.9922	3047.9529
3056.9942	3057.2937	3057.3859
3059.3535	3063.3085	3063.4944
3064.0863	3079.5908	3080.0719
3080.3572	3080.6818	3092.1614
3096.3281	3103.3268	3103.5225
3103.9359	3120.0282	3121.6316
3130.2127	3133.1694	3135.5910
3144.1624	3154.5157	3158.2268
3172.6626	3173.0408	3174.0702
3179.7932	3179.9664	3180.3257
3188.3961	3192.0084	3193.9341
3199.4849	3199.5398	3200.1993
3200.8373	3200.9617	3201.4802
3203.8214	3217.1050	3218.3823
3221.3761	3222.0522	3229.5853

TS3

E(RB3LYP) = -3723.60182263

E(RB3LYP-D3) = -3723.79144483

H - Sum of electronic and thermal Enthalpies= -3722.439511

G - Sum of electronic and thermal Free Energies= -3722.596232

Number of imaginary frequencies: 0

Cartesian Coordinates

C	-5.42021	0.09118	1.93824
C	-5.71024	-0.91072	0.99343
C	-5.87307	-0.58040	-0.36868
C	-5.78216	0.76401	-0.77232
C	-5.53374	1.78113	0.17231
C	-5.33896	1.43686	1.52238
C	-5.22721	-0.28305	3.41062
C	-4.84397	0.90443	4.32773
C	-5.69173	2.12552	3.90998
C	-5.00015	2.49680	2.57589
C	-5.51936	3.25348	-0.25188
C	-5.66753	3.48341	-1.77689
C	-5.92032	1.17083	-2.24301
C	-6.18140	-1.66397	-1.40499
C	-6.20804	-3.09952	-0.83076
C	-5.83208	-2.38532	1.40091
C	-6.92620	-3.05657	0.53604
C	-6.71909	2.49473	-2.32282
C	-2.58968	-4.49022	-0.51713
C	-3.84224	-4.19767	-1.13129
C	-4.81616	-3.54269	-0.41936
C	-4.59248	-3.14089	0.92929
C	-3.40805	-3.42668	1.56286
C	-2.37494	-4.11271	0.85925
C	-2.31149	1.57506	-3.68290
C	-2.19051	2.99238	-3.43710
C	-3.27607	3.68975	-2.83365
C	-4.41905	3.01029	-2.49401
C	-4.55417	1.61813	-2.76370
C	-3.52804	0.91156	-3.34393
C	-1.12314	2.64750	3.02433
C	-1.04091	1.69549	4.10625
C	-2.23431	1.07578	4.57957
C	-3.44429	1.40342	4.01876
C	-3.52893	2.35988	2.96569
C	-2.39852	2.96257	2.46886
C	0.06734	3.26600	2.53869
C	1.26463	2.94371	3.12507
C	1.34067	2.02613	4.20009
C	0.22444	1.40165	4.69363
C	-1.54445	-5.12899	-1.24536
C	-0.35102	-5.36198	-0.61303
C	-0.14856	-5.01750	0.74403
C	-1.12905	-4.41108	1.48556
C	-0.97812	3.66567	-3.76275
C	0.06518	2.93225	-4.26295
C	-0.03993	1.53836	-4.48117
C	-1.20234	0.85759	-4.22307
C	1.29027	1.04214	-4.94212
O	1.62258	-0.08530	-5.25152
N	2.12928	2.17580	-4.96405
C	1.45378	3.34910	-4.59518
O	1.95162	4.46113	-4.56233
C	0.92285	-5.92414	-1.14003
O	1.17839	-6.33598	-2.25833

C	1.24769	-5.38961	1.11441
O	1.79626	-5.31695	2.19639
C	2.64218	3.43644	2.83875
O	3.01157	4.25299	2.01610
C	2.76327	1.93551	4.62905
O	3.25454	1.30621	5.54973
N	3.48064	2.77018	3.75593
N	1.82903	-5.88952	-0.06900
C	3.58234	2.11518	-5.10677
C	3.25490	-6.16312	-0.22989
C	4.92134	2.98942	3.85427
C	7.17872	-0.39495	2.61206
C	7.16506	-0.08315	3.97056
C	6.42697	1.01819	4.40055
C	5.74078	1.77521	3.44503
N	5.76618	1.48630	2.13578
C	6.46032	0.41189	1.71759
C	5.12490	-2.74727	-1.95848
C	5.07835	-3.91677	-2.71694
C	4.49124	-5.06207	-2.17536
C	3.96696	-4.98609	-0.88135
N	4.01841	-3.86726	-0.14735
C	4.58482	-2.76940	-0.66790
C	5.21631	2.88057	-1.25574
C	5.52109	3.77738	-2.27808
C	5.03867	3.52968	-3.56369
C	4.26023	2.38773	-3.77095
N	3.99658	1.50456	-2.79815
C	4.46629	1.73479	-1.56206
C	4.10507	0.70962	-0.50374
C	4.60730	-1.56825	0.27022
C	6.42340	0.09147	0.22693
N	5.13038	-0.33544	-0.31800
H	-6.16132	-0.71739	3.79658
H	-4.46557	-1.06733	3.50296
H	-4.97012	0.61228	5.37587
H	-5.59257	2.94105	4.63607
H	-6.75499	1.89161	3.78540
H	-6.34644	3.77419	0.25378
H	-6.01559	-2.49017	2.47122
H	-7.16343	-1.46032	-1.85686
H	-5.45321	-1.62096	-2.22475
H	-7.86157	-2.48604	0.51506
H	-7.13798	-4.06810	0.90208
H	-4.59801	3.74109	0.08957
H	-5.90282	4.53600	-1.96822
H	-7.64039	2.46935	-1.73010
H	-6.97520	2.72977	-3.36274
H	-4.00509	-4.50460	-2.16302
H	-3.23129	-3.13554	2.59619
H	-6.67282	-3.77601	-1.55624
H	-3.17343	4.75634	-2.64124
H	-3.61245	-0.15556	-3.53889
H	-6.36303	0.37441	-2.84188
H	-2.16510	0.35886	5.39580
H	-2.45068	3.68829	1.65995
H	-5.25667	3.49992	2.23330
H	0.29512	0.69660	5.51803
H	0.01889	3.97914	1.71967
H	-0.95808	-4.13845	2.52390
H	-1.68925	-5.40131	-2.28778
H	-1.27331	-0.21389	-4.39228
H	-0.87828	4.73346	-3.58488
H	3.89707	2.84488	-5.85832
H	3.81304	1.10732	-5.46136
H	3.36425	-7.06897	-0.83169
H	3.65458	-6.33767	0.77218
H	5.14410	3.82960	3.19174
H	5.15665	3.27149	4.88540
H	7.73572	-1.25254	2.24399
H	7.70878	-0.69625	4.68479
H	6.36167	1.27601	5.45283
H	5.54692	-1.82517	-2.34320
H	5.47992	-3.93232	-3.72720
H	4.41087	-5.98019	-2.74956
H	5.52512	3.06482	-0.23106
H	6.09871	4.67457	-2.07014
H	5.21449	4.23029	-4.37449
H	7.14781	-0.70751	0.02416
H	6.75705	0.96803	-0.33705
H	5.19008	-1.85932	1.15463
H	3.58707	-1.42138	0.64876
H	3.20288	0.20325	-0.85502
H	3.87188	1.22484	0.44047

Frequencies

-33.0071	14.4958	17.5296
19.0280	22.7882	25.6235
29.9090	33.6665	39.9808
45.4254	46.9745	53.3866
55.8555	60.3882	63.7724
74.0349	89.4811	96.5728
98.8525	110.0754	116.8206
119.0835	121.8497	130.1622
138.1289	138.8564	145.9703
150.5579	152.8728	158.3324
159.9097	164.4088	172.9827
174.8246	175.9316	185.0738
196.1643	201.3425	204.0642
211.0379	227.1133	228.4943
236.3422	240.1079	244.3895
248.3586	252.3889	255.7492
258.4680	259.7831	263.9642
269.6687	292.5404	296.7492
299.9169	306.2891	308.4520
311.0197	316.0122	319.5877
332.9026	337.7192	347.2932
348.5061	366.3271	371.6063

373.1799	384.8718	388.7492	1143.6065	1155.7476	1162.2020
393.3589	395.2874	401.4864	1165.9305	1166.4618	1175.8969
402.9189	403.9364	411.4843	1176.0407	1176.3533	1177.2474
419.2665	419.9463	427.7606	1178.8348	1179.1607	1182.0875
428.3407	435.6281	438.0978	1189.3546	1189.9250	1190.5043
443.6464	462.1996	468.1520	1190.9935	1191.2886	1227.8384
473.1251	483.5126	484.2327	1229.8974	1230.8114	1232.3798
484.7561	492.6300	497.7621	1236.7601	1239.7611	1244.3139
500.4411	502.5333	527.5958	1247.6883	1249.4363	1249.6167
532.4885	535.4698	547.2801	1254.0782	1254.3075	1254.4932
549.4156	558.5167	566.3706	1259.5007	1263.9666	1271.9409
569.8989	573.1644	573.6429	1272.5587	1277.2844	1277.7010
577.4254	580.4181	583.0409	1278.0279	1281.9971	1290.8489
591.6350	592.4050	601.7847	1291.3735	1297.4607	1299.4597
604.4912	605.3503	609.8467	1300.0099	1301.5204	1305.9237
620.0715	624.0217	628.9185	1313.2734	1313.9739	1318.3945
646.5790	653.0103	654.3830	1318.8993	1322.0399	1326.3002
654.5601	659.6739	660.4912	1329.3310	1339.5530	1339.9200
662.3354	674.4446	700.7636	1341.1866	1344.7888	1345.6129
714.1366	715.9116	720.1111	1349.4471	1350.8601	1357.2783
722.8210	723.6266	727.0217	1365.7065	1370.2191	1373.4999
732.3998	736.9563	740.9726	1376.4268	1376.7423	1378.0894
741.8040	742.0166	743.1923	1379.0044	1390.0871	1396.4549
745.9715	753.1520	762.2706	1400.4352	1408.0513	1409.2185
764.2372	764.8395	768.8876	1411.7512	1413.1490	1414.0590
768.9384	770.7242	773.6375	1417.9838	1423.3528	1451.9662
777.7535	778.0661	781.4635	1451.9766	1470.7896	1471.1311
783.3695	785.1632	790.9753	1471.4203	1473.4302	1473.8311
802.2753	804.1051	811.7266	1474.7603	1475.2445	1475.5403
815.9403	818.3537	823.6590	1475.9765	1483.4579	1484.3470
826.5921	829.9563	837.3094	1484.4250	1486.3815	1489.7107
838.9370	840.7915	843.9369	1490.4737	1493.9544	1495.3393
868.3230	868.7639	869.3559	1497.7249	1498.6647	1501.6371
876.6397	888.0443	888.3735	1502.4991	1502.8669	1508.7977
894.7550	896.4754	896.9634	1510.6781	1521.0035	1521.1103
899.9694	910.9945	912.9400	1521.9358	1533.8152	1535.1475
916.6137	919.6661	920.5301	1535.4176	1606.0764	1607.1783
927.7743	934.7697	935.4652	1626.3574	1626.5886	1628.0885
936.1972	936.7294	938.7053	1636.4668	1638.3304	1639.0772
940.9548	941.0801	941.9541	1647.6845	1648.6519	1649.7484
945.0974	951.5246	954.8915	1673.0048	1676.3965	1676.8474
959.4759	961.1615	966.3070	1677.1606	1679.0745	1679.4864
966.9317	969.7686	974.7590	1769.9056	1772.5422	1773.4942
980.1595	986.1265	995.9744	1819.0190	1821.9277	1823.1753
1005.6937	1006.7053	1008.1427	3012.7348	3014.9555	3016.9024
1009.5023	1010.2765	1011.2409	3017.2633	3029.6624	3048.8125
1013.6556	1014.4126	1015.0752	3056.9124	3057.2798	3057.3782
1015.5400	1015.7120	1018.7522	3061.0944	3063.3686	3064.0060
1039.7997	1043.2585	1044.0497	3064.2507	3079.0247	3079.8385
1066.5873	1075.1834	1077.9917	3080.0142	3080.7924	3088.2437
1078.6861	1095.3240	1103.5072	3094.3860	3103.2006	3103.5253
1104.7259	1107.8186	1108.2487	3103.8182	3103.9292	3117.5983
1115.9318	1120.2440	1123.3074	3127.9352	3132.6058	3134.5415
1135.2152	1139.5711	1139.7371	3138.9404	3141.1580	3146.9118

3172.7596	3172.8875	3174.1511
3179.7150	3179.9717	3180.3392
3187.1228	3188.7266	3188.9338
3199.2983	3199.4650	3200.0855
3200.7011	3200.8505	3201.3008
3201.9729	3208.8535	3211.1566
3214.7565	3218.2058	3228.0102

I3

E(RB3LYP) = -3723.60588586

E(RB3LYP-D3) = -3723.79564383

H - Sum of electronic and thermal Enthalpies= -3722.442595

G - Sum of electronic and thermal Free Energies= -3722.602985

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.87153	1.08391	0.18278
C	5.79060	0.60135	-1.13656
C	5.70012	-0.78468	-1.38586
C	5.66205	-1.68332	-0.30473
C	5.71330	-1.21009	1.02264
C	5.82567	0.17169	1.25815
C	6.05382	2.58388	0.44034
C	6.05953	2.98413	1.93833
C	6.85281	1.92230	2.72812
C	5.85484	0.73999	2.67957
C	5.68277	-2.18686	2.20254
C	5.47684	-3.66821	1.80071
C	5.50600	-3.19136	-0.52341
C	5.68393	-1.32179	-2.81998
C	5.61672	-0.22550	-3.90953
C	5.74861	1.55038	-2.34037
C	6.55891	0.92758	-3.50284
C	6.32946	-3.94947	0.54512
C	1.93043	0.94605	-4.27294
C	3.10018	0.17401	-4.52712
C	4.26771	0.46430	-3.86634
C	4.33544	1.53374	-2.92749
C	3.22861	2.30387	-2.65988
C	1.99486	2.03136	-3.32348
C	1.70228	-4.02318	-0.24447
C	1.70078	-4.34757	1.16198
C	2.91906	-4.25816	1.89646
C	4.07588	-3.88201	1.25913
C	4.08343	-3.59131	-0.13558
C	2.92627	-3.65057	-0.87332
C	2.20930	1.86967	3.50306
C	2.37146	3.25328	3.12440
C	3.63021	3.69566	2.62621
C	4.67196	2.80809	2.52127
C	4.53063	1.45558	2.94501
C	3.32848	0.98997	3.42127
C	0.92625	1.39745	3.91162
C	-0.12362	2.27941	3.93100
C	0.05032	3.64487	3.60508
C	1.26402	4.14501	3.21337
C	0.70083	0.65270	-4.93081
C	-0.40168	1.40837	-4.63052
C	-0.34252	2.47521	-3.70253
C	0.82302	2.80142	-3.05696
C	0.48759	-4.75182	1.79252
C	-0.65917	-4.79826	1.04339
C	-0.66344	-4.45309	-0.32896
C	0.48267	-4.07957	-0.98138
C	-2.05597	-4.59938	-0.83775
O	-2.48770	-4.41130	-1.96016
N	-2.81523	-5.04107	0.26034
C	-2.04383	-5.19677	1.42263
O	-2.46486	-5.60388	2.49026
C	-1.79860	1.31046	-5.13518
O	-2.27288	0.53967	-5.95055
C	-1.70335	3.08079	-3.60975
O	-2.07472	4.03907	-2.95846
C	-1.57109	2.05397	4.20965
O	-2.13970	1.02909	4.53231
C	-1.27119	4.31712	3.70862
O	-1.54328	5.49690	3.55877
N	-2.19352	3.30727	4.02234
N	-2.51145	2.32699	-4.48165
C	-4.24043	-5.30736	0.19690
C	-3.94695	2.50449	-4.62332
C	-3.64286	3.51909	4.07513
C	-5.34931	3.47016	0.17602
C	-4.65073	4.61142	0.56743
C	-4.10907	4.66170	1.84908
C	-4.27200	3.54880	2.68768
N	-4.96261	2.46044	2.32064
C	-5.49828	2.41765	1.08621
C	-6.17978	-0.37635	-2.41910
C	-6.58937	-0.08676	-3.71759
C	-5.86377	0.84076	-4.46997
C	-4.75286	1.44699	-3.88003
N	-4.35573	1.16950	-2.63032
C	-5.04616	0.27395	-1.90923
C	-6.62652	-2.62171	2.47112
C	-6.98642	-3.96694	2.44975
C	-6.20127	-4.86002	1.72278
C	-5.08564	-4.36426	1.04060
N	-4.73344	-3.07264	1.06424
C	-5.48801	-2.20823	1.76471
C	-5.08383	-0.74516	1.74833
C	-4.51210	-0.02624	-0.52049
C	-6.29331	1.17087	0.71327
N	-5.54801	-0.07805	0.51456
H	7.00918	2.90402	-0.00170
H	5.27267	3.15736	-0.07383

H	6.44778	4.00283	2.04465
H	7.01926	2.24642	3.76232
H	7.82018	1.67726	2.27563
H	6.63274	-2.11349	2.75270
H	6.08946	2.55224	-2.07673
H	6.59492	-1.91629	-2.98657
H	4.84114	-2.00936	-2.96019
H	7.55219	0.58548	-3.19105
H	6.67500	1.64729	-4.32185
H	4.89675	-1.89950	2.91192
H	5.71106	-4.31512	2.65308
H	7.35777	-3.58004	0.62860
H	6.35739	-5.02226	0.32047
H	3.04575	-0.64026	-5.24770
H	3.26512	3.11997	-1.94108
H	5.84511	-0.66375	-4.88714
H	2.91070	-4.49749	2.95845
H	2.91664	-3.41632	-1.93571
H	5.76914	-3.48095	-1.54134
H	3.73928	4.73493	2.32113
H	3.19976	-0.04771	3.72178
H	6.07783	-0.03101	3.41780
H	1.37929	5.19210	2.94506
H	0.78441	0.35099	4.16937
H	0.85742	3.62124	-2.34390
H	0.64261	-0.16417	-5.64574
H	0.46825	-3.82587	-2.03829
H	0.47908	-5.01376	2.84757
H	-4.42420	-6.34171	0.50641
H	-4.51410	-5.21117	-0.85949
H	-4.19780	2.49136	-5.68797
H	-4.17273	3.49749	-4.22099
H	-4.06707	2.69127	4.64545
H	-3.81736	4.46159	4.60305
H	-5.76893	3.39024	-0.82231
H	-4.52258	5.44401	-0.11923
H	-3.55341	5.52685	2.19466
H	-6.71194	-1.08963	-1.79724
H	-7.45551	-0.58442	-4.14693
H	-6.14474	1.07652	-5.49274
H	-7.20952	-1.89747	3.03323
H	-7.85518	-4.31759	3.00147
H	-6.43414	-5.92113	1.69991
H	-6.84581	1.37990	-0.21039
H	-7.03863	0.98480	1.49440
H	-3.72295	0.71161	-0.29894
H	-4.03686	-1.01409	-0.54086
H	-3.99415	-0.66358	1.86328
H	-5.52151	-0.23772	2.61017

Frequencies

10.4665	17.0532	18.1561
18.3800	21.9782	24.5460
34.2803	34.8723	35.5887
45.5537	49.3529	50.9123
55.0344	57.9098	70.8534
75.9169	77.5390	91.8071
99.6310	110.0606	113.6805
121.7600	123.3622	127.1797
138.2681	139.0944	147.5770
150.4760	159.2998	160.3799
164.1302	168.7918	172.0226
174.0387	179.1718	189.5444
192.5770	201.2621	212.5257
221.4472	228.4016	232.6920
237.5202	241.4629	242.8381
245.6888	249.8190	253.4476
259.0955	260.2005	262.9134
270.6180	285.6158	294.4103
295.7060	299.4501	301.7795
306.5764	309.6043	317.0874
320.1616	331.5548	347.7494
348.5251	363.1602	372.2481
372.9323	384.1287	385.6690
390.8248	398.2059	400.1337
401.2231	404.6287	405.0884
419.8612	426.9756	428.4666
430.5367	437.6063	440.7246
444.8634	464.0967	469.2008
472.4761	477.3754	483.9251
484.2769	485.1080	499.7738
501.3376	503.2904	527.1892
529.3123	545.0948	547.7598
549.6446	558.9350	567.2173
571.6449	573.6482	575.4666
576.1161	578.1353	581.9347
591.6147	594.0108	601.5022
605.9905	606.7588	609.5997
622.2707	625.3699	626.2744
652.3611	653.0506	654.6663
658.3922	660.6498	661.2127
663.3101	669.3516	700.4933
716.5696	718.2217	721.4851
723.6171	726.2058	726.9127
733.0863	738.2193	739.6052
742.4192	743.2248	743.7490
751.4470	759.5977	760.6213
762.0869	764.8549	765.1188
769.0857	774.2277	777.3394
777.8227	778.5811	781.2255
783.9220	784.1745	785.0007
799.9843	801.4985	802.1204
813.0071	816.8672	822.5125
826.0107	828.6798	836.0615
839.1959	841.8167	853.2779
864.9756	868.6288	869.5905
876.8485	888.0405	888.3949
895.3290	896.5912	897.0587

899.8048	911.1284	912.5111
916.7812	916.8429	920.3630
921.6226	929.5929	933.6741
935.6951	936.2425	936.3488
940.8741	941.2940	941.4952
945.1476	952.9328	955.7705
957.7330	961.7320	965.4254
966.6860	967.3242	968.6919
982.3131	986.3981	1000.9780
1002.3067	1007.0919	1008.6227
1010.5075	1011.6520	1012.8628
1014.3405	1015.3161	1016.1302
1018.0128	1019.8886	1023.0590
1039.7971	1043.1311	1044.3389
1066.6434	1075.1190	1077.8055
1078.7407	1097.0410	1106.3444
1108.1017	1108.1779	1114.7654
1118.1081	1119.9571	1124.2200
1132.4037	1141.2365	1146.3128
1149.7605	1150.2101	1157.0286
1166.2188	1166.6880	1176.1710
1176.5440	1177.4950	1178.1405
1178.4552	1179.1566	1186.2912
1189.4464	1190.1451	1190.7269
1191.9544	1194.0349	1226.8103
1229.7781	1230.3695	1233.0668
1236.2698	1237.1980	1244.2118
1247.8481	1248.6027	1249.7109
1254.1269	1254.2609	1254.5445
1259.6703	1265.1051	1272.4531
1277.1017	1277.7353	1278.0600
1278.2150	1280.1264	1290.4284
1291.1548	1294.2025	1299.3891
1300.1788	1301.6486	1302.9131
1312.8275	1314.3829	1317.9966
1319.4319	1320.4645	1322.7106
1327.3522	1339.6444	1340.0956
1341.4673	1344.9274	1345.4287
1348.1723	1356.1585	1359.6395
1365.6630	1366.3971	1368.0423
1376.1309	1376.7830	1390.3354
1397.2303	1398.1889	1400.6121
1405.1159	1408.8105	1411.1539
1412.3771	1412.8985	1413.5032
1420.1154	1421.7623	1451.8727
1452.4919	1469.6707	1471.5775
1472.5168	1473.7024	1474.7505
1475.4990	1475.6779	1478.2474
1479.1292	1483.5475	1484.2372
1484.5149	1487.4871	1488.3424
1490.3334	1492.1643	1494.4124
1494.7195	1496.5507	1501.9782
1502.9783	1503.1167	1513.7200
1517.8685	1520.9200	1520.9721
1521.8143	1534.1955	1534.7263
1535.8130	1606.7172	1607.3856
1627.4053	1629.4146	1630.6239
1635.1769	1639.1619	1640.0098
1647.9380	1649.3283	1649.5146
1675.6432	1675.7623	1676.4578
1678.4199	1678.8737	1679.0825
1768.2658	1771.8342	1773.9331
1819.3176	1820.8948	1822.5948
2990.1297	3014.4459	3016.2271
3016.3674	3036.5899	3053.9562
3056.7895	3057.1074	3057.1994
3063.5609	3063.8898	3066.8050
3067.8907	3078.0619	3078.9298
3079.4927	3079.8678	3080.6181
3088.8225	3094.3019	3102.9571
3103.2077	3103.8556	3111.6742
3125.1075	3132.6863	3132.7561
3133.8209	3135.0504	3160.5952
3172.5329	3172.9263	3173.5296
3179.0127	3180.4810	3180.9089
3183.3968	3185.2983	3194.6640
3197.5516	3199.3062	3199.4715
3200.0906	3200.5499	3201.2522
3201.5777	3202.3298	3207.0685
3211.8659	3216.7891	3228.0946

TS4

E(RB3LYP) = -3723.60471113

E(RB3LYP-D3) = -3723.79346609

H - Sum of electronic and thermal Enthalpies= -3722.442600

G - Sum of electronic and thermal Free Energies= -3722.600337

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.62516	0.48197	2.07466
C	5.57691	1.59013	1.20872
C	5.69998	1.41382	-0.18627
C	5.85392	0.11815	-0.71204
C	5.89256	-1.00072	0.14533
C	5.78297	-0.81113	1.53393
C	5.54369	0.68678	3.59175
C	5.51806	-0.62561	4.41821
C	6.52388	-1.61435	3.79331
C	5.76627	-1.99822	2.50006
C	6.08505	-2.41204	-0.41698
C	6.09996	-2.48384	-1.96210
C	5.93439	-0.13068	-2.22235
C	5.70957	2.62064	-1.12898
C	5.44954	3.97727	-0.43146
C	5.35415	3.01278	1.73507
C	6.21864	3.99457	0.90702

C	6.92278	-1.29034	-2.49333
C	1.62855	4.45611	0.08720
C	2.89031	4.53202	-0.56971
C	4.01492	4.05034	0.05259
C	3.94590	3.47275	1.35320
C	2.74592	3.37995	2.01714
C	1.55374	3.86850	1.40344
C	2.35317	-1.01814	-3.50407
C	2.46325	-2.44765	-3.33805
C	3.67751	-2.99701	-2.83311
C	4.72593	-2.16718	-2.52134
C	4.61944	-0.75606	-2.68680
C	3.46159	-0.18872	-3.16100
C	1.99568	-2.75247	3.15958
C	1.88067	-1.98938	4.37963
C	3.01835	-1.28738	4.87170
C	4.20796	-1.35363	4.18963
C	4.34016	-2.16005	3.02299
C	3.26200	-2.84133	2.51166
C	0.83482	-3.36215	2.59710
C	-0.36607	-3.20565	3.23983
C	-0.46322	-2.50906	4.46699
C	0.62416	-1.90995	5.04635
C	0.44548	4.94748	-0.53713
C	-0.74518	4.83683	0.13157
C	-0.82326	4.25915	1.42122
C	0.29147	3.78400	2.06399
C	1.36977	-3.28780	-3.69928
C	0.23302	-2.70884	-4.19970
C	0.12253	-1.30730	-4.36106
C	1.14798	-0.46130	-4.02565
C	-1.20498	-1.01799	-4.97413
O	-1.68357	0.05065	-5.30804
N	-1.82056	-2.26756	-5.15103
C	-1.01967	-3.33362	-4.70863
O	-1.31602	-4.51165	-4.78744
C	-2.11689	5.24672	-0.27588
O	-2.48905	5.78888	-1.30129
C	-2.24980	4.29525	1.85628
O	-2.74345	3.92532	2.90530
C	-1.74001	-3.62162	2.83706
O	-2.09675	-4.24452	1.85641
C	-1.88745	-2.51689	4.89105
O	-2.37959	-2.08701	5.92143
N	-2.59605	-3.13595	3.85024
N	-2.95276	4.89471	0.79468
C	-3.10468	-2.44617	-5.79034
C	-4.39649	5.04375	0.75575
C	-4.05776	-3.22946	3.79806
C	-5.86026	0.42864	2.57569
C	-5.33934	0.35747	3.86650
C	-4.76829	-0.83762	4.29386
C	-4.71465	-1.91433	3.39532
N	-5.22842	-1.85198	2.15829
C	-5.80140	-0.70282	1.75425
C	-6.29297	2.12085	-1.69474
C	-6.78148	3.42444	-1.73231
C	-6.16428	4.40526	-0.95285
C	-5.07823	4.03257	-0.15708
N	-4.60653	2.77956	-0.11846
C	-5.19284	1.83813	-0.87302
C	-6.50878	-2.17084	-3.25245
C	-6.70446	-2.33987	-4.61981
C	-5.58783	-2.42577	-5.44940
C	-4.31716	-2.34424	-4.87071
N	-4.12441	-2.19000	-3.55459
C	-5.20037	-2.10301	-2.75365
C	-4.97519	-1.91762	-1.25936
C	-4.56871	0.45404	-0.82027
C	-6.42881	-0.67762	0.36464
N	-5.53984	-0.63859	-0.80024
H	6.41349	1.27650	3.91785
H	4.65844	1.28191	3.84780
H	5.70966	-0.39883	5.47255
H	6.66209	-2.49234	4.43544
H	7.50386	-1.16730	3.59223
H	7.03867	-2.81750	-0.04702
H	5.54773	3.07998	2.80635
H	6.68958	2.67434	-1.62640
H	4.96933	2.48615	-1.92721
H	7.25978	3.66599	0.81284
H	6.20381	4.99505	1.35538
H	5.30233	-3.08141	-0.03945
H	6.47696	-3.46174	-2.28070
H	7.88039	-1.16108	-1.97641
H	7.11318	-1.39085	-3.56839
H	2.94051	4.98034	-1.56048
H	2.67829	2.93738	3.00886
H	5.71610	4.79579	-1.10889
H	3.75705	-4.07660	-2.71742
H	3.36733	0.88752	-3.28988
H	6.19092	0.77823	-2.76776
H	2.91703	-0.69056	5.77646
H	3.34248	-3.43250	1.60199
H	6.15756	-2.90377	2.03553
H	0.53000	-1.35578	5.97679
H	0.90243	-3.90712	1.65901
H	0.22077	3.34210	3.05467
H	0.49281	5.39289	-1.52765
H	1.05475	0.61321	-4.16155
H	1.44662	-4.36637	-3.58723
H	-3.09070	-3.43550	-6.26039
H	-3.18755	-1.69188	-6.58023
H	-4.63710	6.06165	0.43466
H	-4.74406	4.91107	1.78585
H	-4.30116	-3.99427	3.05888
H	-4.40417	-3.54726	4.78666
H	-6.30725	1.34679	2.20619

H	-5.37524	1.21995	4.52681
H	-4.35367	-0.94107	5.29048
H	-6.73787	1.32586	-2.28526
H	-7.62466	3.67963	-2.36961
H	-6.50841	5.43580	-0.97180
H	-7.35087	-2.08552	-2.57189
H	-7.70768	-2.40323	-5.03437
H	-5.69629	-2.55225	-6.52409
H	-7.08717	0.19875	0.31119
H	-7.06559	-1.56236	0.25888
H	-3.87736	0.43102	0.03809
H	-3.95690	0.32468	-1.72259
H	-3.90187	-2.00414	-1.04513
H	-5.46536	-2.73125	-0.71601

Frequencies

-15.9907	9.1804	17.5274
18.3951	19.6379	23.5962
28.3998	34.0024	35.2060
44.2531	48.8710	51.7908
56.2565	58.9054	71.3064
74.9208	79.2280	95.4436
101.5339	111.8177	114.1092
121.8663	122.0206	126.6187
138.3568	138.6933	148.2170
149.6203	159.5743	160.2812
162.9751	166.3910	170.4469
174.9076	179.2486	184.5047
190.8498	200.2030	211.4126
218.7889	225.3756	234.5899
235.1592	239.5545	241.4942
245.0205	248.5984	251.3088
257.0169	261.5027	267.5066
270.8598	279.2975	290.8703
295.2567	297.9995	300.8593
306.2877	309.1209	317.2723
321.8882	331.3346	346.3809
347.8351	349.2616	370.4441
373.3859	374.7807	385.7489
389.9226	398.3893	399.1355
401.2231	403.0176	404.4011
419.5477	427.4384	429.3150
430.2732	436.1676	439.5992
445.0278	468.5847	470.9954
474.1628	477.8063	482.8402
484.2363	485.0625	499.7906
502.0234	503.8496	527.2245
529.2902	542.7839	548.6635
549.4394	556.5069	567.4966
571.7289	572.7303	575.0529
575.8572	577.5942	582.1958
591.9718	595.3776	605.5280
606.2986	607.3838	609.9290
622.9224	625.2603	638.5791
649.7832	652.7250	653.6410
654.9948	658.9474	660.5091
661.5622	663.8286	700.1295
716.4455	718.0071	720.7090
721.6007	725.8923	726.4442
731.3467	733.9844	739.7472
742.2114	743.1102	743.1878
750.7853	753.9672	759.4773
762.1262	764.3647	764.5107
768.2146	769.2584	776.7452
778.1329	779.0221	781.0904
781.5200	785.1410	786.2083
797.6434	798.7605	801.4190
810.0653	815.9207	822.3454
826.6158	827.3846	835.5949
839.5895	841.7493	852.1277
866.5310	868.7263	869.2946
876.4084	887.9149	888.1392
895.0497	896.0728	896.6069
899.9847	908.3484	912.2836
916.6125	917.0995	920.6921
921.6714	926.8506	934.8969
935.6289	936.0610	936.3615
940.6862	941.2452	941.4352
945.4250	953.8061	956.9253
958.3354	962.2368	965.0417
966.5581	967.1998	968.9869
979.0215	986.6440	997.8095
1001.2162	1007.0002	1008.6237
1009.7501	1010.7485	1012.2958
1012.9486	1015.1617	1016.5082
1018.2125	1020.9591	1031.0302
1039.9682	1043.5241	1044.5102
1066.7551	1075.1810	1077.7358
1078.7181	1097.2802	1107.4438
1108.4105	1108.5265	1117.8209
1118.0640	1119.9887	1125.5505
1134.4927	1144.1007	1147.7807
1154.2048	1157.0061	1157.4932
1166.3104	1167.0387	1176.2782
1176.7961	1177.6453	1178.3562
1178.5781	1179.4016	1186.0513
1189.4022	1190.2575	1190.7290
1192.1470	1194.6232	1226.4839
1227.6969	1229.9944	1231.4620
1233.4528	1237.4821	1244.4054
1247.8213	1248.9172	1249.5310
1254.1289	1254.2796	1254.3687
1259.8619	1264.6474	1272.9013
1273.9858	1276.9692	1277.5353
1277.6075	1278.2605	1290.6697
1291.0548	1293.7376	1299.4139
1300.7960	1301.8481	1302.9410
1313.4573	1315.7657	1318.3748

1319.1790	1321.5283	1322.5969
1327.4098	1339.8042	1340.2901
1341.5120	1345.3923	1345.4923
1348.2978	1358.2089	1365.8451
1367.6054	1369.0752	1372.0630
1376.3006	1377.2765	1386.2857
1392.8179	1400.8921	1403.9107
1406.2725	1407.4070	1410.9255
1412.5199	1412.6935	1413.5601
1417.7678	1422.0067	1452.0708
1452.8222	1468.0777	1469.9553
1472.7702	1473.9577	1474.5271
1475.5411	1476.1564	1476.9686
1478.8386	1481.9022	1483.6155
1484.2704	1484.6002	1487.8838
1488.1608	1490.4220	1493.1809
1494.2779	1494.5108	1501.8406
1502.8556	1503.1806	1513.7276
1515.5328	1520.9569	1521.0614
1521.8737	1534.2362	1534.5892
1535.8250	1606.7230	1607.8477
1628.5441	1630.1207	1631.3950
1635.4297	1638.3241	1639.2478
1648.0588	1649.1367	1649.7865
1675.5680	1675.7542	1676.5312
1678.3846	1678.8969	1678.9805
1768.6254	1772.2344	1774.1850
1820.1952	1821.1072	1823.3258
2995.1064	3015.4756	3015.6083
3016.0717	3043.1263	3046.9367
3056.8798	3057.0659	3057.1414
3062.6111	3064.0272	3064.1614
3065.3210	3068.3943	3075.5738
3079.5047	3079.6763	3080.6865
3084.3730	3092.6748	3103.0547
3103.2263	3103.6180	3109.0570
3112.1545	3121.5598	3131.6126
3132.0106	3134.5836	3159.9648
3172.5681	3173.0536	3173.4930
3178.7619	3179.4584	3179.7768
3181.4028	3184.9564	3193.5783
3194.0732	3199.4803	3199.5350
3200.0319	3200.7079	3200.7627
3201.5810	3201.7722	3208.4452
3210.9131	3215.9484	3231.8043

I4

E(RB3LYP) = -3723.60528569

E(RB3LYP-D3) = -3723.79355999

H - Sum of electronic and thermal Enthalpies= -3722.442287

G - Sum of electronic and thermal Free Energies= -3722.602868

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.65786	0.55379	2.01154
C	5.60601	1.63089	1.10778
C	5.71737	1.40633	-0.28124
C	5.90463	0.09665	-0.76063
C	5.96815	-0.98903	0.13731
C	5.83458	-0.75472	1.51698
C	5.54754	0.80802	3.51908
C	5.48789	-0.47750	4.38444
C	6.51221	-1.48571	3.82406
C	5.79716	-1.91034	2.52000
C	6.21102	-2.41299	-0.36993
C	6.24532	-2.53905	-1.91030
C	6.00426	-0.20388	-2.26147
C	5.66629	2.57609	-1.26797
C	5.38706	3.95027	-0.61307
C	5.38368	3.06894	1.59011
C	6.20055	4.03339	0.69676
C	7.03338	-1.33935	-2.47936
C	1.57975	4.40484	0.04006
C	2.81175	4.45971	-0.67468
C	3.96742	4.01527	-0.08124
C	3.95733	3.49439	1.24505
C	2.78849	3.41986	1.96308
C	1.56768	3.87376	1.38203
C	2.46932	-1.26186	-3.54477
C	2.61547	-2.67550	-3.29276
C	3.84353	-3.16334	-2.75995
C	4.86601	-2.28873	-2.48850
C	4.71684	-0.89037	-2.71697
C	3.54957	-0.38325	-3.23483
C	2.00598	-2.64492	3.07819
C	1.85016	-1.84099	4.26709
C	2.97086	-1.12028	4.77182
C	4.18371	-1.21033	4.13435
C	4.35424	-2.05595	3.00080
C	3.29298	-2.75300	2.47551
C	0.86674	-3.28482	2.50514
C	-0.35219	-3.12292	3.11158
C	-0.49011	-2.38533	4.31051
C	0.57440	-1.75110	4.89538
C	0.36678	4.87064	-0.54626
C	-0.79009	4.79149	0.18444
C	-0.80459	4.26616	1.49846
C	0.33942	3.81538	2.10499
C	1.54011	-3.56222	-3.58983
C	0.38806	-3.04316	-4.11921
C	0.24883	-1.66043	-4.38492
C	1.25457	-0.77029	-4.10861
C	-1.08930	-1.44557	-5.00690

O	-1.58609	-0.41781	-5.43104
N	-1.69416	-2.71128	-5.05387
C	-0.86331	-3.72657	-4.54749
O	-1.14017	-4.91135	-4.51630
C	-2.17911	5.19948	-0.16450
O	-2.60158	5.70846	-1.18738
C	-2.20475	4.33012	2.00626
O	-2.64454	4.00254	3.09265
C	-1.70560	-3.59759	2.70469
O	-2.02557	-4.27522	1.74812
C	-1.91964	-2.42791	4.71628
O	-2.43753	-1.99545	5.73261
N	-2.59337	-3.10019	3.68520
N	-2.95869	4.89702	0.96252
C	-3.00099	-2.96589	-5.63040
C	-4.39788	5.07637	1.00831
C	-4.04195	-3.32006	3.65630
C	-6.27110	0.17471	2.68835
C	-5.79366	0.04510	3.99130
C	-5.07355	-1.09656	4.33015
C	-4.83751	-2.06004	3.33804
N	-5.30525	-1.94155	2.08621
C	-6.01825	-0.84667	1.76507
C	-6.51368	2.21203	-1.32556
C	-6.99497	3.51915	-1.29357
C	-6.30661	4.47832	-0.55019
C	-5.15883	4.08135	0.14216
N	-4.69712	2.82547	0.11753
C	-5.35231	1.90354	-0.60518
C	-6.28483	-1.26531	-3.53502
C	-6.33102	-1.29689	-4.92529
C	-5.24485	-1.82490	-5.62220
C	-4.16012	-2.31640	-4.89075
N	-4.11116	-2.28702	-3.55165
C	-5.15029	-1.76648	-2.88038
C	-5.08163	-1.78528	-1.35614
C	-4.72264	0.52031	-0.63670
C	-6.59669	-0.76014	0.35616
N	-5.67405	-0.58065	-0.76714
H	6.41681	1.39799	3.84664
H	4.66398	1.42056	3.73589
H	5.64463	-0.21863	5.43717
H	6.62893	-2.34329	4.49727
H	7.49856	-1.04475	3.64132
H	7.17222	-2.77332	0.02641
H	5.61682	3.17657	2.65033
H	6.62893	2.64182	-1.79651
H	4.90776	2.38756	-2.03792
H	7.24411	3.72061	0.57845
H	6.18130	5.04933	1.10860
H	5.44541	-3.09359	0.02197
H	6.65631	-3.51496	-2.19069
H	7.98100	-1.15867	-1.95951
H	7.23760	-1.47413	-3.54812
H	2.81515	4.86758	-1.68402
H	2.76798	3.02270	2.97577
H	5.61170	4.74920	-1.32804
H	3.95327	-4.23280	-2.58824
H	3.42563	0.68168	-3.42041
H	6.23644	0.69307	-2.83697
H	2.83929	-0.49358	5.65218
H	3.40366	-3.37384	1.58908
H	6.20381	-2.82915	2.09678
H	0.45003	-1.16959	5.80537
H	0.96620	-3.86514	1.59141
H	0.31736	3.41609	3.11581
H	0.36605	5.27653	-1.55475
H	1.13674	0.29027	-4.31618
H	1.63965	-4.62817	-3.40123
H	-3.11937	-4.05506	-5.62147
H	-3.00156	-2.63111	-6.67360
H	-4.63739	6.09881	0.70009
H	-4.68488	4.95323	2.05823
H	-4.22631	-4.06709	2.88237
H	-4.33887	-3.71997	4.63167
H	-6.83538	1.05276	2.38684
H	-5.97804	0.82099	4.72985
H	-4.67719	-1.23935	5.32907
H	-7.00981	1.43599	-1.89871
H	-7.88766	3.79212	-1.85112
H	-6.64248	5.51125	-0.51803
H	-7.09901	-0.85216	-2.94952
H	-7.19399	-0.90819	-5.46068
H	-5.23188	-1.84544	-6.70856
H	-7.31006	0.07455	0.34626
H	-7.17223	-1.67161	0.16157
H	-4.07497	0.42593	0.25016
H	-4.05907	0.48049	-1.51086
H	-4.03794	-1.94633	-1.05193
H	-5.63558	-2.65869	-0.99367

Frequencies

10.2851	14.1604	17.1142
18.5958	20.7928	27.1023
33.2106	35.9190	36.1944
45.3953	48.4530	50.8383
56.3803	59.1009	68.6102
79.7315	82.3976	97.1847
100.7418	113.9435	114.9560
120.7999	125.7070	128.6474
138.1632	138.3843	148.3259
149.8521	159.2685	160.7411
166.4088	171.7039	173.8920
177.9441	179.5606	183.0843
192.5195	202.3056	206.7497
218.8898	225.0645	232.7464
238.2964	238.7465	239.6169
243.5901	245.7455	249.4446

255.5563	260.9075	265.1669	1040.0439	1043.5266	1044.8110
270.8604	275.1312	290.5231	1066.7771	1075.2276	1077.9237
294.3570	295.9583	299.6001	1078.2377	1098.0308	1107.7252
302.7582	308.8788	317.4322	1108.3880	1108.9435	1114.2736
326.1331	329.9791	345.1226	1117.6351	1119.8136	1127.8803
347.3309	349.6813	368.5407	1136.7797	1148.2388	1150.5972
372.6837	373.7366	385.4511	1151.9680	1156.9914	1166.5611
389.9553	396.4073	398.7831	1166.9968	1167.3828	1176.1852
401.2463	402.7807	403.8064	1177.0647	1177.8626	1178.2886
419.5308	427.4535	428.8865	1178.6533	1179.0202	1185.1392
435.1624	435.8991	439.4622	1187.6711	1189.9099	1190.9179
448.1922	467.7488	470.5955	1191.7723	1194.0927	1227.4657
474.6523	482.6877	483.9098	1228.6728	1230.1706	1231.9833
484.8175	490.7272	499.8422	1232.9821	1237.4979	1244.3816
501.7217	505.2340	527.2968	1247.6183	1249.0599	1249.3079
529.4126	538.2164	548.7410	1254.0379	1254.2286	1254.3914
549.4797	550.7562	567.9979	1259.9748	1266.3933	1271.2087
571.6009	573.3290	575.6323	1273.1547	1274.9134	1277.5763
576.6110	577.3488	580.9706	1277.7110	1278.0231	1290.4093
592.4673	594.9312	605.7093	1290.7685	1292.8028	1299.4820
606.6119	607.6794	610.6188	1300.6375	1301.0239	1301.8922
622.1614	625.0804	633.7410	1312.1172	1313.7701	1318.4103
651.2800	652.5487	653.7720	1318.8242	1319.8019	1322.6556
656.9936	659.2198	661.5107	1327.1289	1339.5022	1340.0593
663.0754	665.0277	701.0358	1341.5374	1345.1023	1345.5547
714.3275	716.3334	720.0420	1346.8147	1352.2879	1358.5353
721.5048	725.6373	726.0867	1365.8006	1368.5832	1371.3562
731.6171	734.9954	739.9342	1376.4778	1377.3269	1380.5707
741.4815	742.6862	743.0392	1394.1944	1400.7990	1401.1372
748.3189	753.0540	757.4681	1407.9997	1409.3903	1412.0749
762.1858	764.1405	764.7823	1412.3386	1413.3082	1413.6802
768.1508	769.6218	774.2306	1420.1364	1424.3353	1452.2101
777.3085	778.5964	779.1624	1452.7501	1470.2597	1471.1839
780.9538	784.4437	785.5122	1472.6163	1474.4031	1474.8743
797.7506	801.7869	806.7485	1475.1791	1476.2964	1476.8421
810.6697	814.4807	822.7019	1479.7261	1483.8562	1484.0941
825.7643	827.0251	835.5905	1484.4744	1485.9940	1487.5641
840.1472	843.4963	853.7196	1489.4562	1492.4550	1493.7457
867.5251	868.8838	869.3846	1494.5160	1496.9331	1501.5338
876.3738	887.7501	888.0899	1502.4589	1503.3430	1509.1166
894.9062	895.8710	896.5182	1512.9229	1520.9280	1521.0026
900.0028	910.2739	912.6722	1521.8314	1534.3787	1534.9819
913.8483	917.1996	920.7784	1535.5206	1606.6752	1607.8441
921.4599	931.8095	935.3037	1629.5609	1630.0258	1631.3321
935.5128	935.9657	936.1330	1635.7669	1637.8959	1639.3727
940.9170	941.1062	941.4191	1648.8100	1649.3285	1649.4455
949.5340	955.1314	958.3370	1675.3476	1675.8031	1676.8628
960.4148	964.7776	965.4805	1678.3117	1678.3959	1679.3842
966.9628	969.1954	969.4985	1769.0863	1772.7099	1773.6997
982.3572	987.2711	1000.9369	1820.6627	1821.2978	1823.0554
1003.8647	1005.8268	1009.4036	2998.1675	3015.1053	3015.2225
1010.5569	1011.1333	1011.7305	3016.3851	3033.3199	3038.1303
1013.3975	1014.9300	1016.4031	3056.7936	3057.0112	3057.0990
1016.9530	1022.2580	1023.9430	3057.1800	3063.1295	3064.3070

3064.8810	3066.7073	3073.3475
3078.2449	3079.4413	3079.5753
3080.6126	3084.3960	3093.4981
3103.1889	3103.2525	3103.5291
3108.2322	3118.3927	3129.2191
3131.2346	3136.1633	3156.8203
3172.3304	3173.1597	3173.3516
3179.4044	3179.4643	3181.5594
3183.2680	3184.8695	3190.4015
3199.4242	3199.5511	3200.1197
3200.7250	3200.7710	3200.7942
3201.8635	3201.9250	3206.3086
3221.4775	3224.8230	3234.9835

TS5

E(RB3LYP) = -3723.59829981

E(RB3LYP-D3) = -3723.78643709

H - Sum of electronic and thermal Enthalpies= -3722.436560

G - Sum of electronic and thermal Free Energies= -3722.595243

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.53911	0.68945	1.90749
C	5.64545	1.66011	0.89385
C	5.86799	1.27157	-0.44372
C	6.03556	-0.09066	-0.75443
C	5.94484	-1.06933	0.25603
C	5.70344	-0.67290	1.58410
C	5.23344	1.11832	3.34482
C	5.00958	-0.05960	4.32405
C	6.08691	-1.12594	4.02858
C	5.54250	-1.70758	2.70313
C	6.09391	-2.55517	-0.07956
C	6.20546	-2.85039	-1.59356
C	6.25190	-0.55704	-2.20022
C	5.91348	2.31389	-1.56207
C	5.59479	3.75077	-1.09157
C	5.46764	3.15394	1.20113
C	6.34756	3.98406	0.23773
C	7.16329	-1.80618	-2.20795
C	1.76426	4.32684	-0.67226
C	3.02018	4.23519	-1.34333
C	4.14855	3.88754	-0.64153
C	4.07597	3.58224	0.74908
C	2.89129	3.68394	1.43485
C	1.70587	4.07512	0.74742
C	2.72721	-1.35886	-3.65988
C	2.67584	-2.73731	-3.23577
C	3.80184	-3.29874	-2.56370
C	4.90555	-2.52162	-2.30886
C	4.94235	-1.15347	-2.70605
C	3.88866	-0.58404	-3.37652
C	1.74644	-2.54748	2.99634
C	1.42176	-1.53950	3.97685
C	2.45421	-0.67873	4.45532
C	3.73896	-0.82454	3.99036
C	4.05738	-1.82787	3.02939
C	3.08950	-2.66761	2.53701
C	0.72681	-3.41838	2.51354
C	-0.54419	-3.27896	3.00583
C	-0.86263	-2.30051	3.97754
C	0.08512	-1.43634	4.46415
C	0.57390	4.67858	-1.37390
C	-0.59694	4.79116	-0.66875
C	-0.64352	4.59040	0.73116
C	0.47134	4.23185	1.44268
C	1.49985	-3.50644	-3.47988
C	0.43944	-2.90573	-4.10817
C	0.49890	-1.55941	-4.53878
C	1.61084	-0.78566	-4.33504
C	-0.80514	-1.21847	-5.17085
O	-1.16192	-0.17423	-5.68662
N	-1.58962	-2.37693	-5.07340
C	-0.91103	-3.43906	-4.44751
O	-1.36693	-4.55127	-4.26051
C	-1.96826	5.14635	-1.12873
O	-2.36333	5.39679	-2.25306
C	-2.03321	4.86627	1.19262
O	-2.47935	4.88671	2.32456
C	-1.77225	-4.07109	2.72297
O	-1.91695	-5.02828	1.98653
C	-2.29973	-2.46328	4.33780
O	-2.96143	-1.86502	5.16765
N	-2.77836	-3.51094	3.53440
N	-2.76283	5.16776	0.03067
C	-2.99287	-2.41966	-5.44464
C	-4.17541	5.47517	0.02456
C	-4.11191	-4.07708	3.65203
C	-7.33394	-1.62194	2.37471
C	-7.40930	-2.20152	3.64070
C	-6.34243	-2.97804	4.08268
C	-5.24151	-3.15038	3.23362
N	-5.16219	-2.58516	2.02281
C	-6.18908	-1.83121	1.59481
C	-6.71784	2.17151	0.88207
C	-7.29234	3.42870	0.70176
C	-6.46571	4.50956	0.40636
C	-5.08849	4.28365	0.29658
N	-4.53850	3.07427	0.44245
C	-5.33128	2.02777	0.73629
C	-5.40606	0.00157	-2.90589
C	-5.68851	-0.00707	-4.27082
C	-4.90487	-0.78532	-5.12179
C	-3.86281	-1.53238	-4.56402
N	-3.59254	-1.53201	-3.25361
C	-4.34243	-0.77746	-2.43482

C	-3.94394	-0.80740	-0.96076
C	-4.64465	0.68166	0.94277
C	-6.09373	-1.22907	0.19583
N	-4.97539	-0.33121	-0.05437
H	6.06689	1.72424	3.73071
H	4.35076	1.76899	3.35913
H	5.02278	0.31349	5.35388
H	6.10488	-1.89764	4.80718
H	7.09335	-0.70454	3.92666
H	6.99452	-2.95159	0.41313
H	5.66739	3.37182	2.25164
H	6.91444	2.32015	-2.01869
H	5.21551	2.03372	-2.36036
H	7.38823	3.64185	0.20780
H	6.33234	5.04260	0.52266
H	5.24791	-3.11882	0.33149
H	6.52338	-3.88805	-1.74254
H	8.08085	-1.66815	-1.62483
H	7.43571	-2.07451	-3.23548
H	3.06293	4.46331	-2.40700
H	2.83213	3.47927	2.50164
H	5.85873	4.46189	-1.88195
H	3.76449	-4.34442	-2.26283
H	3.91045	0.45681	-3.69197
H	6.63276	0.24851	-2.82974
H	2.20448	0.07564	5.19945
H	3.32215	-3.43546	1.80255
H	6.00419	-2.66012	2.43945
H	-0.16853	-0.69052	5.21335
H	0.96082	-4.18087	1.77506
H	0.42300	4.07101	2.51669
H	0.60080	4.85374	-2.44645
H	1.64031	0.25047	-4.66249
H	1.44481	-4.54243	-3.15502
H	-3.29892	-3.46673	-5.34805
H	-3.09644	-2.12246	-6.49297
H	-4.39592	5.90163	-0.95959
H	-4.36667	6.24659	0.77991
H	-4.11209	-4.96498	3.01125
H	-4.26850	-4.39733	4.68788
H	-8.15000	-1.01406	1.99291
H	-8.27891	-2.04290	4.27344
H	-6.35145	-3.43425	5.06819
H	-7.33199	1.31775	1.14965
H	-8.36558	3.56721	0.80785
H	-6.87339	5.50952	0.27845
H	-5.97966	0.60199	-2.20795
H	-6.50039	0.59655	-4.66937
H	-5.08347	-0.80052	-6.19344
H	-7.05302	-0.73117	-0.01928
H	-6.01781	-2.05384	-0.52173
H	-4.88720	0.31687	1.95232
H	-3.56743	0.86656	0.92759
H	-3.05897	-0.17075	-0.84424
H	-3.62085	-1.83248	-0.72261

Frequencies

-22.6387	6.8708	15.1792
18.2087	23.5250	24.5369
27.8951	33.9982	37.5516
43.5588	47.2347	49.8909
51.5444	54.7753	60.3616
69.3169	78.4420	98.2810
104.6452	110.4221	112.4725
119.0584	120.5863	123.8828
138.0528	138.8937	149.0964
150.9180	158.9079	160.4609
163.3821	169.2389	171.4508
176.1923	177.6744	183.7137
191.4038	197.9291	204.1223
211.9617	230.7758	233.6899
236.1726	236.7297	240.6360
243.7256	247.4619	250.5932
254.5209	258.4316	263.3715
267.6422	271.0550	287.3126
289.1602	297.3870	298.8687
301.0148	306.1652	313.2279
320.0390	328.1557	337.9124
347.4126	347.8674	355.9945
371.6587	372.4245	374.5745
386.5450	396.8210	399.6814
401.3841	404.8165	405.1048
419.7861	425.3864	428.8621
429.8097	436.0194	438.6524
452.6361	467.5211	472.2718
475.7331	483.1311	483.7851
484.6484	492.1671	501.8998
502.4807	503.2314	524.0620
530.5437	534.3718	547.6215
548.6038	549.0791	568.5891
571.9346	573.2631	575.5229
577.0058	577.5960	579.5936
594.4130	594.9246	604.4129
606.5741	606.9114	612.8135
622.4090	623.6799	631.9210
648.0231	649.8864	653.1798
655.7081	658.0552	659.9394
660.8230	663.6874	692.3606
712.5827	716.2140	718.7106
720.7704	723.6726	725.6912
727.4292	734.3261	740.2152
741.2221	743.1518	743.7866
747.6221	750.1869	752.9890
762.6562	763.8195	764.4065
764.8141	767.5008	767.7513
769.1321	779.4436	779.8689
782.3091	785.5465	785.8189
796.0022	799.5853	805.0041

809.5981	817.4317	821.6749
825.8864	827.4077	830.6692
839.5865	842.1071	844.8694
863.0803	869.4240	869.5430
876.5574	887.8598	888.1835
894.5363	895.9284	896.5962
899.8804	903.9893	907.7348
912.1140	914.2820	919.3196
920.3872	921.1027	934.5642
935.5434	935.9533	940.7009
941.1909	941.5029	947.1692
950.3792	958.3057	959.0580
961.4112	964.8637	966.2694
966.8989	969.7940	972.1611
989.0345	990.1218	999.7159
1000.8850	1001.5575	1003.2965
1009.3490	1011.0985	1012.2815
1013.0653	1015.4070	1016.5298
1020.7109	1021.2556	1029.7998
1040.1896	1044.6423	1045.2635
1066.9603	1074.8899	1077.3687
1077.6879	1107.2464	1107.9092
1109.6832	1114.1046	1117.2335
1117.8041	1119.4132	1127.3533
1145.6549	1148.5299	1151.5408
1155.5265	1160.3437	1166.6422
1166.8888	1177.6150	1178.2264
1178.4189	1178.8607	1179.3694
1179.7926	1182.5871	1185.6968
1189.5511	1190.9791	1191.1570
1191.9633	1194.3084	1222.1242
1228.3410	1229.7601	1231.2086
1231.5500	1236.5680	1237.8225
1244.7575	1248.9917	1249.0900
1253.7478	1254.0325	1254.2000
1260.6357	1264.3391	1266.4285
1270.8777	1271.8722	1277.7140
1278.1231	1278.1471	1289.7464
1290.0934	1299.3265	1299.5855
1299.8391	1301.7449	1307.3473
1314.8859	1315.6764	1318.5947
1319.2055	1321.5387	1325.8460
1333.6696	1339.1961	1339.5607
1341.0807	1345.4416	1345.8740
1352.5165	1354.9427	1359.1171
1365.0467	1376.9699	1377.4557
1377.8934	1387.0118	1391.7579
1395.0598	1400.5764	1400.8120
1407.8340	1412.6256	1413.0044
1413.3375	1416.1731	1416.8020
1422.3981	1426.8889	1452.3533
1452.5425	1469.8048	1470.4786
1472.3200	1474.3237	1474.5686
1475.0727	1475.4232	1477.2926
1478.7592	1481.4805	1483.8307
1484.3017	1484.4642	1485.7249
1488.7343	1491.4343	1495.0862
1495.8526	1497.7286	1500.5710
1501.1637	1501.8111	1502.4951
1517.6685	1521.1778	1521.2921
1522.1066	1534.1178	1534.3888
1534.9833	1606.7457	1607.4743
1629.2217	1630.1381	1632.5797
1636.5574	1636.9639	1638.7716
1648.6230	1649.2545	1649.8225
1674.9428	1676.2231	1677.2867
1677.9864	1678.8611	1679.7214
1771.0138	1774.1164	1775.0415
1821.2188	1822.3639	1824.1436
2987.2421	3010.9484	3014.9335
3016.0022	3016.3150	3016.6126
3057.1547	3057.3454	3057.4670
3061.9283	3067.0119	3068.5056
3069.9548	3070.1047	3074.1170
3078.0970	3078.5726	3079.0261
3079.5661	3082.2257	3103.0377
3103.4022	3103.6125	3111.2475
3115.4371	3116.3797	3118.7353
3124.0199	3127.0082	3128.8107
3172.0161	3172.7692	3173.1836
3180.2138	3180.5111	3181.0029
3181.5690	3184.1591	3184.3446
3195.9099	3197.9295	3199.3398
3199.4250	3199.5005	3200.6320
3200.8286	3201.8393	3202.1635
3210.1805	3216.2733	3223.1133

I5

E(RB3LYP) = -3723.59974092

E(RB3LYP-D3) = -3723.79027105

H - Sum of electronic and thermal Enthalpies= -3722.436885

G - Sum of electronic and thermal Free Energies= -3722.596751

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.35532	1.36485	1.77195
C	5.58134	1.84213	0.46692
C	5.86994	0.94094	-0.57924
C	6.02180	-0.42946	-0.29614
C	5.84077	-0.91075	1.01635
C	5.50176	-0.01064	2.04309
C	4.92856	2.33519	2.87602
C	4.55810	1.64920	4.21402
C	5.62592	0.56851	4.49145
C	5.20425	-0.50565	3.46264
C	5.99676	-2.40029	1.33172

C	6.21619	-3.28800	0.08486
C	6.32758	-1.44488	-1.40568
C	5.99438	1.43517	-2.02108
C	5.71392	2.94531	-2.18938
C	5.47240	3.33878	0.13750
C	6.42838	3.67736	-1.02993
C	7.22492	-2.56922	-0.83763
C	1.90424	3.77776	-2.24116
C	3.17295	3.36424	-2.74921
C	4.25930	3.29753	-1.91052
C	4.12637	3.60226	-0.52400
C	2.93470	4.04274	-0.00672
C	1.79554	4.15877	-0.85376
C	2.90108	-2.84051	-2.63373
C	2.80376	-3.91924	-1.67998
C	3.87866	-4.13748	-0.76830
C	4.97245	-3.30680	-0.78727
C	5.05028	-2.22196	-1.70798
C	4.05069	-1.99894	-2.62186
C	1.37596	-1.21252	3.66421
C	0.98035	0.09939	4.11720
C	1.98263	1.09727	4.31132
C	3.30439	0.79712	4.08225
C	3.69063	-0.50515	3.64970
C	2.75505	-1.48664	3.43703
C	0.38833	-2.22092	3.46853
C	-0.92150	-1.91822	3.73246
C	-1.31199	-0.63899	4.19493
C	-0.39600	0.36528	4.38485
C	0.74825	3.82678	-3.07581
C	-0.43654	4.25935	-2.53559
C	-0.52378	4.68828	-1.19046
C	0.55492	4.64214	-0.34781
C	1.63024	-4.72927	-1.64821
C	0.61517	-4.45106	-2.52693
C	0.72408	-3.40967	-3.47804
C	1.83620	-2.61333	-3.55281
C	-0.54102	-3.36497	-4.26071
O	-0.84632	-2.63680	-5.18837
N	-1.36131	-4.36501	-3.71780
C	-0.73287	-5.07197	-2.67507
O	-1.22222	-5.99968	-2.05942
C	-1.79537	4.36857	-3.13981
O	-2.16298	4.08304	-4.26436
C	-1.92033	5.13227	-0.93422
O	-2.39925	5.62123	0.07312
C	-2.13225	-2.78036	3.66965
O	-2.22548	-3.95346	3.36105
C	-2.78114	-0.67406	4.45148
O	-3.50641	0.19246	4.90661
N	-3.20099	-1.96547	4.09164
N	-2.61955	4.89580	-2.12791
C	-2.76100	-4.52904	-4.08201
C	-4.05964	5.03942	-2.25273
C	-4.54291	-2.47942	4.30484
C	-7.64909	-0.63737	2.06513
C	-7.89188	-0.95332	3.39973
C	-6.86688	-1.52795	4.14757
C	-5.64137	-1.78023	3.52073
N	-5.40872	-1.48762	2.23423
C	-6.39007	-0.91908	1.51530
C	-6.07318	2.75828	0.72161
C	-6.62406	3.98427	0.34917
C	-5.98667	4.73904	-0.63314
C	-4.81918	4.22819	-1.21061
N	-4.30958	3.03727	-0.88016
C	-4.91546	2.30901	0.07255
C	-4.97609	-1.03799	-3.06976
C	-5.13343	-1.56597	-4.35005
C	-4.42719	-2.71505	-4.70331
C	-3.58459	-3.29267	-3.74942
N	-3.44707	-2.80168	-2.51164
C	-4.12442	-1.69378	-2.17189
C	-3.87570	-1.18570	-0.75423
C	-4.26464	0.98188	0.42939
C	-6.13305	-0.59641	0.04117
N	-4.80666	-0.14000	-0.34161
H	5.74351	3.04658	3.07747
H	4.07782	2.93484	2.53146
H	4.47536	2.40611	5.00153
H	5.53895	0.17646	5.51164
H	6.65014	0.92667	4.33771
H	6.85386	-2.53979	2.00782
H	5.64813	3.95305	1.02275
H	7.00949	1.23683	-2.39538
H	5.31401	0.86569	-2.66650
H	7.45112	3.32075	-0.86321
H	6.45518	4.76025	-1.19858
H	5.11698	-2.76432	1.87530
H	6.53375	-4.28869	0.39757
H	8.10083	-2.18594	-0.30207
H	7.56566	-3.23055	-1.64298
H	3.25920	3.12340	-3.80741
H	2.83460	4.31385	1.04194
H	6.03849	3.26828	-3.18457
H	3.80947	-4.96592	-0.06524
H	4.10511	-1.18050	-3.33648
H	6.75815	-0.96240	-2.28436
H	1.67891	2.08384	4.65711
H	3.04009	-2.48184	3.10330
H	5.66282	-1.47652	3.65513
H	-0.70433	1.34445	4.74281
H	0.67583	-3.21149	3.12561
H	0.47004	4.95618	0.68942
H	0.80921	3.51422	-4.11522
H	1.90062	-1.80771	-4.27977
H	1.53870	-5.53385	-0.92287
H	-3.11950	-5.39501	-3.51680

H	-2.83225	-4.75325	-5.15095
H	-4.30778	4.70315	-3.26535
H	-4.33327	6.09696	-2.16870
H	-4.49966	-3.53521	4.01535
H	-4.77708	-2.43021	5.37442
H	-8.41861	-0.17292	1.45352
H	-8.85595	-0.73955	3.85465
H	-7.00543	-1.76356	5.19892
H	-6.51604	2.16694	1.51808
H	-7.51994	4.35922	0.83802
H	-6.36293	5.71727	-0.92048
H	-5.47845	-0.12818	-2.76060
H	-5.78230	-1.07550	-5.07164
H	-4.50104	-3.13623	-5.70190
H	-6.87831	0.15193	-0.26477
H	-6.35638	-1.49454	-0.54866
H	-4.34543	0.81516	1.51558
H	-3.20366	1.07199	0.18747
H	-2.86093	-0.77214	-0.72933
H	-3.86964	-2.04987	-0.07378

Frequencies

13.6269	16.3395	19.2333
23.3503	24.9585	25.5666
31.5241	37.3205	41.3047
44.3188	47.9929	51.6042
52.8381	58.9923	60.9224
73.8773	81.1733	96.7864
104.6724	114.6685	115.7382
118.6527	120.2634	130.1164
138.4822	139.5322	150.1799
150.9942	159.2374	160.9130
166.5642	171.1540	177.6238
179.7545	183.5947	187.1966
191.8455	199.3873	205.1030
213.5537	229.3280	232.9932
236.5218	239.7181	245.2528
247.0891	250.2780	252.2763
256.4258	260.1717	262.7895
264.9416	271.3381	289.0365
293.1796	298.5717	300.4068
301.8414	307.4892	313.9908
320.4597	327.8037	339.4439
346.8652	347.7093	355.1627
371.0843	372.3561	384.1203
386.5493	398.3704	399.1096
402.5314	404.8743	406.1524
419.9311	428.1088	428.7420
429.9231	436.7737	437.7307
452.2550	468.4953	471.6784
475.0328	483.2472	483.8844
484.8551	492.8047	500.5476
501.9562	502.7529	528.3694
531.1998	536.3766	547.5612
549.4887	551.8575	567.6668
571.8001	573.2889	575.6737
577.4032	579.2647	581.2696
594.3090	594.5388	601.5184
606.3002	606.9696	615.6518
620.8122	625.8636	629.8496
646.4528	652.7055	654.4506
656.9495	659.8382	660.7584
663.3177	667.9227	682.0964
710.7785	715.8486	718.1241
720.8316	724.1085	725.4703
733.0598	738.2862	740.4673
741.2228	743.2211	743.9041
746.6979	750.1243	759.4233
762.6844	762.8472	764.6633
765.4233	768.1334	770.3651
778.3330	779.1187	780.8138
782.4395	785.4090	786.0657
802.9365	805.0212	806.6299
807.8349	810.6932	818.1654
826.1217	827.2259	829.3340
840.2860	842.5471	847.0947
869.2676	869.5419	875.9980
876.6752	887.9843	888.3582
894.5982	896.0243	896.7659
899.5968	905.3373	911.6675
916.0627	919.2503	919.5694
920.3207	933.2129	934.8331
935.8027	936.4107	941.1172
941.4310	941.8716	951.1236
952.5361	960.0051	960.8629
962.0948	965.5464	966.1173
968.4016	970.3631	978.6202
989.5730	991.6056	1001.6804
1002.6314	1004.3149	1009.9560
1010.1608	1012.1354	1013.7958
1014.5692	1015.6409	1016.5191
1016.9173	1020.8111	1022.2701
1039.6421	1044.4556	1045.2107
1066.8323	1074.5721	1077.0221
1077.8320	1106.1266	1107.2520
1108.5487	1114.3906	1115.2933
1117.9757	1121.7602	1127.2969
1145.7063	1147.2426	1147.5226
1154.6156	1158.4126	1166.1608
1166.6754	1177.1638	1177.5148
1177.6268	1178.5657	1178.9118
1179.4388	1179.8568	1184.2681
1189.4662	1190.3696	1190.6396
1192.0051	1193.1313	1221.8647
1229.0247	1230.3203	1230.9988
1232.7493	1235.6622	1236.8380
1244.7945	1248.4923	1249.4255
1253.5577	1253.9160	1254.1498

1259.5532	1260.4301	1265.7147
1268.1207	1275.9461	1277.7170
1277.7753	1278.0098	1289.6148
1289.9599	1297.6012	1298.2488
1299.3117	1301.3367	1302.6580
1310.2101	1314.7431	1317.7457
1319.0150	1321.1551	1325.3237
1325.5741	1337.6640	1339.1858
1339.7977	1341.1659	1345.1327
1345.9799	1349.6888	1350.8475
1362.3110	1364.5590	1376.7117
1377.3359	1386.2584	1391.3557
1394.2647	1397.1641	1399.6255
1400.4180	1412.0000	1412.6013
1412.8932	1415.0341	1416.6015
1423.0516	1430.0329	1451.8992
1452.0282	1469.9644	1471.8644
1472.0134	1473.4680	1474.7697
1475.0939	1475.3945	1478.3766
1480.3650	1483.3979	1484.3687
1484.4968	1485.8798	1487.3014
1494.8086	1495.9907	1497.6107
1499.0667	1500.8658	1501.5484
1501.9928	1502.3559	1505.9057
1518.7495	1521.0467	1521.4291
1522.2159	1533.6276	1534.9318
1535.2644	1605.8401	1607.0114
1628.9605	1630.5652	1631.8281
1636.2159	1638.5507	1639.1650
1647.5699	1649.2719	1650.0082
1673.8271	1676.3424	1677.1298
1677.4359	1679.4458	1679.7868
1770.3024	1773.2857	1774.6769
1820.8801	1821.6484	1823.9090
3000.0476	3014.4369	3015.8852
3018.1361	3019.6393	3026.8138
3057.1879	3057.3073	3057.8651
3060.9767	3064.8598	3066.0633
3066.3869	3071.0050	3073.8879
3077.0204	3078.4149	3079.0658
3079.5318	3081.0182	3103.1746
3103.3633	3104.0172	3106.5133
3109.4764	3119.3804	3123.9436
3126.7412	3127.3703	3129.0008
3171.7558	3173.0450	3173.4430
3180.2674	3181.2937	3181.9424
3182.9861	3183.2846	3185.7048
3195.0762	3197.8340	3199.0730
3199.2463	3199.4179	3200.5963
3200.7531	3202.1560	3204.7528
3206.9916	3207.4313	3228.2267

TS6

E(RB3LYP) = -3723.59892863

E(RB3LYP-D3) = -3723.78991560

H - Sum of electronic and thermal Enthalpies= -3722.437137

G - Sum of electronic and thermal Free Energies= -3722.594133

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.37039	1.33860	1.73671
C	5.63455	1.72576	0.40927
C	5.89816	0.75117	-0.57559
C	6.00440	-0.60255	-0.20453
C	5.78213	-0.99518	1.13102
C	5.45434	-0.02248	2.09336
C	4.96420	2.39122	2.77040
C	4.52642	1.80219	4.13310
C	5.53858	0.69694	4.50653
C	5.09995	-0.41921	3.53103
C	5.87818	-2.46683	1.53999
C	6.10035	-3.43574	0.35570
C	6.30642	-1.69301	-1.24179
C	6.03408	1.14839	-2.04594
C	5.79278	2.65189	-2.30911
C	5.58529	3.20282	-0.01154
C	6.54196	3.43229	-1.20404
C	7.15417	-2.80527	-0.58127
C	2.00894	3.60552	-2.38158
C	3.25745	3.11487	-2.87259
C	4.35181	3.06903	-2.04235
C	4.24499	3.47431	-0.67935
C	3.07701	3.99446	-0.18351
C	1.93201	4.08896	-1.02439
C	2.87483	-3.06345	-2.47920
C	2.71500	-4.07230	-1.45971
C	3.75845	-4.26531	-0.50652
C	4.87906	-3.47193	-0.54748
C	5.01580	-2.45106	-1.53232
C	4.05076	-2.25955	-2.48905
C	1.24114	-0.95974	3.68360
C	0.88972	0.39689	4.02824
C	1.92785	1.36511	4.17984
C	3.24133	0.99627	4.01219
C	3.58301	-0.34614	3.67510
C	2.61262	-1.30225	3.50637
C	0.21867	-1.94444	3.55635
C	-1.08182	-1.57545	3.78055
C	-1.43018	-0.24765	4.12497
C	-0.47957	0.73501	4.24556
C	0.84174	3.63015	-3.20218
C	-0.32192	4.13557	-2.67844
C	-0.37479	4.66318	-1.36706
C	0.71517	4.64644	-0.53852
C	1.51065	-4.83455	-1.40428
C	0.52601	-4.57606	-2.32298

C	0.69801	-3.60661	-3.33855
C	1.84214	-2.86042	-3.43917
C	-0.55093	-3.55555	-4.14513
O	-0.80722	-2.87584	-5.12326
N	-1.42775	-4.47514	-3.55089
C	-0.84817	-5.14189	-2.45380
O	-1.39044	-6.00180	-1.78668
C	-1.68891	4.23733	-3.26686
O	-2.08453	3.88055	-4.36107
C	-1.75436	5.16070	-1.12070
O	-2.20299	5.73053	-0.14220
C	-2.31869	-2.40247	3.80763
O	-2.44971	-3.59800	3.62248
C	-2.89919	-0.21093	4.38096
O	-3.59524	0.71712	4.75167
N	-3.35838	-1.52053	4.15777
N	-2.48088	4.85847	-2.28235
C	-2.83778	-4.56709	-3.90698
C	-3.92094	5.02304	-2.38572
C	-4.69477	-1.97242	4.48112
C	-7.76562	-1.27057	1.62261
C	-8.10806	-1.79671	2.86488
C	-7.09743	-2.01708	3.79746
C	-5.77884	-1.71164	3.44130
N	-5.44339	-1.21749	2.24299
C	-6.41920	-0.99215	1.34750
C	-5.89727	2.96588	0.77182
C	-6.41622	4.19502	0.36384
C	-5.79164	4.87722	-0.67784
C	-4.66859	4.29434	-1.27587
N	-4.19061	3.10138	-0.90892
C	-4.78486	2.44221	0.10014
C	-4.75161	-0.86023	-3.06453
C	-4.88914	-1.39009	-4.34587
C	-4.28867	-2.61317	-4.64432
C	-3.56617	-3.25792	-3.63721
N	-3.45111	-2.76366	-2.39741
C	-4.02901	-1.58760	-2.10958
C	-3.81610	-1.08225	-0.68447
C	-4.18281	1.10222	0.48884
C	-6.07933	-0.39982	-0.02708
N	-4.72004	0.00038	-0.31655
H	5.80756	3.07409	2.95335
H	4.15267	3.00868	2.36860
H	4.45340	2.60716	4.87247
H	5.40656	0.37121	5.54503
H	6.58108	1.00284	4.36297
H	6.71139	-2.59281	2.24779
H	5.79244	3.86246	0.83354
H	7.04241	0.90101	-2.40916
H	5.33713	0.55620	-2.65199
H	7.55342	3.05174	-1.02205
H	6.60421	4.50070	-1.44146
H	4.97194	-2.76767	2.07892
H	6.37849	-4.42431	0.73699
H	8.02741	-2.41507	-0.04637
H	7.49493	-3.52495	-1.33491
H	3.32182	2.79747	-3.91199
H	2.99960	4.34393	0.84356
H	6.11728	2.90089	-3.32536
H	3.64335	-5.04355	0.24612
H	4.15154	-1.49267	-3.25397
H	6.77440	-1.27736	-2.13555
H	1.65717	2.38441	4.44988
H	2.86411	-2.32916	3.25071
H	5.51217	-1.39444	3.79345
H	-0.75535	1.75017	4.52013
H	0.47373	-2.97063	3.30448
H	0.65569	5.03658	0.47435
H	0.87702	3.24092	-4.21662
H	1.95369	-2.10747	-4.21523
H	1.37098	-5.58356	-0.62882
H	-3.25184	-5.37436	-3.29555
H	-2.92623	-4.84092	-4.96277
H	-4.19867	4.62677	-3.36839
H	-4.17221	6.08907	-2.36399
H	-4.61913	-3.05134	4.65548
H	-4.99104	-1.49540	5.42241
H	-8.52621	-1.07370	0.87049
H	-9.14339	-2.02515	3.10579
H	-7.32265	-2.41491	4.78399
H	-6.33019	2.42715	1.61041
H	-7.27727	4.62660	0.86818
H	-6.14225	5.85505	-0.99706
H	-5.17231	0.10212	-2.79414
H	-5.43871	-0.84605	-5.11021
H	-4.34694	-3.04038	-5.64123
H	-6.74118	0.46542	-0.17846
H	-6.38456	-1.13106	-0.78744
H	-4.32166	0.93326	1.56637
H	-3.10902	1.16052	0.29496
H	-2.78784	-0.70770	-0.61723
H	-3.87026	-1.94578	-0.00410

Frequencies

-23.5394	13.9480	17.4500
18.7424	22.4295	25.7394
29.2841	35.4913	41.2796
45.4181	47.6352	52.7105
52.8777	60.9467	61.4474
74.6274	82.1238	96.1468
103.7592	114.6864	116.1514
119.1872	120.8118	130.7106
139.4918	139.6989	150.1807
151.1676	154.4555	158.9751
161.6549	169.8770	174.5376
180.4398	182.8767	189.4167
192.5537	199.3954	207.0882

212.5487	228.6076	233.9688	1010.4552	1010.9388	1013.3899
235.3936	238.6812	243.2289	1014.6366	1015.6811	1016.6489
248.0726	250.2248	252.7211	1017.4881	1020.3266	1030.7788
254.7476	262.1008	263.4982	1039.7263	1044.7634	1045.0592
265.7284	271.6210	290.7382	1066.8419	1074.3692	1076.7514
294.2356	299.1603	300.6704	1078.0491	1104.8181	1106.9602
302.1434	308.5388	314.9777	1108.2934	1113.8634	1117.6751
320.2165	321.9030	328.1535	1118.1704	1120.8145	1123.0382
346.9902	347.7506	359.1556	1144.7102	1146.9502	1151.7854
370.7857	372.6250	383.3852	1154.6460	1163.7624	1166.3684
386.7316	397.6026	399.4105	1166.7485	1176.9677	1177.2773
402.6412	405.6159	406.4084	1177.7373	1178.8132	1178.9136
419.9534	428.1598	428.7045	1179.7329	1180.6323	1184.4512
430.6287	433.7536	437.2180	1188.9422	1190.2946	1190.7695
450.7697	467.6218	472.1090	1191.8467	1192.7486	1215.6609
477.2602	483.2837	483.9789	1229.2348	1230.6489	1230.6793
485.1477	488.1127	499.9426	1233.6817	1234.7996	1236.6720
502.4337	504.3131	531.3102	1244.6774	1248.2985	1249.5029
535.5019	538.0226	547.5653	1253.5259	1253.9322	1254.2381
549.8512	553.4805	567.6083	1259.0065	1260.3848	1261.1427
571.4062	572.9856	575.3813	1268.8580	1275.1481	1277.5450
577.1318	579.2694	582.0231	1277.7930	1278.1887	1289.4405
594.1584	595.5156	602.4750	1290.0110	1296.6615	1298.1198
605.8074	607.0648	617.5567	1299.5208	1301.3934	1303.3322
622.4170	626.2819	633.5469	1309.3158	1314.8034	1317.7775
647.5358	652.7512	653.9842	1319.0023	1321.0916	1325.1946
655.0978	659.9717	660.5983	1326.8045	1337.4558	1339.0204
662.9022	664.3361	668.8842	1339.4895	1341.0549	1345.0037
714.5108	715.9846	719.0213	1346.2045	1350.5342	1359.9724
720.8121	723.7445	724.6665	1364.5410	1371.7027	1377.0173
733.0183	738.0423	738.6204	1377.3677	1383.9421	1389.2756
740.9767	742.4697	744.2174	1391.3160	1400.4742	1404.2127
745.1812	751.1526	754.1909	1405.5707	1411.6352	1412.4641
760.4567	762.7436	764.5207	1412.8435	1414.4837	1415.9259
764.9890	768.1866	770.9134	1418.8287	1429.7931	1451.7928
778.0994	778.6575	779.8601	1452.1850	1468.2235	1470.5889
782.1598	784.9454	785.3134	1471.5455	1472.9856	1474.4843
785.8353	803.6647	805.8452	1474.9778	1475.7010	1476.6602
809.3324	810.3461	817.5183	1477.7462	1481.1145	1483.6071
826.1742	826.9110	828.3100	1484.3357	1484.5356	1487.2492
840.8952	842.3681	846.7814	1488.8689	1494.1292	1495.4337
869.2925	869.8465	877.0827	1498.4332	1501.0345	1501.6574
880.7182	888.0890	888.6548	1502.3148	1502.5881	1504.3420
894.6983	896.2863	896.8911	1521.1415	1521.1523	1521.5379
899.5971	902.7354	911.5342	1522.3237	1533.3527	1534.9489
917.3694	918.6101	919.8119	1535.4248	1605.8125	1606.9890
920.3271	934.8001	935.7449	1628.3898	1630.5524	1632.6596
936.1579	937.1269	941.0828	1635.4386	1638.0451	1639.0697
941.1608	942.1515	950.6089	1647.3265	1648.8123	1650.0942
954.2702	958.1519	960.3650	1673.4216	1676.2886	1676.6763
960.9520	965.0023	966.0960	1677.6372	1679.7540	1680.0384
966.4857	969.3601	970.6593	1770.5166	1773.4922	1774.6488
989.9382	991.7174	1002.0779	1821.4105	1821.6470	1824.0318
1002.4956	1003.2830	1009.8338	3013.9457	3014.7751	3015.2132

3018.4785	3021.0576	3029.9996
3057.2076	3057.3228	3057.8916
3057.9289	3062.2283	3066.1658
3067.4178	3070.2236	3076.5345
3077.2975	3078.4565	3079.1252
3080.0659	3080.2128	3103.1627
3103.3758	3103.9920	3107.1000
3111.1087	3117.3869	3119.5053
3125.8146	3128.7352	3129.7827
3171.6863	3173.0062	3173.2655
3177.8779	3180.6091	3182.1757
3182.3906	3183.4582	3186.5627
3187.1349	3196.6536	3199.0358
3199.2331	3199.4332	3200.5600
3200.6840	3201.5827	3201.9561
3206.3314	3206.5442	3226.7482

I6

E(RB3LYP) = -3723.60398033

E(RB3LYP-D3) = -3723.79485308

H - Sum of electronic and thermal Enthalpies= -3722.440741

G - Sum of electronic and thermal Free Energies= -3722.600472

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.56019	1.17722	1.15525
C	5.67621	1.37957	-0.23301
C	5.73061	0.27713	-1.11018
C	5.74909	-1.02894	-0.58545
C	5.65192	-1.24095	0.80486
C	5.56772	-0.13485	1.67148
C	5.39354	2.38013	2.08498
C	5.12094	1.99966	3.55860
C	6.09340	0.85637	3.92649
C	5.42153	-0.32407	3.18805
C	5.61441	-2.65963	1.37660
C	5.59687	-3.77183	0.30193
C	5.83143	-2.25408	-1.50622
C	5.73660	0.48708	-2.62496
C	5.60200	1.96677	-3.05079
C	5.69717	2.79483	-0.83017
C	6.53166	2.79237	-2.13188
C	6.61589	-3.37932	-0.79127
C	1.93060	3.27596	-2.87139
C	3.07286	2.61654	-3.41945
C	4.24090	2.55244	-2.69811
C	4.31662	3.11167	-1.38862
C	3.25413	3.78629	-0.84344
C	2.03725	3.89948	-1.57460
C	2.20669	-3.41517	-2.34120
C	2.03399	-4.27736	-1.19702
C	3.11871	-4.44371	-0.28430
C	4.29823	-3.76968	-0.49009
C	4.45039	-2.89091	-1.60213
C	3.43974	-2.72334	-2.51486
C	1.61646	-0.47662	4.01302
C	1.41066	0.94626	4.13791
C	2.52855	1.82338	3.99974
C	3.77440	1.31045	3.72842
C	3.96180	-0.09273	3.55895
C	2.91742	-0.97006	3.70885
C	0.52020	-1.36843	4.19376
C	-0.71794	-0.84295	4.45354
C	-0.93146	0.55312	4.54084
C	0.10065	1.44681	4.40159
C	0.69210	3.33263	-3.57789
C	-0.36368	3.99722	-3.00590
C	-0.23762	4.65026	-1.75755
C	0.92720	4.61259	-1.03830
C	0.78604	-4.93893	-0.99632
C	-0.22249	-4.73310	-1.90325
C	-0.03994	-3.90785	-3.03766
C	1.14137	-3.25572	-3.27333
C	-1.31437	-3.88678	-3.80473
O	-1.57897	-3.30869	-4.84375
N	-2.20721	-4.69537	-3.08493
C	-1.62752	-5.23409	-1.92055
O	-2.19297	-5.96366	-1.12787
C	-1.76963	4.17213	-3.47370
O	-2.30120	3.75199	-4.48449
C	-1.54107	5.28997	-1.43421
O	-1.84386	5.97650	-0.47484
C	-2.01853	-1.52595	4.68719
O	-2.26155	-2.71807	4.75725
C	-2.38327	0.78167	4.79628
O	-2.98091	1.82967	4.95173
N	-2.96584	-0.50193	4.84368
N	-2.40201	4.95710	-2.49101
C	-3.62900	-4.75167	-3.38270
C	-3.83095	5.22175	-2.46013
C	-4.38955	-0.75185	5.05718
C	-6.19791	-2.42558	1.59026
C	-6.02392	-3.25368	2.69790
C	-5.44104	-2.72532	3.84829
C	-5.05833	-1.37990	3.84392
N	-5.24284	-0.57717	2.78616
C	-5.79643	-1.08494	1.67021
C	-5.58970	3.38030	0.95156
C	-6.07171	4.62976	0.56033
C	-5.52338	5.24407	-0.56400
C	-4.50755	4.57614	-1.25648
N	-4.06717	3.36539	-0.90233
C	-4.59250	2.76846	0.18082
C	-5.40477	-0.93148	-2.74144
C	-5.82065	-1.66923	-3.84878
C	-5.26199	-2.92690	-4.08033

C	-4.30282	-3.39976	-3.18068
N	-3.91932	-2.70494	-2.10349
C	-4.44984	-1.49241	-1.88455
C	-3.88515	-0.75060	-0.68197
C	-4.03291	1.40180	0.53041
C	-5.97070	-0.14536	0.48111
N	-4.74310	0.31768	-0.17955
H	6.30312	2.99865	2.05860
H	4.57952	3.01754	1.71999
H	5.22117	2.88890	4.19042
H	6.10351	0.67411	5.00751
H	7.11990	1.04197	3.59070
H	6.49524	-2.82055	2.01596
H	6.04918	3.52780	-0.10183
H	6.67316	0.09840	-3.05140
H	4.92776	-0.09742	-3.08042
H	7.52164	2.33961	-2.00548
H	6.65652	3.81527	-2.50582
H	4.73936	-2.77522	2.02760
H	5.80184	-4.73899	0.77377
H	7.57452	-3.03900	-0.38361
H	6.80092	-4.21259	-1.47926
H	2.99934	2.18621	-4.41678
H	3.31581	4.24633	0.14030
H	5.83402	2.06186	-4.11718
H	2.99212	-5.11688	0.56195
H	3.55400	-2.06989	-3.37699
H	6.25451	-1.99448	-2.47805
H	2.37267	2.89330	4.12672
H	3.05649	-2.04370	3.60339
H	5.80103	-1.29565	3.50856
H	-0.07056	2.51735	4.48218
H	0.66874	-2.44263	4.11877
H	1.00497	5.10305	-0.07130
H	0.58961	2.84416	-4.54368
H	1.26350	-2.61401	-4.14221
H	0.63803	-5.57777	-0.12924
H	-4.05255	-5.49970	-2.70452
H	-3.76956	-5.09412	-4.41239
H	-4.23277	4.81776	-3.39544
H	-4.00287	6.30314	-2.44998
H	-4.50130	-1.40230	5.93059
H	-4.83809	0.22101	5.27272
H	-6.63161	-2.80953	0.67103
H	-6.32076	-4.29857	2.65942
H	-5.25604	-3.34435	4.72031
H	-5.95818	2.89535	1.85111
H	-6.84309	5.13016	1.14049
H	-5.84616	6.23397	-0.87538
H	-5.78448	0.06461	-2.53884
H	-6.55559	-1.25981	-4.53759
H	-5.54138	-3.51415	-4.95084
H	-6.52650	0.74086	0.80472
H	-6.59194	-0.65199	-0.26698
H	-4.04920	1.25234	1.61696
H	-2.99038	1.39029	0.20364
H	-2.94244	-0.29264	-1.00463
H	-3.61770	-1.50442	0.07808

Frequencies

9.1176	15.5424	17.3928
19.7411	24.3779	27.8229
34.7651	37.0335	45.3233
48.1651	49.3359	52.8586
56.2058	61.2102	63.5477
76.9520	83.1419	95.2211
99.8428	112.7645	113.9556
119.5216	123.9681	127.7187
138.3090	138.9388	149.9873
151.3619	159.9325	160.5493
164.1761	172.1497	175.6710
177.9874	181.4243	189.6983
195.7175	200.1422	209.8500
226.4640	230.6306	234.5768
237.7946	242.7026	243.4380
246.9224	252.1086	253.3334
254.6884	260.8098	263.9114
271.0332	279.3431	294.4070
299.0565	300.9577	303.0523
308.0313	311.6222	319.8022
322.7115	329.7750	346.1669
346.7436	353.5593	370.1683
372.8721	381.7027	385.1760
389.7033	396.8674	401.5165
402.4205	405.8589	406.7779
419.9749	425.3645	427.8810
429.0200	437.6238	439.4280
448.6421	469.4752	470.8989
473.4617	483.2891	483.6086
484.5444	486.4924	499.0140
501.8376	502.4287	530.5085
534.3081	540.2375	548.0647
549.4229	553.8422	567.4911
570.4786	572.0901	575.2549
578.3106	579.2053	581.0387
593.6133	594.7784	601.8517
604.8556	606.1410	613.6402
618.8130	623.8004	630.9291
649.1190	653.5087	653.7595
657.8755	658.9507	659.7125
663.0415	668.0158	700.5225
714.0478	716.1776	718.2424
721.6171	723.6593	727.7616
734.8804	738.9134	739.3612
740.4127	743.2601	745.5859
751.4947	754.9705	761.4941
762.8086	764.1457	764.7932
767.9148	767.9970	771.6856

779.0859	780.1029	781.5827
781.7685	786.5591	787.0403
802.0361	803.0748	804.0298
808.8247	816.1273	822.0562
825.4467	826.5182	838.0019
842.6273	845.1647	847.3908
867.9139	869.3097	869.6544
876.7339	888.0437	888.2281
894.4541	896.2873	896.6254
899.2261	910.6372	912.8149
917.4918	918.5849	919.5988
920.1669	932.9775	934.8930
935.9484	936.3499	939.7789
941.1716	941.5279	942.4589
945.4648	956.8942	959.6921
962.0728	965.1641	966.4380
967.5173	970.6429	973.5224
990.2393	994.3465	1003.3706
1003.7253	1006.7476	1008.5407
1010.8049	1011.4633	1014.0945
1014.5703	1014.8533	1015.6197
1018.4333	1019.0937	1020.7166
1039.7461	1044.9754	1045.2620
1066.7884	1074.6555	1076.8574
1077.5261	1104.0049	1105.7441
1107.2238	1108.3929	1112.9734
1116.5930	1120.0193	1121.2361
1135.0605	1142.8976	1146.2921
1147.2431	1153.8643	1158.6929
1166.0327	1166.2915	1176.6879
1178.1336	1178.2586	1178.4817
1179.5595	1179.8230	1184.5217
1188.9315	1189.8916	1190.9272
1191.7022	1191.8989	1229.1601
1229.9086	1230.3776	1231.6552
1233.3365	1236.4115	1242.4714
1244.9218	1248.7619	1249.4137
1253.5740	1254.0765	1254.2081
1259.8403	1260.6249	1271.0849
1271.2789	1276.6181	1277.6539
1277.7146	1277.9074	1289.6149
1290.2578	1298.5634	1298.8847
1299.6821	1300.7860	1302.8370
1313.4470	1315.4357	1317.9741
1318.5748	1320.4154	1325.2098
1326.2716	1337.9449	1338.8966
1340.6194	1341.6734	1345.4521
1345.8092	1348.5597	1353.4221
1364.3388	1365.0938	1376.7438
1377.0809	1378.0469	1385.3934
1389.7778	1393.0083	1398.6966
1400.2612	1410.1663	1412.1022
1412.5134	1414.1153	1415.4650
1417.4026	1427.6908	1451.5824
1451.8229	1471.0196	1471.5450
1472.0578	1474.2889	1474.7226
1474.8307	1475.6962	1478.0845
1478.6245	1483.8049	1484.2283
1484.4212	1488.1625	1491.5076
1494.1180	1495.4805	1496.3089
1499.8568	1501.2192	1501.7084
1501.7250	1501.8695	1504.4497
1521.3970	1521.6532	1522.3628
1522.4690	1534.1270	1534.6997
1534.9882	1605.9973	1606.2333
1627.5359	1629.0736	1630.7936
1637.5366	1638.4860	1639.3315
1648.1547	1648.7825	1649.2408
1674.2528	1676.2397	1676.6253
1677.9346	1679.2587	1679.3519
1769.9829	1773.0637	1773.9624
1819.4402	1821.7131	1823.2228
2982.8979	3016.4482	3016.6698
3017.8050	3054.0567	3057.5385
3057.6580	3057.8708	3058.6388
3068.3424	3069.3149	3070.4586
3071.3835	3074.2049	3077.8346
3078.5776	3078.7851	3079.3063
3080.2406	3100.9257	3103.5256
3103.7148	3103.9281	3115.1213
3120.2546	3122.6750	3123.5821
3124.4770	3125.2666	3140.5320
3172.3631	3173.0914	3173.5296
3180.6383	3181.2569	3182.1228
3184.2416	3185.5935	3190.0389
3198.6304	3199.2515	3199.3033
3199.9017	3200.5013	3200.6275
3201.2162	3202.3784	3205.1866
3208.8425	3219.0022	3222.1796

TS7

E(RB3LYP) = -3723.60259793

E(RB3LYP-D3) = -3723.79214354

H - Sum of electronic and thermal Enthalpies= -3722.440545

G - Sum of electronic and thermal Free Energies= -3722.598300

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.82063	0.95161	1.05491
C	5.75122	1.59292	-0.19570
C	5.71590	0.83636	-1.38422
C	5.79638	-0.56714	-1.31615
C	5.86925	-1.21866	-0.06792
C	5.90757	-0.45454	1.11419
C	5.75753	1.78491	2.33545
C	5.66210	0.93706	3.62295

C	6.69483	-0.20609	3.49655
C	5.96398	-1.12803	2.49457
C	5.86758	-2.74624	0.01382
C	5.66886	-3.44787	-1.35026
C	5.73825	-1.42543	-2.58721
C	5.55551	1.52383	-2.74114
C	5.33221	3.05084	-2.64753
C	5.64483	3.12054	-0.29728
C	6.32607	3.60020	-1.59966
C	6.56130	-2.71735	-2.37863
C	1.65646	3.95458	-1.71138
C	2.75899	3.60783	-2.54925
C	3.99873	3.39128	-1.99784
C	4.19356	3.48314	-0.58857
C	3.16221	3.82891	0.24798
C	1.86870	4.08586	-0.29027
C	2.00018	-2.26910	-3.29443
C	1.93257	-3.45276	-2.47207
C	3.11078	-3.89869	-1.79996
C	4.28295	-3.19232	-1.92625
C	4.33356	-2.00300	-2.71083
C	3.22822	-1.55386	-3.38852
C	2.28017	-1.74079	3.59434
C	2.04486	-0.42712	4.14306
C	3.12666	0.50307	4.19918
C	4.35556	0.15807	3.68957
C	4.55706	-1.11357	3.07700
C	3.55865	-2.05363	3.05209
C	1.22911	-2.70104	3.58171
C	-0.00392	-2.32751	4.04495
C	-0.25679	-1.02266	4.52832
C	0.73974	-0.08208	4.60603
C	0.35982	4.19812	-2.25333
C	-0.65081	4.56908	-1.40307
C	-0.43279	4.72428	-0.01366
C	0.79188	4.48729	0.55244
C	0.69644	-4.15531	-2.35254
C	-0.39845	-3.68483	-3.03270
C	-0.32099	-2.53833	-3.85826
C	0.84279	-1.83004	-3.99993
C	-1.66057	-2.31375	-4.46699
O	-2.01615	-1.45614	-5.25516
N	-2.48247	-3.33301	-3.96318
C	-1.79931	-4.19413	-3.08513
O	-2.28976	-5.15656	-2.52373
C	-2.07101	4.92117	-1.68679
O	-2.66403	4.93481	-2.75036
C	-1.69911	5.20789	0.60412
O	-1.92024	5.52660	1.75749
C	-1.26509	-3.10797	4.13335
O	-1.44993	-4.29120	3.90357
C	-1.70480	-0.93663	4.87805
O	-2.32946	-0.00176	5.33995
N	-2.24502	-2.20593	4.57245
N	-2.62483	5.28891	-0.44888
C	-3.90610	-3.41124	-4.23166
C	-3.98217	5.75859	-0.28519
C	-3.65394	-2.56269	4.75039
C	-5.60015	-3.33946	1.04725
C	-5.02952	-4.41667	1.72299
C	-4.40265	-4.18500	2.94451
C	-4.35509	-2.87336	3.43533
N	-4.91437	-1.83767	2.79228
C	-5.53375	-2.06322	1.61956
C	-6.77148	2.88226	1.14798
C	-7.23410	4.14897	0.80243
C	-6.32245	5.08613	0.32030
C	-4.97894	4.71327	0.20580
N	-4.53178	3.49429	0.53072
C	-5.40941	2.58797	0.99603
C	-6.10007	-0.22868	-2.44045
C	-6.54580	-0.73186	-3.66067
C	-5.83195	-1.76341	-4.27211
C	-4.69657	-2.25872	-3.62465
N	-4.27016	-1.78377	-2.44831
C	-4.94802	-0.78201	-1.86656
C	-4.35980	-0.24302	-0.57237
C	-4.88360	1.20565	1.35432
C	-6.21047	-0.87666	0.93930
N	-5.35846	0.18531	0.40225
H	6.65248	2.42050	2.41179
H	4.90070	2.46719	2.28931
H	5.81479	1.57900	4.49739
H	6.83861	-0.72214	4.45307
H	7.66948	0.13675	3.13129
H	6.82073	-3.09545	0.43838
H	6.04350	3.60910	0.59338
H	6.45348	1.34942	-3.35258
H	4.72035	1.07122	-3.28875
H	7.34086	3.20482	-1.72169
H	6.36854	4.69534	-1.62704
H	5.08495	-3.07778	0.70639
H	5.89182	-4.51548	-1.24752
H	7.57397	-2.52364	-2.00714
H	6.63140	-3.28073	-3.31649
H	2.59825	3.54113	-3.62395
H	3.30759	3.92419	1.32172
H	5.44241	3.49789	-3.64152
H	3.06013	-4.80857	-1.20425
H	3.26351	-0.65878	-4.00549
H	6.05318	-0.85984	-3.46577
H	2.95578	1.47725	4.65418
H	3.71364	-3.03850	2.61744
H	6.40299	-2.12560	2.43558
H	0.54190	0.91344	4.99539
H	1.40371	-3.70199	3.19555
H	0.94820	4.60952	1.62122
H	0.18428	4.09776	-3.32149

H	0.88760	-0.94610	-4.63101
H	0.62867	-5.04196	-1.72715
H	-4.24111	-4.36440	-3.80823
H	-4.06547	-3.44060	-5.31445
H	-4.30478	6.14799	-1.25608
H	-3.96064	6.59035	0.42834
H	-3.70613	-3.42687	5.42119
H	-4.12770	-1.70265	5.22765
H	-6.09083	-3.48084	0.08839
H	-5.06484	-5.41751	1.30069
H	-3.92809	-4.98919	3.49554
H	-7.45135	2.12658	1.53110
H	-8.28500	4.40549	0.91219
H	-6.64173	6.08823	0.04368
H	-6.61516	0.57963	-1.93086
H	-7.42958	-0.31653	-4.13887
H	-6.13973	-2.16524	-5.23388
H	-6.89799	-0.41603	1.65695
H	-6.82612	-1.26638	0.11869
H	-5.21008	0.93776	2.36361
H	-3.78879	1.24544	1.38382
H	-3.75442	0.63650	-0.82504
H	-3.66544	-1.00382	-0.17809

Frequencies

-18.4593	11.1743	15.3979
17.6386	19.8778	23.4776
28.5689	34.7748	37.0442
45.4229	48.5312	51.9223
54.7797	59.7212	65.2575
73.3973	79.7076	96.4544
101.6712	109.7624	111.1120
119.6947	120.9546	126.4700
139.0083	140.3949	150.0371
150.6269	159.4639	160.9332
163.7610	165.8799	171.8249
177.0194	179.3215	186.2695
188.5047	200.6175	210.6696
222.9818	228.8991	233.4381
234.3548	236.5161	242.3175
244.0083	247.5725	249.7037
255.6950	261.1099	266.6805
270.4584	272.8103	284.9061
294.7572	299.1709	301.2862
307.0662	308.4823	315.7527
320.7196	326.9281	346.0630
346.7118	350.0019	369.1366
372.1862	376.8015	385.8361
392.1094	393.3405	400.1885
400.9407	405.7207	406.1499
420.0810	427.8494	427.9208
429.7060	435.0491	440.0133
448.8935	468.8660	470.7724
476.6305	480.0790	483.1577
484.0954	485.3253	499.0222
502.5880	504.3860	528.2285
533.0725	545.4163	547.6160
548.2084	552.0314	567.7917
571.7921	572.8498	576.0686
576.5280	577.3645	579.9941
593.8773	595.7854	604.7767
606.2652	607.2631	610.0577
621.5133	625.5111	636.6976
648.0690	652.5420	653.5585
655.6975	658.8136	659.4290
660.2374	664.2337	700.4062
714.9063	716.1408	717.8888
721.0749	724.0034	725.1509
728.6164	735.2895	739.6169
739.9565	742.9890	744.8015
750.5505	753.6268	757.4894
762.8887	763.8083	763.8708
766.3802	767.2649	769.8592
776.8486	779.0248	780.4001
781.6482	785.5346	785.9322
796.2704	797.8155	802.9251
809.5833	816.6998	822.1073
825.9539	826.2275	836.8853
843.1422	843.1472	853.3494
864.5597	869.5545	869.8594
876.9544	887.9980	888.0998
894.6410	896.2794	896.6137
899.5805	908.1269	911.3659
914.6084	916.5555	919.5597
920.0103	921.9259	934.0451
934.4953	935.5983	935.9526
941.0608	941.3107	942.0277
944.2557	956.6128	958.0071
961.8406	964.1371	965.9216
966.8357	968.6497	969.9224
982.0264	991.4063	999.7348
1000.6875	1005.3721	1008.1598
1009.2835	1009.6275	1011.2929
1012.3729	1015.6585	1015.9899
1016.1358	1022.5572	1030.5944
1040.1089	1045.0303	1045.9763
1067.0334	1074.5479	1076.8894
1077.0840	1099.9901	1107.2416
1107.8387	1109.8581	1117.1680
1117.6268	1120.0488	1126.1562
1135.6141	1144.7979	1149.3749
1152.6434	1154.9264	1156.2777
1166.4425	1166.5800	1176.6440
1178.2014	1178.7449	1179.1503
1179.4145	1179.8064	1185.6805
1189.6818	1190.4785	1191.0517
1192.0864	1193.3530	1227.6239
1228.4802	1230.9719	1231.4532

1232.4021	1236.3102	1244.2744
1244.7001	1248.4627	1249.1174
1253.6596	1254.0413	1254.2471
1260.8924	1264.1799	1272.0612
1273.1322	1275.8005	1277.7814
1278.0099	1278.0592	1289.1232
1289.8628	1298.3360	1298.5976
1299.5250	1300.8362	1301.0256
1314.8443	1315.4584	1318.6940
1318.9403	1320.7793	1324.0151
1325.4342	1338.6824	1339.1168
1341.0053	1345.3111	1345.8823
1346.9304	1354.7658	1364.2890
1368.4338	1372.6599	1373.5440
1377.1127	1377.7972	1386.3642
1393.7439	1400.6387	1403.6838
1405.1589	1411.6586	1412.2349
1413.4496	1413.6024	1415.9763
1417.4829	1421.6952	1451.7690
1451.9878	1468.6970	1470.8261
1472.6834	1474.0843	1474.4663
1475.8049	1476.4994	1477.3222
1479.3008	1482.6342	1483.9514
1484.1572	1484.6527	1488.5224
1490.0314	1492.6033	1493.9370
1495.2210	1496.7989	1500.7424
1501.6763	1502.2656	1510.4961
1517.2454	1521.3606	1521.6197
1522.4593	1534.1391	1534.4360
1535.3735	1606.0218	1606.7726
1628.8643	1629.7503	1631.5966
1636.5993	1638.1666	1639.1230
1648.6276	1648.9881	1649.1577
1675.7128	1675.8159	1676.4130
1678.7063	1679.1037	1679.5735
1769.5838	1772.9116	1774.5228
1820.2952	1821.3986	1823.7437
2988.8638	3016.1527	3016.2230
3016.4051	3044.4897	3057.4522
3057.5534	3057.7057	3059.5701
3066.1633	3070.4018	3071.0831
3072.8582	3073.6097	3074.6293
3076.7930	3078.7810	3079.0071
3079.0739	3090.0824	3103.3528
3103.4696	3103.7635	3114.3854
3114.4425	3115.7910	3122.0750
3123.7843	3124.1143	3151.2726
3172.3836	3172.7951	3173.1045
3178.9891	3181.6178	3182.0957
3182.1637	3184.0249	3191.8478
3192.8754	3199.3369	3199.4239
3200.0718	3200.0780	3200.6352
3200.7190	3201.3265	3206.3645
3207.4806	3217.2409	3232.1506

I7

E(RB3LYP) = -3723.60383617

E(RB3LYP-D3) = -3723.79284547

H - Sum of electronic and thermal Enthalpies= -3722.440889

G - Sum of electronic and thermal Free Energies= -3722.601234

Number of imaginary frequencies: 0

Cartesian Coordinates

C	-5.97478	-0.74162	0.79590
C	-5.88278	-1.28282	-0.49940
C	-5.71338	-0.43979	-1.61581
C	-5.70506	0.95600	-1.43426
C	-5.81979	1.50935	-0.14207
C	-5.96465	0.65752	0.96966
C	-6.04187	-1.67868	2.00234
C	-5.92273	-0.94979	3.35852
C	-6.85577	0.28094	3.30088
C	-6.02153	1.21821	2.39963
C	-5.76257	3.02405	0.06500
C	-5.46730	3.82571	-1.22406
C	-5.51831	1.90959	-2.62181
C	-5.50944	-1.02997	-3.01286
C	-5.42177	-2.57477	-3.03737
C	-5.89449	-2.80008	-0.72425
C	-6.52548	-3.11420	-2.10031
C	-6.31254	3.21122	-2.36210
C	-1.90440	-3.87200	-1.96183
C	-2.91999	-3.37930	-2.83595
C	-4.16835	-3.08604	-2.34171
C	-4.46136	-3.26039	-0.95756
C	-3.51493	-3.74042	-0.08807
C	-2.21234	-4.06060	-0.56497
C	-1.71786	2.68577	-3.02802
C	-1.67443	3.80554	-2.11888
C	-2.87926	4.23153	-1.48380
C	-4.05725	3.57007	-1.73317
C	-4.08953	2.44283	-2.60511
C	-2.95406	2.01038	-3.24393
C	-2.32859	1.42256	3.61754
C	-2.21837	0.05259	4.05747
C	-3.37648	-0.78159	4.01878
C	-4.55972	-0.29085	3.52062
C	-4.63817	1.03902	3.01239
C	-3.56282	1.88785	3.08152
C	-1.20039	2.28667	3.70653
C	-0.01559	1.77149	4.16016
C	0.11489	0.41370	4.53297
C	-0.95859	-0.44134	4.51111
C	-0.60061	-4.19436	-2.44274
C	0.32957	-4.67344	-1.55524
C	0.02234	-4.85863	-0.18662

C	-1.21673	-4.56805	0.31853
C	-0.43681	4.47487	-1.88524
C	0.68319	4.03948	-2.54646
C	0.63298	2.95842	-3.45811
C	-0.53120	2.27914	-3.70514
C	1.99422	2.77628	-4.03459
O	2.37548	1.98700	-4.87981
N	2.79876	3.74976	-3.42234
C	2.08494	4.54434	-2.50761
O	2.55533	5.46108	-1.85897
C	1.74091	-5.10470	-1.76839
O	2.39172	-5.13621	-2.79760
C	1.22622	-5.41269	0.49184
O	1.36456	-5.75104	1.65216
C	1.29857	2.43609	4.35970
O	1.57762	3.61879	4.25902
C	1.53771	0.17925	4.91536
O	2.06761	-0.83760	5.31796
N	2.19046	1.42060	4.73460
N	2.20787	-5.51565	-0.50971
C	4.22098	3.88374	-3.66741
C	3.54883	-6.01917	-0.26963
C	3.60252	1.64682	5.05138
C	5.93037	2.94506	1.73489
C	5.34509	3.91752	2.54350
C	4.58628	3.50899	3.63628
C	4.42471	2.13611	3.86712
N	4.99395	1.19864	3.09418
C	5.74253	1.59334	2.04853
C	6.59116	-3.05166	-0.35357
C	6.82043	-4.24633	-1.02812
C	5.82091	-5.22023	-1.03256
C	4.63325	-4.95601	-0.34701
N	4.40677	-3.80275	0.30026
C	5.36371	-2.86343	0.30000
C	6.52412	0.61648	-2.19920
C	7.00305	1.32385	-3.30059
C	6.25148	2.38438	-3.80411
C	5.04638	2.70405	-3.16945
N	4.58992	2.03569	-2.10528
C	5.30446	1.00202	-1.63040
C	4.67135	0.23654	-0.47911
C	5.09420	-1.58986	1.09614
C	6.44329	0.51669	1.22466
N	5.62297	-0.39704	0.42902
H	-6.99317	-2.23186	1.99388
H	-5.24934	-2.43193	1.92886
H	-6.15504	-1.64590	4.17185
H	-6.98980	0.72767	4.29306
H	-7.84203	0.04997	2.88267
H	-6.72364	3.37421	0.47055
H	-6.38967	-3.32147	0.09670
H	-6.34212	-0.72988	-3.66623
H	-4.60155	-0.60964	-3.46268
H	-7.49348	-2.62227	-2.24858
H	-6.65705	-4.19577	-2.22185
H	-5.00576	3.26862	0.81976
H	-5.66588	4.88842	-1.04727
H	-7.35311	3.02524	-2.07297
H	-6.30265	3.84994	-3.25310
H	-2.68723	-3.25814	-3.89254
H	-3.73397	-3.89086	0.96652
H	-5.50409	-2.92829	-4.07091
H	-2.84450	5.09445	-0.82088
H	-2.97287	1.16271	-3.92548
H	-5.78759	1.43052	-3.56451
H	-3.29915	-1.80129	4.39230
H	-3.62242	2.91349	2.72438
H	-6.37728	2.24979	2.41370
H	-0.85522	-1.47882	4.81892
H	-1.28098	3.32843	3.40698
H	-1.44211	-4.71837	1.37122
H	-0.35552	-4.06078	-3.49344
H	-0.55673	1.44664	-4.40369
H	-0.38929	5.31381	-1.19551
H	4.52925	4.80163	-3.15462
H	4.38760	4.01999	-4.74133
H	3.75946	-6.81647	-0.98938
H	3.52880	-6.45248	0.73598
H	3.65878	2.37377	5.86957
H	3.99035	0.68631	5.39638
H	6.52799	3.22484	0.87173
H	5.47310	4.97402	2.32276
H	4.09839	4.22930	4.28296
H	7.33508	-2.26242	-0.33062
H	7.75887	-4.41712	-1.55019
H	5.95221	-6.15702	-1.56675
H	7.06492	-0.22690	-1.78363
H	7.94244	1.04307	-3.77071
H	6.58393	2.94467	-4.67413
H	7.05008	-0.09513	1.90135
H	7.14109	1.02569	0.54651
H	5.57471	-1.68527	2.07638
H	4.01647	-1.52545	1.29909
H	4.05772	-0.56141	-0.91750
H	3.97319	0.91715	0.03521

Frequencies

13.1521	15.4202	16.6721
19.3356	19.9112	26.9879
34.2833	34.9802	38.8263
45.1576	47.4745	50.3692
55.2302	59.9886	64.2315
78.3816	84.9790	97.1592
100.7751	110.5237	115.9285
119.7899	123.4903	128.7071
138.9367	139.1566	149.6462
150.4162	160.2014	161.0989

167.5955	171.3516	173.9570	966.4988	969.6672	969.8128
179.2087	180.3366	183.1378	985.5493	990.9435	1001.6787
187.6241	201.9433	207.6220	1003.9809	1005.1058	1008.5648
221.8598	227.2469	230.2239	1010.0387	1010.4693	1011.0455
234.6837	236.3718	240.8082	1012.8041	1015.5807	1015.6670
243.1301	246.5110	247.6352	1016.1976	1021.1891	1024.7385
257.2285	261.3887	264.7773	1039.9421	1044.5155	1046.0856
268.9941	271.7259	287.4356	1067.0058	1074.4544	1076.7784
292.8636	297.6761	300.6008	1077.3655	1100.7418	1107.2227
305.2616	308.3676	319.1237	1107.8170	1110.0425	1112.3627
326.3217	328.5136	345.7119	1117.1156	1120.6805	1128.7213
346.9790	350.3121	367.4559	1137.2661	1148.1435	1150.1861
371.6932	372.1305	385.6620	1153.3821	1154.8900	1166.2970
391.8549	393.6881	398.8870	1166.5050	1168.0329	1176.4723
400.6071	404.5324	406.0259	1177.8482	1178.5165	1178.8566
419.9865	428.1147	428.9905	1179.0560	1179.6536	1185.2551
433.8768	435.8229	439.6191	1187.6256	1189.6937	1191.1462
453.1315	465.3587	471.1932	1191.6643	1193.6019	1227.1926
475.8110	482.3574	483.9416	1230.1460	1230.8269	1231.5312
484.6319	491.1083	498.9619	1234.8367	1236.6222	1244.4206
502.6606	505.8464	527.5730	1245.5886	1248.2469	1249.4028
532.6112	538.6761	547.5924	1253.6716	1253.9970	1254.2920
548.4795	549.1363	567.8810	1260.6800	1266.4423	1271.1872
571.6758	574.2291	575.8050	1272.3408	1274.0736	1277.5549
576.6126	576.9725	579.5523	1277.7649	1278.6097	1288.5663
594.1291	594.9583	604.7340	1290.1287	1294.8674	1298.1526
606.5499	607.8001	609.9988	1298.7085	1299.3061	1301.1086
620.9162	625.3159	631.1589	1311.9422	1314.8566	1318.6853
650.9492	653.1116	653.3301	1319.3331	1320.6069	1321.2711
657.9524	659.0369	660.1303	1325.5323	1338.6965	1338.9070
663.0287	667.6412	701.5853	1340.9185	1342.7514	1345.6294
713.8137	715.5118	717.4591	1345.8167	1352.2943	1358.6778
720.5993	724.1495	725.6217	1364.5120	1370.3058	1373.2441
729.1504	736.0243	739.8749	1376.9073	1377.6117	1380.8596
740.2010	741.6565	743.8951	1396.3934	1397.4313	1400.4359
747.8696	752.6875	755.5650	1409.2279	1412.0226	1412.5158
762.7513	763.7245	764.0582	1412.9966	1413.9626	1417.3681
767.1930	768.5848	769.7949	1419.8041	1423.4303	1451.8998
774.3900	778.8025	780.2263	1452.3061	1470.2922	1471.2441
781.8093	783.1395	785.7878	1472.5688	1474.0795	1474.6401
793.6552	803.0109	805.4880	1475.3601	1476.1901	1476.7043
813.5167	815.4458	821.2458	1479.6340	1483.8066	1483.8803
825.2506	828.2396	836.1779	1484.4263	1485.6359	1487.6600
840.4374	843.6992	855.3012	1490.2556	1491.9689	1494.9359
866.6939	869.1981	869.7715	1495.7692	1499.0369	1501.0169
876.6193	887.5693	888.1450	1501.5443	1502.0336	1507.9501
894.3856	895.7681	896.4794	1513.3930	1521.2016	1521.5676
899.4124	909.7734	912.2038	1522.3726	1534.1042	1534.7467
913.0072	915.5697	919.2518	1535.2350	1606.2339	1606.9596
920.1335	931.9979	934.0200	1629.1084	1629.5209	1631.6391
934.3103	935.4354	935.7549	1637.0732	1637.9295	1639.6972
940.6840	940.9703	942.1866	1648.7513	1648.8669	1649.3570
948.1901	956.6258	960.2738	1675.4000	1675.5592	1676.8703
962.1798	964.2075	966.0381	1678.2289	1679.0053	1679.8191

1769.7932	1773.3372	1773.9781
1820.8267	1821.3820	1823.5168
2996.5581	3015.2806	3016.1958
3017.0301	3034.9231	3038.7839
3057.4217	3057.5513	3057.7326
3059.8871	3067.4221	3067.6852
3068.8463	3072.4883	3072.7829
3077.6713	3078.7459	3079.1528
3080.9084	3084.3531	3092.6578
3103.4038	3103.5373	3103.7823
3110.0827	3118.7693	3123.1565
3124.5846	3125.1675	3149.1708
3172.2162	3172.7990	3172.9992
3180.9629	3182.1552	3183.3523
3183.4271	3184.4875	3190.5722
3199.3662	3199.4427	3199.6866
3200.2163	3200.6841	3200.9252
3201.4306	3203.6208	3206.1046
3219.9508	3226.2895	3233.8891

TS8

E(RB3LYP) = -3723.60140460

E(RB3LYP-D3) = -3723.78880059

H - Sum of electronic and thermal Enthalpies= -3722.439460

G - Sum of electronic and thermal Free Energies= -3722.597141

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.87117	-1.19152	-0.60842
C	5.89053	-0.98539	0.78309
C	5.80847	0.31802	1.31321
C	5.77925	1.42046	0.43885
C	5.75531	1.22530	-0.95758
C	5.79918	-0.08247	-1.47631
C	5.91246	-2.61677	-1.16259
C	5.69542	-2.70123	-2.69015
C	6.54271	-1.59076	-3.34957
C	5.70019	-0.34659	-2.98515
C	5.67795	2.42003	-1.91106
C	5.56077	3.79012	-1.20182
C	5.73457	2.85752	0.97283
C	5.72917	0.54038	2.82518
C	5.63875	-0.76623	3.64922
C	5.92356	-2.16909	1.75814
C	6.66183	-1.75826	3.05260
C	6.52001	3.77907	0.00921
C	2.03513	-2.25771	3.62331
C	3.12308	-1.43966	4.05377
C	4.33121	-1.50477	3.40187
C	4.51097	-2.37865	2.29007
C	3.49254	-3.18751	1.85282
C	2.22830	-3.15126	2.50699
C	2.01937	4.00706	1.24792
C	1.90223	4.53219	-0.09113
C	3.03633	4.48815	-0.95541
C	4.21685	3.94545	-0.50970
C	4.32373	3.41133	0.80732
C	3.25721	3.44202	1.67067
C	1.92913	-0.91954	-3.80267
C	1.91202	-2.33808	-3.53663
C	3.12706	-2.99124	-3.17438
C	4.28796	-2.26573	-3.06253
C	4.29300	-0.85738	-3.28193
C	3.14826	-0.19645	-3.65349
C	0.73205	-0.26511	-4.21614
C	-0.41726	-1.00392	-4.32528
C	-0.44301	-2.38691	-4.02809
C	0.68886	-3.06222	-3.64942
C	0.76831	-2.21568	4.27805
C	-0.23785	-3.02837	3.82035
C	-0.04295	-3.90593	2.72764
C	1.15721	-3.98443	2.07269
C	0.66305	5.09053	-0.52334
C	-0.39160	5.11040	0.35288
C	-0.27062	4.60553	1.66907
C	0.90043	4.06276	2.12850
C	-1.58031	4.78271	2.35374
O	-1.89866	4.50022	3.49531
N	-2.42750	5.37767	1.40732
C	-1.78537	5.61039	0.17646
O	-2.29587	6.13556	-0.79486
C	-1.63863	-3.20164	4.30137
O	-2.21184	-2.65334	5.22542
C	-1.30948	-4.65453	2.49885
O	-1.55190	-5.52199	1.68063
C	-1.77777	-0.60431	-4.78026
O	-2.15939	0.47004	-5.21002
C	-1.83056	-2.88074	-4.24981
O	-2.27144	-4.00920	-4.14378
N	-2.57513	-1.75362	-4.65817
N	-2.20671	-4.18163	3.47145
C	-3.84142	5.61618	1.64582
C	-3.58420	-4.61863	3.56767
C	-3.95676	-1.84318	-5.11910
C	-6.72203	0.82492	-3.30571
C	-6.42207	1.00688	-4.65470
C	-5.49805	0.15482	-5.25169
C	-4.90770	-0.84897	-4.47401
N	-5.18746	-1.02017	-3.17432
C	-6.07958	-0.19768	-2.59427
C	-6.39297	-1.89493	1.89199
C	-6.81040	-2.72529	2.93290
C	-5.89688	-3.60543	3.50552
C	-4.59196	-3.62794	2.99795
N	-4.19056	-2.83844	1.99850
C	-5.06700	-1.97638	1.45357

C	-6.04251	1.97999	1.88251
C	-6.27126	2.95001	2.85800
C	-5.56013	4.14800	2.80597
C	-4.63980	4.32612	1.76822
N	-4.41892	3.39800	0.83062
C	-5.10504	2.24517	0.87911
C	-4.81026	1.27894	-0.26522
C	-4.50345	-1.11440	0.32737
C	-6.40884	-0.42605	-1.12298
N	-5.38919	-0.05210	-0.13873
H	6.88702	-3.07165	-0.92895
H	5.15896	-3.23531	-0.66183
H	5.93509	-3.71106	-3.04058
H	6.58638	-1.71835	-4.43764
H	7.56557	-1.54207	-2.95934
H	6.57993	2.44050	-2.54056
H	6.34969	-3.05964	1.29340
H	6.61802	1.09184	3.16610
H	4.86658	1.17612	3.05972
H	7.63993	-1.30285	2.86036
H	6.80006	-2.62813	3.70539
H	4.83022	2.29840	-2.59682
H	5.76152	4.59204	-1.92057
H	7.51616	3.39187	-0.23293
H	6.62594	4.78202	0.43911
H	2.97612	-0.78073	4.90785
H	3.62391	-3.86477	1.01200
H	5.80294	-0.54147	4.70870
H	2.94786	4.90419	-1.95757
H	3.33248	3.04887	2.68219
H	6.09831	2.91160	2.00024
H	3.11263	-4.06612	-3.00220
H	3.14518	0.87562	-3.83829
H	5.97190	0.53487	-3.56758
H	0.66115	-4.12852	-3.43978
H	0.73845	0.79822	-4.44186
H	1.29515	-4.66355	1.23524
H	0.60912	-1.54787	5.12099
H	0.97907	3.67468	3.14085
H	0.56156	5.48483	-1.53132
H	-4.19765	6.20125	0.79184
H	-3.95344	6.21624	2.55409
H	-3.81564	-4.81817	4.61855
H	-3.64478	-5.56257	3.01448
H	-3.97384	-1.70882	-6.20703
H	-4.27698	-2.86339	-4.89051
H	-7.44483	1.46417	-2.80551
H	-6.89595	1.80001	-5.22729
H	-5.22217	0.26969	-6.29522
H	-7.07461	-1.18770	1.43422
H	-7.83317	-2.67703	3.29904
H	-6.18047	-4.25282	4.33109
H	-6.55809	1.02735	1.89441
H	-6.98440	2.76821	3.65841
H	-5.69377	4.91512	3.56337
H	-6.62861	-1.48925	-0.98382
H	-7.33633	0.12292	-0.90085
H	-4.19684	-1.78221	-0.49340
H	-3.58183	-0.66104	0.70707
H	-3.71912	1.23036	-0.38620
H	-5.17050	1.75661	-1.18526

Frequencies

-25.3991	12.5348	17.7368
18.7308	23.6983	25.9522
29.4082	35.7043	41.8989
44.6356	45.8834	46.3351
50.5206	57.0375	60.3689
63.9124	89.8297	97.4578
100.7141	113.0935	115.9814
118.5129	120.0221	133.4731
138.1679	138.5830	148.9479
150.5744	157.0045	159.2271
161.2387	164.1906	174.4835
179.2511	180.1379	181.6702
185.3292	194.2852	201.6834
210.2685	225.4935	226.4213
229.3313	236.4456	237.9030
242.9518	246.8815	249.4058
255.6440	260.6963	262.5845
270.2956	271.5615	285.9032
290.5655	299.2921	300.7455
307.6685	311.1982	319.3693
327.1344	329.5609	341.4873
346.5430	348.8864	357.8087
370.8257	372.4244	384.5641
387.3269	395.8254	400.3854
401.1956	404.7925	406.1289
419.7664	427.7544	428.3925
431.5779	436.6701	437.5410
458.0686	465.2770	470.6811
479.6558	483.2785	484.2816
485.2043	491.7387	500.0858
502.1078	505.3617	529.8048
531.5487	533.9592	539.9346
548.0227	550.3088	568.5103
571.2588	573.7702	575.5347
576.7593	577.7510	578.8950
594.0546	595.4325	603.8617
606.9234	607.4519	610.4060
622.5588	623.7511	631.0716
645.2584	649.7939	652.6508
654.8894	658.1598	660.3269
661.1910	662.5015	699.7188
713.9090	715.0381	717.3574
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729.4247	734.6201	738.8166
740.9041	741.8888	742.5951

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762.6552	763.9679	764.6168
766.9591	768.0746	768.6824
771.4849	779.0250	779.6596
783.0113	784.4034	784.8328
794.6474	803.6509	805.2762
806.4322	814.1965	822.3261
825.7836	827.1034	835.0538
840.4801	842.2570	848.9864
861.6373	869.1129	869.8287
876.6818	887.7259	888.5113
894.6539	896.4638	896.6012
899.7727	905.2300	910.3692
911.8886	914.9827	919.4639
920.3698	930.6713	934.6838
935.8609	936.1085	940.7396
941.1656	941.8240	944.1831
952.7542	954.2790	960.3056
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987.7376	989.8692	994.2977
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1007.5129	1010.6111	1013.3277
1013.7891	1015.0715	1016.1877
1016.7442	1018.7283	1025.6705
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1078.1865	1104.7723	1107.5086
1107.8382	1111.0987	1114.4325
1116.8495	1120.3597	1129.1074
1141.6859	1146.5844	1150.8752
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1178.0576	1178.1862	1178.9278
1179.5441	1179.8724	1183.6031
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1229.4342	1230.5828	1231.7522
1233.7153	1237.1375	1239.6643
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1253.8824	1254.2141	1254.2941
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1278.2127	1278.3041	1289.4316
1290.6923	1298.8401	1299.9824
1301.2239	1301.6637	1312.2360
1315.0681	1316.3697	1318.7231
1319.3641	1321.4994	1325.9225
1335.6775	1338.9474	1339.5622
1341.0800	1344.3746	1345.4431
1346.1105	1350.7483	1361.1257
1365.1794	1376.9554	1377.3740
1379.6020	1382.0835	1383.1577
1392.5718	1397.1078	1400.7330
1405.4726	1410.8570	1412.5296
1412.9822	1413.7779	1416.9728
1421.3159	1425.5026	1452.0596
1452.7810	1468.8792	1470.4637
1472.9681	1474.1880	1474.2567
1474.6169	1475.3265	1475.9300
1477.4839	1480.0171	1482.8924
1483.9970	1484.6372	1485.4922
1489.3002	1491.0494	1493.7248
1497.8609	1499.6912	1501.1597
1502.1594	1502.6219	1503.6105
1511.6702	1521.2010	1521.3553
1522.1385	1534.3746	1534.5742
1535.0670	1606.7273	1607.2261
1628.8403	1629.4475	1632.5379
1637.3930	1637.6623	1640.6211
1648.9042	1649.1123	1649.7457
1674.8135	1676.5885	1676.9117
1677.8388	1679.4176	1679.4852
1770.7645	1773.6888	1774.8094
1820.7610	1821.8566	1823.8108
3005.5884	3010.5243	3014.4860
3016.7158	3016.9865	3029.1775
3057.1330	3057.4631	3057.6764
3062.1418	3063.6092	3067.9203
3068.0428	3071.2685	3076.1974
3077.0460	3079.0619	3079.1740
3079.7898	3094.1770	3099.7641
3103.1677	3103.3165	3103.9518
3116.8178	3123.2609	3124.6203
3125.2329	3127.6010	3129.6682
3172.7972	3172.8475	3172.8853
3180.6883	3180.9063	3182.8068
3183.2424	3186.4152	3186.4302
3199.2816	3199.5469	3200.1702
3200.3423	3200.8053	3200.9134
3200.9653	3201.4288	3205.3712
3215.6784	3231.1870	3242.5042

I8

E(RB3LYP) = -3723.60197479

E(RB3LYP-D3) = -3723.79038867

H - Sum of electronic and thermal Enthalpies= -3722.439017

G - Sum of electronic and thermal Free Energies= -3722.598818

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.92770	-1.37447	-0.19445
C	5.93358	-0.78022	1.08070
C	5.86848	0.62101	1.21624
C	5.86615	1.42846	0.06353
C	5.83912	0.84316	-1.21923

C	5.87030	-0.55871	-1.34320
C	5.96489	-2.89875	-0.31863
C	5.74881	-3.41446	-1.75876
C	6.60189	-2.54372	-2.70722
C	5.76752	-1.24208	-2.71405
C	5.76413	1.71706	-2.47341
C	5.65476	3.23262	-2.18222
C	5.84280	2.95876	0.16683
C	5.76921	1.26600	2.60051
C	5.61528	0.24971	3.75742
C	5.91353	-1.63755	2.35231
C	6.62533	-0.89102	3.50280
C	6.62474	3.56013	-1.02499
C	1.96428	-1.10366	4.00439
C	3.06614	-0.22546	4.23559
C	4.29292	-0.50066	3.67973
C	4.47921	-1.65699	2.86714
C	3.44685	-2.52831	2.62746
C	2.16278	-2.27687	3.18831
C	2.13595	4.16118	0.13068
C	2.00493	4.27329	-1.30199
C	3.13177	3.97977	-2.12654
C	4.31667	3.58626	-1.55335
C	4.43482	3.45554	-0.13899
C	3.37770	3.74133	0.68797
C	1.98816	-1.99732	-3.32181
C	1.96311	-3.27835	-2.65713
C	3.17672	-3.81078	-2.13033
C	4.34325	-3.09400	-2.23851
C	4.35616	-1.80734	-2.85169
C	3.21328	-1.27214	-3.39295
C	0.79256	-1.48047	-3.90118
C	-0.36297	-2.20841	-3.78397
C	-0.39662	-3.44403	-3.09623
C	0.73372	-3.99193	-2.54617
C	0.67899	-0.85209	4.57105
C	-0.33901	-1.73642	4.31677
C	-0.13914	-2.88474	3.51455
C	1.07772	-3.17000	2.95524
C	0.75891	4.67873	-1.86557
C	-0.28856	4.94881	-1.02243
C	-0.15241	4.85076	0.38241
C	1.02568	4.46993	0.96828
C	-1.45541	5.21776	0.99996
O	-1.75492	5.29633	2.17872
N	-2.32145	5.48860	-0.06918
C	-1.68719	5.37180	-1.32218
O	-2.20561	5.60214	-2.39774
C	-1.75401	-1.75039	4.78939
O	-2.33136	-0.96851	5.52285
C	-1.41682	-3.64628	3.46283
O	-1.65835	-4.70447	2.91233
C	-1.72252	-1.94959	-4.33427
O	-2.09317	-1.05019	-5.06797
C	-1.78889	-3.96871	-3.15869
O	-2.23540	-5.01568	-2.73089
N	-2.53033	-3.00118	-3.87169
N	-2.32683	-2.90834	4.23821
C	-3.72972	5.81847	0.11003
C	-3.69451	-3.32312	4.46806
C	-3.90746	-3.23224	-4.30171
C	-6.73219	-0.14769	-3.56247
C	-6.30725	-0.34792	-4.87364
C	-5.35665	-1.33371	-5.12147
C	-4.86712	-2.08246	-4.04506
N	-5.26417	-1.88156	-2.77916
C	-6.18098	-0.92759	-2.53532
C	-6.63974	-1.23820	2.21271
C	-7.01940	-1.85063	3.40776
C	-6.05682	-2.51219	4.16298
C	-4.74233	-2.54827	3.67897
N	-4.37556	-1.96991	2.53291
C	-5.30211	-1.31399	1.81037
C	-5.98658	2.47855	1.47597
C	-5.91610	3.60069	2.29946
C	-5.18333	4.70951	1.87672
C	-4.54064	4.64481	0.63712
N	-4.59666	3.56369	-0.15186
C	-5.30915	2.50042	0.25061
C	-5.38724	1.36129	-0.75747
C	-4.78670	-0.64762	0.53885
C	-6.65312	-0.73428	-1.09791
N	-5.81489	0.08110	-0.20481
H	6.93780	-3.26976	0.03815
H	5.20888	-3.34780	0.33515
H	5.98200	-4.48375	-1.80612
H	6.64358	-2.97719	-3.71344
H	7.62549	-2.39184	-2.34657
H	6.66341	1.55395	-3.08571
H	6.32706	-2.63142	2.17440
H	6.67022	1.86622	2.79704
H	4.92534	1.96599	2.62037
H	7.62141	-0.52808	3.22502
H	6.71952	-1.54275	4.37934
H	4.91302	1.40877	-3.09333
H	5.85199	3.79630	-3.10056
H	7.61635	3.11187	-1.15388
H	6.74050	4.64309	-0.89954
H	2.91386	0.65041	4.86403
H	3.58129	-3.41628	2.01409
H	5.75539	0.76268	4.71513
H	3.03368	4.08748	-3.20544
H	3.46239	3.65977	1.76933
H	6.21833	3.29760	1.13396
H	3.15641	-4.79050	-1.65598
H	3.21565	-0.29812	-3.87751
H	6.04370	-0.56558	-3.52403
H	0.70003	-4.95163	-2.03668

H	0.80492	-0.52931	-4.42728
H	1.21952	-4.05854	2.34540
H	0.51669	0.02495	5.19265
H	1.11590	4.39508	2.04895
H	0.64632	4.76237	-2.94360
H	-4.09790	6.11684	-0.87551
H	-3.80670	6.66926	0.79411
H	-3.90849	-3.23804	5.53847
H	-3.74100	-4.38248	4.19133
H	-3.90373	-3.46689	-5.37297
H	-4.24031	-4.11776	-3.75425
H	-7.48859	0.59832	-3.33356
H	-6.71102	0.25035	-5.68634
H	-4.98813	-1.51745	-6.12557
H	-7.35590	-0.69749	1.60473
H	-8.05094	-1.80171	3.74838
H	-6.31028	-2.98591	5.10787
H	-6.54297	1.59543	1.76679
H	-6.41839	3.60787	3.26365
H	-5.08606	5.59207	2.50164
H	-6.76551	-1.72072	-0.63828
H	-7.65142	-0.27527	-1.13366
H	-4.28276	-1.40868	-0.07728
H	-4.00831	0.06273	0.84084
H	-4.42091	1.30716	-1.28528
H	-6.11840	1.66470	-1.51684

Frequencies

13.9845	17.6364	19.3164
20.9302	25.2056	26.3411
36.2120	41.1683	43.8452
44.5523	45.9792	49.9231
53.6232	56.6059	61.0291
70.5521	95.7662	97.2302
102.5692	112.7540	115.9797
119.3253	120.0936	134.6058
137.8965	138.4603	149.0495
150.4236	159.1677	161.6367
166.3691	169.6234	176.0194
182.0157	182.9922	184.2018
185.4525	197.9000	200.3075
211.1098	223.1906	226.0276
229.3808	237.1046	238.5475
242.1603	245.3749	246.3966
256.3204	260.6354	262.7404
269.3034	270.8354	284.3020
287.3054	298.1793	298.7767
305.8112	306.2574	318.7324
321.7591	327.1635	340.4488
347.1713	349.0477	370.3503
371.7411	376.4634	386.0025
391.5852	395.8153	400.2391
402.2262	405.4029	406.9629
419.8276	424.9004	427.9722
429.1318	436.7472	437.5919
448.8865	461.0855	469.8231
477.2939	483.3360	483.6649
484.7518	486.8902	499.0506
502.2132	504.8089	530.3988
532.6619	538.9144	542.1942
548.0158	550.7853	568.1258
571.7657	573.9049	575.1863
576.6899	577.7940	579.0456
593.5343	595.5336	601.9817
606.9557	608.0387	609.2333
622.4103	628.3848	633.3421
649.1044	650.8074	652.4331
655.5455	659.1171	660.6050
661.1356	664.6184	702.6506
714.5095	715.1402	718.0186
720.6763	723.5373	727.4787
731.1326	735.4706	740.5086
741.3333	741.8312	742.9151
746.9923	750.2630	756.0175
762.6651	763.8615	764.8989
767.8647	768.2936	770.2684
774.4904	779.2327	779.9644
782.9384	783.6919	784.7728
793.7268	804.4237	806.3202
813.8039	817.3952	822.0563
826.8318	828.5466	838.1962
840.3789	842.4918	853.9490
863.6976	869.2910	869.8254
876.8143	887.8577	888.2947
894.8835	896.3132	896.8793
899.9342	909.9424	912.2557
916.3011	918.4863	919.7406
921.0250	929.7765	934.8129
935.8005	936.1624	940.7731
941.0722	941.5421	942.9902
948.3892	953.6099	960.0525
961.1260	964.3507	966.0702
966.3332	969.3434	971.0796
988.9753	990.2837	996.7493
1005.6007	1006.3902	1009.1637
1010.4765	1010.5695	1012.8229
1013.1263	1014.8106	1015.4347
1017.0515	1018.9075	1027.5481
1039.8627	1044.3780	1045.6602
1067.0650	1074.5802	1076.8903
1077.9909	1103.4577	1107.2164
1107.8244	1110.3403	1115.1606
1118.1326	1120.5583	1128.7671
1139.9995	1143.4336	1152.0831
1155.3484	1155.8039	1166.5301
1167.0016	1171.5981	1176.9809
1177.3540	1177.5833	1178.7077
1179.6045	1179.8517	1185.2749

1187.5728	1189.7751	1190.9495
1191.4387	1193.4204	1225.5416
1229.1758	1231.0719	1231.1505
1236.7663	1240.0883	1241.1490
1244.4399	1248.1810	1249.6855
1253.8361	1254.1420	1254.2436
1260.2866	1260.7989	1268.4947
1274.9557	1276.3576	1277.7856
1278.3169	1278.4794	1288.8912
1290.3528	1298.2352	1298.9743
1300.4728	1301.5462	1303.8353
1313.8342	1314.8817	1318.7439
1319.4979	1321.4740	1322.1522
1326.0207	1338.7225	1339.4061
1341.0823	1342.2806	1345.3677
1346.3486	1351.9584	1363.0244
1364.9793	1374.5753	1376.7909
1377.3899	1379.1965	1383.3401
1388.0073	1400.7743	1401.3773
1404.4378	1408.3563	1412.4225
1413.1858	1413.6429	1418.4282
1421.1722	1425.9477	1452.0418
1452.7120	1469.2892	1472.2626
1472.9510	1474.0764	1474.2328
1475.0527	1475.6257	1475.9786
1476.8608	1480.3206	1483.8978
1484.5246	1484.7100	1487.4027
1489.7820	1491.4860	1493.9046
1497.2409	1500.8816	1502.0746
1502.8624	1503.4756	1505.0405
1509.8859	1521.3034	1521.3974
1522.1930	1534.2167	1534.6641
1535.1805	1606.5259	1607.1861
1628.9813	1629.5503	1633.2469
1636.6576	1637.8368	1640.0019
1648.6762	1648.9834	1649.7999
1674.8992	1676.3077	1676.8855
1677.7987	1679.4226	1679.6351
1770.4023	1773.2947	1775.0372
1820.8790	1821.5124	1823.9364
2995.2654	3012.9795	3013.9048
3015.9502	3017.2790	3023.4329
3057.0890	3057.4217	3057.7881
3058.8733	3064.1926	3067.8757
3069.6681	3071.6444	3077.4774
3079.1403	3079.2670	3080.5700
3080.7265	3082.9442	3103.0689
3103.2363	3104.0853	3109.0715
3112.0501	3122.5386	3126.2986
3129.3563	3131.7603	3133.3638
3172.3878	3172.6676	3172.8633
3180.6287	3181.8549	3182.1609
3182.5096	3186.3081	3189.7472
3198.8630	3199.2444	3199.6379
3200.1573	3200.9209	3201.1949
3201.3178	3201.4225	3211.7090
3217.8314	3228.9013	3239.3982

TS9

E(RB3LYP) = -3723.60003780

E(RB3LYP-D3) = -3723.78665395

H - Sum of electronic and thermal Enthalpies= -3722.438209

G - Sum of electronic and thermal Free Energies= -3722.596243

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.81776	-1.29385	-0.08864
C	5.82505	-0.64918	1.16182
C	5.78314	0.75801	1.24068
C	5.79509	1.51915	0.05700
C	5.80572	0.88327	-1.20171
C	5.81311	-0.52211	-1.26860
C	5.80799	-2.82275	-0.15515
C	5.64040	-3.39034	-1.58404
C	6.55075	-2.57274	-2.52631
C	5.74571	-1.25539	-2.61381
C	5.81277	1.70536	-2.49295
C	5.69544	3.23177	-2.27213
C	5.75017	3.05170	0.09341
C	5.71910	1.46116	2.59857
C	5.61570	0.49754	3.80472
C	5.81960	-1.45188	2.46856
C	6.59542	-0.67048	3.55462
C	6.59507	3.61177	-1.07564
C	1.97700	-0.79865	4.31881
C	3.09663	0.07726	4.44306
C	4.28357	-0.23519	3.82585
C	4.41037	-1.42388	3.04966
C	3.35775	-2.29348	2.91029
C	2.11406	-2.00811	3.54376
C	2.02510	4.16786	-0.21538
C	1.98680	4.23791	-1.65639
C	3.16960	3.94642	-2.39736
C	4.32212	3.59720	-1.73732
C	4.35400	3.51259	-0.31520
C	3.23784	3.79387	0.43327
C	1.98205	-1.95815	-3.36316
C	1.91298	-3.23807	-2.69977
C	3.08827	-3.77048	-2.09216
C	4.26558	-3.06482	-2.14306
C	4.32843	-1.79484	-2.78682
C	3.21863	-1.24986	-3.38430
C	0.82027	-1.42849	-3.99785
C	-0.34160	-2.15456	-3.95577
C	-0.41183	-3.40562	-3.29766
C	0.68085	-3.95513	-2.67793

C	0.73391	-0.50747	4.95436
C	-0.30385	-1.39218	4.80834
C	-0.16480	-2.58083	4.05331
C	1.01046	-2.90226	3.42714
C	0.77390	4.59847	-2.31356
C	-0.33239	4.86887	-1.55061
C	-0.29066	4.81222	-0.13734
C	0.85316	4.47278	0.53669
C	-1.63902	5.17761	0.37843
O	-2.02446	5.27704	1.52971
N	-2.42678	5.42146	-0.75643
C	-1.71145	5.26078	-1.95728
O	-2.16197	5.44094	-3.07310
C	-1.69043	-1.35464	5.35356
O	-2.22155	-0.51481	6.05761
C	-1.45448	-3.32296	4.11328
O	-1.74736	-4.39796	3.62364
C	-1.67125	-1.88121	-4.56935
O	-2.02465	-0.94587	-5.26513
C	-1.78873	-3.94523	-3.47453
O	-2.25097	-5.00925	-3.10878
N	-2.48360	-2.97108	-4.21884
N	-2.30432	-2.53685	4.90950
C	-3.83916	5.75114	-0.69416
C	-3.69181	-2.86153	5.15759
C	-3.83226	-3.16025	-4.72329
C	-6.89994	-0.71773	-3.09198
C	-6.81315	-0.82667	-4.47806
C	-5.78031	-1.58477	-5.02526
C	-4.87564	-2.20947	-4.15918
N	-4.93794	-2.07917	-2.82700
C	-5.93014	-1.34528	-2.29567
C	-6.41118	-0.98618	2.47020
C	-6.90425	-1.49069	3.67472
C	-6.02296	-2.08867	4.57017
C	-4.66975	-2.16693	4.21570
N	-4.19567	-1.68931	3.06355
C	-5.04394	-1.10032	2.20155
C	-6.26741	2.52598	0.64822
C	-6.53656	3.80177	1.13936
C	-5.74183	4.86911	0.72394
C	-4.70395	4.61111	-0.17657
N	-4.43832	3.38572	-0.64539
C	-5.20338	2.35735	-0.24625
C	-4.88173	1.00885	-0.88318
C	-4.39677	-0.54357	0.94090
C	-6.01302	-1.26958	-0.78087
N	-5.33053	-0.14086	-0.10517
H	6.75105	-3.21214	0.25714
H	5.00917	-3.21954	0.48248
H	5.85461	-4.46461	-1.57954
H	6.62392	-3.04368	-3.51371
H	7.56184	-2.42804	-2.12923
H	6.74759	1.51045	-3.03961
H	6.20446	-2.46188	2.31886
H	6.62061	2.07666	2.73539
H	4.86976	2.15537	2.61836
H	7.58382	-0.33870	3.21700
H	6.71778	-1.28502	4.45424
H	4.99984	1.37827	-3.15265
H	5.94452	3.75698	-3.20063
H	7.59502	3.16665	-1.12905
H	6.69752	4.69987	-0.98845
H	2.99175	0.97904	5.04391
H	3.44812	-3.20789	2.32809
H	5.80923	1.04968	4.73082
H	3.13880	4.01676	-3.48334
H	3.25300	3.73946	1.51971
H	6.06249	3.43878	1.06439
H	3.03218	-4.74310	-1.60635
H	3.25762	-0.28317	-3.88172
H	6.06790	-0.61719	-3.43763
H	0.61733	-4.92149	-2.18412
H	0.86420	-0.47041	-4.50951
H	1.10536	-3.81828	2.84964
H	0.61763	0.40066	5.54057
H	0.87181	4.42960	1.62272
H	0.73266	4.65039	-3.39863
H	-4.13235	6.00877	-1.71746
H	-3.97201	6.63493	-0.06188
H	-3.92685	-2.59949	6.19380
H	-3.78541	-3.94747	5.04558
H	-3.81294	-3.07305	-5.81484
H	-4.10442	-4.18845	-4.46194
H	-7.70330	-0.15282	-2.62630
H	-7.53847	-0.33356	-5.12014
H	-5.67497	-1.69382	-6.10075
H	-7.06526	-0.50747	1.75101
H	-7.96223	-1.41107	3.91273
H	-6.36912	-2.48377	5.52191
H	-6.85078	1.66509	0.95252
H	-7.34744	3.96116	1.84601
H	-5.90655	5.87370	1.10335
H	-5.59467	-2.20350	-0.39180
H	-7.08080	-1.26156	-0.51172
H	-3.65982	-1.28378	0.58357
H	-3.82096	0.34127	1.24012
H	-3.80033	0.98390	-1.09224
H	-5.36848	0.99505	-1.86319

Frequencies

-39.3710	12.5643	15.7890
18.8714	21.5226	25.3275
28.8642	32.5819	40.2900
44.0414	45.6657	48.8538
49.7713	55.3621	61.0283
65.4835	91.0844	97.0046
101.8317	109.8241	114.7540

118.7864	120.3312	129.8657	941.3478	942.0554	945.0118
138.2286	138.8183	148.3173	951.7896	955.0499	958.7819
150.9611	159.4941	160.9485	961.3406	963.5395	966.3211
166.6136	172.2218	174.0671	966.4734	969.4757	970.2065
176.7484	178.9391	181.1805	989.1899	996.1923	1001.4363
186.5094	194.3105	202.5310	1003.3331	1005.1757	1006.2093
212.2848	227.5159	230.2810	1010.4571	1011.1558	1012.2545
232.6642	236.9330	239.2717	1013.4913	1015.3681	1016.2814
242.5260	247.0749	249.4996	1021.4890	1023.7882	1027.9962
258.1433	260.7535	268.2977	1039.9390	1044.3553	1044.8703
271.5096	272.5382	282.0609	1066.8871	1075.0756	1077.5869
290.8182	298.0835	300.8240	1078.1018	1106.3840	1107.8364
305.3102	306.6575	312.6814	1108.2598	1112.8168	1114.4006
319.2888	322.5532	328.8174	1117.4772	1118.7874	1126.0612
346.8423	348.3024	354.5299	1146.2096	1148.6897	1151.9745
369.5636	372.6618	374.8442	1155.7698	1156.3697	1166.7299
386.7856	396.3073	400.3277	1166.9655	1177.4542	1178.3119
401.2333	404.2127	405.2317	1178.4783	1178.7690	1179.0669
418.6550	419.4308	428.5595	1179.9116	1180.9213	1186.1114
429.0267	436.9707	438.4318	1188.0111	1190.2013	1191.1218
450.0112	462.8585	470.0545	1191.8972	1193.2872	1225.4503
476.8942	482.5177	484.0284	1228.9893	1230.0248	1231.6828
484.3962	485.3358	501.7458	1232.6598	1236.8994	1237.9237
503.0093	504.3961	529.4212	1244.7092	1249.0062	1249.6290
531.4755	542.1557	548.2312	1254.0100	1254.2307	1254.3711
549.0419	554.2143	569.2999	1260.4123	1263.2165	1268.1691
571.6334	573.1289	575.8924	1273.3598	1277.7031	1278.1027
576.6214	577.8659	578.4639	1278.1555	1278.2674	1290.0364
594.7040	595.7511	605.3782	1290.5302	1299.0716	1299.2293
607.2305	607.8655	613.4831	1300.0912	1301.8673	1305.8448
623.5478	631.7438	633.6998	1314.9915	1316.7522	1319.0517
648.5368	652.3903	653.0980	1319.3259	1321.7477	1325.1277
654.3430	658.5160	660.2276	1326.3715	1337.0621	1339.3162
660.9309	662.9070	694.8621	1339.8537	1341.1406	1345.3474
714.2044	715.4524	718.5338	1346.0195	1354.2261	1363.7814
720.0931	724.1911	727.7241	1365.1919	1365.8204	1376.9914
733.9459	735.6931	740.3549	1377.3320	1383.5249	1387.1319
740.9087	742.8340	743.2004	1394.0938	1399.5089	1400.7533
748.0835	750.9465	754.4387	1409.5024	1412.7053	1412.8921
762.6243	764.1291	764.4280	1413.3854	1417.2092	1420.6272
767.1324	768.4957	769.5957	1424.7076	1429.5985	1452.2737
773.2376	779.3319	779.9663	1452.6535	1468.6962	1470.9340
783.4061	784.3855	786.5031	1471.7302	1474.3493	1474.7542
789.1797	805.0855	805.7995	1475.3124	1475.3687	1476.6694
806.8759	813.9991	823.6741	1478.0176	1479.3411	1484.1603
825.7682	827.6099	835.3246	1484.3089	1484.9007	1486.0074
841.0328	842.2509	842.6603	1489.2837	1489.6392	1494.5527
857.6135	869.3195	869.7534	1494.9115	1498.6519	1501.4421
876.8841	888.2294	888.4832	1502.1851	1502.4715	1504.7400
895.0857	896.6851	896.9519	1521.0864	1521.2050	1522.0010
900.0229	906.7008	911.0277	1525.3922	1534.1838	1534.5917
912.1601	916.5901	920.0180	1535.0090	1607.0090	1607.1984
920.3606	929.3892	935.4647	1629.4788	1630.1265	1633.4809
936.2540	936.4338	941.1237	1636.4909	1637.2524	1639.4926

1648.7774	1649.4876	1649.8575
1675.2462	1676.7968	1676.9749
1678.0588	1679.3884	1679.4681
1771.3546	1774.3119	1774.8134
1821.4240	1821.9498	1823.8915
2979.4182	2992.3370	3002.7173
3015.1639	3015.7259	3016.9208
3057.1221	3057.2283	3057.4359
3065.0105	3066.3860	3068.0003
3068.9096	3071.7382	3072.1136
3072.3211	3078.9917	3079.1185
3079.4180	3091.3208	3099.4455
3103.1272	3103.3052	3103.5429
3114.7236	3117.0180	3118.1842
3125.5094	3127.8209	3130.1857
3172.5288	3172.8735	3173.2284
3180.6273	3181.1952	3182.1727
3182.5099	3185.6790	3185.9636
3198.8079	3198.8999	3199.3405
3199.5583	3200.1753	3200.8186
3200.8638	3201.3847	3203.8435
3210.4748	3231.9878	3238.4077

B(–)

E(RB3LYP) = -3723.61525060

E(RB3LYP-D3) = -3723.80357478

H - Sum of electronic and thermal Enthalpies= -3722.452452

G - Sum of electronic and thermal Free Energies= -3722.613242

Number of imaginary frequencies: 0

Cartesian Coordinates

C	-5.66270	0.98765	1.00625
C	-5.66849	-0.37632	1.35152
C	-5.66211	-1.36823	0.34902
C	-5.66703	-0.98520	-1.00491
C	-5.66104	0.37901	-1.36257
C	-5.66805	1.36003	-0.35398
C	-5.67157	2.05141	2.10729
C	-5.59003	3.50644	1.58663
C	-6.50241	3.62097	0.34582
C	-5.64974	2.85485	-0.69407
C	-5.66770	0.80055	-2.83438
C	-5.58397	-0.37787	-3.83400
C	-5.64670	-2.02707	-2.12933
C	-5.67073	-2.85365	0.71996
C	-5.58976	-3.13008	2.24050
C	-5.65026	-0.82904	2.81608
C	-6.50260	-2.11292	2.95961
C	-6.49719	-1.50976	-3.31438
C	-1.91994	-2.88784	3.51289
C	-3.08957	-3.49184	2.96486
C	-4.22943	-2.74530	2.79412
C	-4.26229	-1.36685	3.15396
C	-3.15526	-0.74903	3.68159
C	-1.95437	-1.49187	3.87782
C	-1.94934	-2.61500	-3.22922
C	-1.91344	-1.60077	-4.25542
C	-3.08253	-0.82367	-4.50554
C	-4.22342	-1.04911	-3.77527
C	-4.25769	-2.05028	-2.76176
C	-3.15114	-2.81631	-2.48921
C	-1.95405	4.10647	-0.64958
C	-1.91979	4.48700	0.74221
C	-3.08956	4.31380	1.53896
C	-4.22943	3.79339	0.97720
C	-4.26196	3.41660	-0.39674
C	-3.15484	3.56540	-1.19536
C	-0.79110	4.27880	-1.45627
C	0.33814	4.80026	-0.88030
C	0.37134	5.17439	0.48409
C	-0.72444	5.03245	1.29549
C	-0.72451	-3.63941	3.70946
C	0.37122	-3.00698	4.23737
C	0.33780	-1.63798	4.59421
C	-0.79148	-0.87873	4.42977
C	-0.71731	-1.39589	-5.00363
C	0.37768	-2.17014	-4.71929
C	0.34294	-3.16347	-3.71197
C	-0.78705	-3.40008	-2.97311
C	1.68277	-3.81153	-3.65641
O	2.07697	-4.70879	-2.93387
N	2.44693	-3.18712	-4.65610
C	1.74008	-2.17084	-5.32118
O	2.19009	-1.47693	-6.21453
C	1.73322	-3.52919	4.53835
O	2.18207	-4.65024	4.38372
C	1.67803	-1.26729	5.12779
O	2.07312	-0.19365	5.54460
C	1.67853	5.07747	-1.46758
O	2.07390	4.90243	-2.60581
C	1.73325	5.69596	0.78656
O	2.18187	6.12175	1.83516
N	2.44154	5.62945	-0.42530
N	2.44127	-2.44581	5.08579
C	3.86185	-3.42074	-4.83628
C	3.85604	-2.48677	5.37868
C	3.85638	5.90352	-0.53566
C	6.27989	2.49253	0.28048
C	6.90965	3.69205	-0.04927
C	6.12916	4.81516	-0.31715
C	4.73722	4.69060	-0.24341
N	4.13105	3.54156	0.06999
C	4.88147	2.45823	0.33167
C	6.28049	-1.48270	2.01888
C	6.90979	-1.79573	3.22312
C	6.12895	-2.12702	4.32894

C	4.73715	-2.13135	4.18293
N	4.13142	-1.82926	3.03063
C	4.88218	-1.51261	1.96230
C	6.28332	-1.00037	-2.29615
C	6.91389	-1.88643	-3.16876
C	6.13408	-2.68238	-4.00585
C	4.74201	-2.55807	-3.93434
N	4.13508	-1.71138	-3.09725
C	4.88483	-0.94048	-2.29172
C	4.14058	0.03564	-1.40001
C	4.13917	-1.22765	0.67056
C	4.13786	1.19697	0.72929
N	4.58981	0.00184	0.00037
H	-6.59656	1.95420	2.69491
H	-4.84547	1.87535	2.80747
H	-5.84879	4.19924	2.39473
H	-6.62831	4.66741	0.04384
H	-7.49242	3.17531	0.49479
H	-6.59262	1.35755	-3.04558
H	-5.97312	-0.03111	3.48613
H	-6.59550	-3.31416	0.34173
H	-4.84440	-3.37204	0.21780
H	-7.49250	-2.01943	2.49889
H	-6.62870	-2.37447	4.01686
H	-4.84167	1.49542	-3.03068
H	-5.84097	-0.02446	-4.83851
H	-7.48782	-1.15800	-3.00482
H	-6.62158	-2.29458	-4.06980
H	-3.06001	-4.54755	2.70075
H	-3.17016	0.30225	3.96133
H	-5.84837	-4.17635	2.43646
H	-3.05190	-0.06707	-5.28771
H	-3.16714	-3.58451	-1.71896
H	-5.96977	-3.00645	-1.77400
H	-3.06014	4.61218	2.58552
H	-3.16960	3.28284	-2.24590
H	-5.97227	3.03617	-1.72020
H	-0.68771	5.32234	2.34258
H	-0.80467	3.99398	-2.50528
H	-0.80515	0.17241	4.70660
H	-0.68773	-4.69145	3.43810
H	-0.80172	-4.16534	-2.20118
H	-0.67950	-0.63487	-5.77900
H	4.09988	-3.22041	-5.88597
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H	4.04747	6.26264	-1.55217
H	4.09326	6.70990	0.16600
H	6.84833	1.59374	0.49678
H	7.99436	3.75229	-0.09439
H	6.58602	5.76666	-0.57861
H	6.84921	-1.21934	1.13292
H	7.99441	-1.78463	3.29883
H	6.58542	-2.37552	5.28409
H	6.85129	-0.36178	-1.62729
H	7.99868	-1.95416	-3.19879
H	6.59158	-3.38487	-4.69841
H	3.05741	1.37856	0.60131
H	4.30564	1.01656	1.79814
H	3.05850	-1.20927	0.89084
H	4.30878	-2.06287	-0.01993
H	3.06010	-0.16478	-1.49520
H	4.31027	1.05119	-1.77814

Frequencies

9.1359	14.1304	14.3842
24.5118	26.3509	26.6136
27.4322	31.2179	31.4147
46.1033	46.3411	49.3315
53.9848	60.6930	60.7681
78.2602	91.6535	91.8296
107.8882	117.1102	117.2417
121.8812	125.2319	125.4501
138.3649	138.5834	148.1703
151.1942	159.4434	159.6474
167.9430	168.1598	170.4557
177.4378	178.7943	178.8101
191.8744	192.0056	210.4059
224.4439	224.4903	231.9267
239.3272	241.4679	241.4992
253.2638	253.3326	254.4390
260.3189	260.3658	266.7564
271.3534	271.4961	272.6526
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323.5954	323.8546	323.9243
334.9059	337.5258	337.5598
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3200.7785 3200.8000 3200.8151
3217.9355 3218.1498 3218.9219

B(+)⊂CCl_4

E(RB3LYP) = -5602.47162552

E(RB3LYP-D3) = -5602.69504063

H - Sum of electronic and thermal Enthalpies= -5601.291172

G - Sum of electronic and thermal Free Energies= -5601.472471

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.62119	0.47240	1.32900
C	5.63161	1.38324	0.25537

C	5.61976	0.91723	-1.07618
C	5.63109	-0.46802	-1.32820
C	5.62066	-1.38807	-0.25879
C	5.63286	-0.91373	1.06687
C	5.60153	0.99394	2.76746
C	5.52357	-0.11587	3.84240
C	6.47029	-1.25718	3.40841
C	5.64035	-1.87962	2.25997
C	5.60007	-2.89461	-0.52626
C	5.52066	-3.27081	-2.02474
C	5.63700	-1.01851	-2.76119
C	5.59900	1.90246	-2.24692
C	5.52057	3.38814	-1.82306
C	5.63806	2.89940	0.49555
C	6.46742	3.58336	-0.61780
C	6.46675	-2.32441	-2.79709
C	1.88254	4.46519	-0.94247
C	3.02121	4.20704	-1.76215
C	4.17698	3.72531	-1.19754
C	4.25265	3.46639	0.20190
C	3.18515	3.72136	1.02636
C	1.97252	4.23275	0.47878
C	1.97105	-1.70094	-3.90513
C	1.88183	-3.04812	-3.39607
C	3.02103	-3.62853	-2.76324
C	4.17660	-2.89826	-2.62882
C	4.25156	-1.55681	-3.10432
C	3.18349	-0.97062	-3.73667
C	1.97541	-2.53174	3.42443
C	1.88576	-1.41724	4.33652
C	3.02449	-0.57829	4.52244
C	4.18000	-0.82632	3.82247
C	4.25532	-1.90881	2.89851
C	3.18776	-2.75029	2.70736
C	0.85133	-3.39029	3.24643
C	-0.30355	-3.11366	3.93043
C	-0.40007	-2.00690	4.80673
C	0.66445	-1.17149	5.03028
C	0.66098	4.94262	-1.50204
C	-0.40342	5.16665	-0.66662
C	-0.30657	4.96155	0.73005
C	0.84855	4.50786	1.31149
C	0.66053	-3.77194	-3.52966
C	-0.40436	-3.16068	-4.14080
C	-0.30831	-1.84826	-4.66084
C	0.84657	-1.11750	-4.55893
C	-1.62156	-1.49196	-5.26760
O	-1.94802	-0.47820	-5.85547
N	-2.44846	-2.61138	-5.05997
C	-1.79140	-3.64953	-4.38058
O	-2.29770	-4.71595	-4.07932
C	-1.79061	5.61853	-0.96961
O	-2.29746	5.89024	-2.04368
C	-1.61955	5.30917	1.34248
O	-1.94536	5.31227	2.51454
C	-1.61661	-3.81765	3.92521
O	-1.94264	-4.83395	3.34150
C	-1.78713	-1.97054	5.34995
O	-2.29367	-1.17660	6.12289
N	-2.44381	-3.07821	4.79062
N	-2.44706	5.68834	0.26942
C	-3.85880	-2.63903	-5.38982
C	-3.85731	5.98795	0.41098
C	-3.85397	-3.35080	4.97979
C	-6.36477	-1.23246	2.26381
C	-6.89293	-1.60405	3.49999
C	-6.08184	-2.27909	4.41143
C	-4.76035	-2.55684	4.04439
N	-4.24642	-2.18521	2.86796
C	-5.02774	-1.54041	1.98603
C	-6.36691	2.57517	-0.06162
C	-6.89614	3.83121	-0.35734
C	-6.08551	4.95852	-0.22964
C	-4.76331	4.78030	0.19255
N	-4.24839	3.57598	0.45836
C	-5.02933	2.48936	0.34224
C	-6.36765	-1.34321	-2.19681
C	-6.89673	-2.22792	-3.13625
C	-6.08637	-2.68045	-4.17683
C	-4.76457	-2.22469	-4.23444
N	-4.24983	-1.39163	-3.32491
C	-5.03052	-0.94933	-2.32543
C	-4.37803	0.05213	-1.39117
C	-4.37657	1.17937	0.74143
C	-4.37627	-1.23117	0.65129
N	-4.85032	0.00003	0.00089
H	6.51373	1.57948	2.95456
H	4.76108	1.68646	2.90111
H	5.76126	0.30955	4.82349
H	6.61080	-1.98420	4.21687
H	7.45312	-0.90075	3.07974
H	6.51236	-3.34989	-0.11345
H	5.99513	3.14182	1.49759
H	6.51092	1.77214	-2.84807
H	4.75825	1.67181	-2.91304
H	7.45050	3.12110	-0.76236
H	6.60735	4.64707	-0.39233
H	4.75977	-3.35596	0.00747
H	5.75815	-4.33319	-2.14701
H	7.45004	-2.21807	-2.32502
H	6.60624	-2.66108	-3.83106
H	2.95465	4.40867	-2.82993
H	3.23866	3.54093	2.09789
H	5.75774	4.02533	-2.68198
H	2.95504	-4.65415	-2.40407
H	3.23646	0.04747	-4.11644
H	5.99338	-0.27202	-3.47262
H	2.95816	0.24560	5.23100

H	3.24111	-3.58810	2.01537
H	5.99738	-2.86861	1.96881
H	0.58186	-0.32843	5.71184
H	0.91153	-4.23799	2.56867
H	0.90904	4.34516	2.38455
H	0.57812	5.11101	-2.57297
H	0.90650	-0.10667	-4.95416
H	0.57823	-4.78379	-3.14043
H	-4.11421	-3.64820	-5.72531
H	-4.00038	-1.94699	-6.22762
H	-4.11299	6.78310	-0.29514
H	-3.99840	6.36751	1.42927
H	-3.99508	-4.42225	4.79823
H	-4.10919	-3.13800	6.02181
H	-6.96044	-0.70376	1.52686
H	-7.92333	-1.36606	3.75258
H	-6.45901	-2.57371	5.38729
H	-6.96221	1.67226	-0.15017
H	-7.92705	3.93039	-0.68835
H	-6.46358	5.95074	-0.46191
H	-6.96272	-0.96883	-1.37026
H	-7.92730	-2.56504	-3.05592
H	-6.46433	-3.37816	-4.91962
H	-4.58532	-2.06889	-0.02606
H	-3.28473	-1.22155	0.80489
H	-4.58445	1.01157	1.80580
H	-3.28526	1.30856	0.65520
H	-4.58744	1.05756	-1.77787
H	-3.28664	-0.08591	-1.46090
C	0.27442	0.00021	0.00268
Cl	2.06205	0.00760	0.00097
Cl	-0.32681	0.54473	1.60161
Cl	-0.33161	1.10848	-1.26968
Cl	-0.31946	-1.65998	-0.32240

Frequencies

15.5592	16.2255	16.5153
18.7879	19.3805	20.6444
25.9371	27.1750	28.3213
30.9890	31.9738	32.0609
35.1027	35.1781	39.8669
48.3038	48.4673	52.8907
57.1228	63.1833	63.4793
89.7859	93.5013	93.6377
106.4612	119.9987	120.1051
121.3057	128.2588	128.3538
140.2454	140.3537	149.1343
151.5158	159.2883	160.2207
167.5884	171.5442	171.6919
175.8049	175.8238	178.2530
195.4164	195.4661	208.2859
214.3388	214.8187	221.4050
221.4711	231.3642	235.8155
243.0182	243.1169	251.7589
251.9763	252.0225	257.9436
258.1801	268.9906	275.1859
276.1232	276.2487	300.6432
300.7429	306.4074	313.4723
313.7861	315.3741	315.4076
315.8009	320.2705	324.2167
324.3339	331.3578	341.4027
346.6258	347.2892	373.0580
373.1224	382.1262	388.4467
398.3079	399.5588	399.6513
405.8271	405.9608	419.5020
429.5304	429.8669	437.0614
437.0827	439.5520	450.8806
459.5948	459.6833	468.1831
479.8064	479.8324	484.6530
485.0830	485.5179	501.3058
503.4819	503.5311	529.3874
530.8624	548.9642	549.0359
552.9158	552.9700	569.1479
571.8951	571.9059	575.2518
578.0399	578.1070	579.8380
595.1765	595.1940	606.0068
606.7551	606.7626	623.8398
629.6474	645.5027	645.5380
653.2212	653.2900	653.6710
657.4494	659.4224	659.5135
660.4766	661.3483	661.4675
715.9241	715.9416	718.3051
723.5842	723.6509	727.1002
734.1111	734.1288	736.7451
737.3172	737.5218	740.7705
744.2748	744.3109	744.7967
749.7435	752.1798	752.2268
762.8593	767.2258	767.3779
769.2196	771.8425	775.5601
775.6656	779.4827	779.5491
785.9479	786.2443	786.2736
800.0554	800.1264	800.4542
812.3823	812.4942	817.1163
825.3575	825.4178	827.6341
841.1310	841.1950	842.3512
869.1069	869.3693	876.8087
883.3029	888.2020	888.6717
894.1409	896.9058	897.6085
900.3671	911.0813	913.9691
914.0685	915.2626	919.2035
919.4056	935.3851	935.4165
936.6404	937.2486	937.5969
941.2937	941.4245	941.8781
954.6472	956.3450	956.4216
962.9224	962.9987	967.3799
967.5853	971.0474	976.3365
987.7483	1005.1954	1005.8046
1005.8755	1010.8373	1010.8672

1012.1083	1013.9508	1014.0920
1015.5238	1015.5733	1024.6686
1024.8332	1024.8359	1035.2847
1039.3123	1043.9257	1044.0049
1066.4731	1075.0019	1077.6520
1077.6704	1106.4336	1106.5065
1107.4068	1107.4953	1110.2073
1117.4729	1117.5077	1117.7954
1147.4731	1147.8017	1147.8944
1151.4449	1151.6053	1153.9106
1165.7259	1165.7666	1177.8065
1178.4692	1178.5212	1178.9451
1180.0152	1180.0751	1184.9983
1185.0731	1186.5058	1190.9058
1191.7538	1191.7892	1227.5959
1227.6220	1229.6675	1231.7095
1231.7433	1233.5620	1236.8119
1245.2566	1249.8941	1249.9542
1253.8191	1254.1343	1254.1714
1259.1214	1270.8939	1271.8958
1272.0116	1277.4160	1277.4933
1277.5047	1287.7620	1288.0182
1290.9059	1291.0080	1291.5732
1299.2909	1299.3738	1299.9414
1315.1511	1318.1338	1318.1868
1319.8717	1320.2680	1321.9351
1322.1059	1325.6797	1338.9491
1338.9687	1340.1729	1345.3292
1345.4236	1360.7273	1361.8765
1362.0416	1365.1630	1376.8609
1376.9780	1385.1901	1389.8730
1389.9033	1400.1676	1406.8702
1406.9463	1408.5566	1412.6718
1412.7294	1413.7022	1416.2798
1416.3995	1421.2385	1450.0934
1450.3061	1468.5066	1468.5455
1469.9243	1474.0743	1474.3129
1474.3725	1475.9501	1475.9639
1477.5233	1482.0428	1482.1084
1483.3413	1484.5036	1484.5354
1484.5718	1491.8249	1491.8761
1495.5246	1500.4532	1501.1800
1501.6697	1510.4726	1510.5703
1511.4434	1520.9937	1521.1651
1521.9819	1534.4184	1534.4414
1534.7704	1604.1302	1604.3427
1630.3808	1630.4106	1631.9939
1636.7927	1636.8070	1638.1196
1648.7213	1648.7440	1648.8534
1675.5578	1675.6732	1675.7140
1678.1443	1678.2581	1678.2923
1771.2704	1773.8146	1773.8318
1821.6333	1821.6504	1823.4072
2999.2427	2999.9063	3004.9834
3017.5399	3017.6384	3017.7746
3057.4328	3057.4471	3057.5435
3064.4783	3064.5418	3064.7236
3065.6415	3066.5949	3066.7592
3073.1986	3073.3034	3073.3336
3078.7157	3078.7593	3078.9133
3103.3103	3103.3319	3103.6133
3124.0602	3124.1252	3124.1446
3126.7943	3127.1578	3127.2413
3172.5854	3172.6311	3172.6587
3179.4765	3179.9612	3179.9986
3184.2664	3184.2834	3184.3651
3197.7699	3197.7893	3197.8051
3200.0835	3200.1001	3200.3126
3200.5493	3200.5724	3200.6055
3219.0008	3219.1437	3220.6024

TS1⊂CCl_4

E(RB3LYP) = -5602.45888363

E(RB3LYP-D3) = -5602.67854487

H - Sum of electronic and thermal Enthalpies= -5601.279238

G - Sum of electronic and thermal Free Energies= -5601.459076

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.81309	-1.38503	-0.22122
C	5.84044	-0.80559	1.06109
C	5.79425	0.59607	1.21351
C	5.76982	1.41798	0.07071
C	5.76247	0.84720	-1.21932
C	5.78717	-0.55306	-1.35966
C	5.81329	-2.90864	-0.36744
C	5.66478	-3.40427	-1.82550
C	6.56801	-2.52207	-2.71535
C	5.73809	-1.21700	-2.74184
C	5.74057	1.73482	-2.46607
C	5.64018	3.24898	-2.16572
C	5.73001	2.94751	0.18629
C	5.77752	1.22826	2.60754
C	5.73140	0.20413	3.76709
C	5.88165	-1.67376	2.32541
C	6.70147	-0.94583	3.41694
C	6.56266	3.55957	-0.96630
C	2.10785	-1.10540	4.33636
C	3.23982	-0.24941	4.48039
C	4.40279	-0.53271	3.80665
C	4.49710	-1.67831	2.96406
C	3.43641	-2.53673	2.81631
C	2.21203	-2.27298	3.49502
C	2.02766	4.16900	-0.00095
C	1.96658	4.30734	-1.43598
C	3.12802	4.01926	-2.21158

C	4.28105	3.60642	-1.59043
C	4.33416	3.44962	-0.17499
C	3.23988	3.72771	0.60647
C	2.00178	-1.95376	-3.57792
C	1.94698	-3.26596	-2.98002
C	3.12633	-3.80871	-2.38863
C	4.28947	-3.07758	-2.38391
C	4.33542	-1.77521	-2.96102
C	3.22517	-1.22407	-3.55061
C	0.83314	-1.40210	-4.17839
C	-0.32594	-2.13205	-4.15402
C	-0.38410	-3.41586	-3.56187
C	0.72027	-3.99342	-2.98892
C	0.87447	-0.81762	4.99116
C	-0.19158	-1.65478	4.78365
C	-0.08607	-2.80224	3.96293
C	1.08511	-3.13000	3.33235
C	0.75361	4.73254	-2.05287
C	-0.33158	4.99746	-1.25798
C	-0.26781	4.87535	0.15012
C	0.87818	4.47357	0.78573
C	-1.59581	5.25753	0.70740
O	-1.95583	5.32071	1.86867
N	-2.39158	5.58567	-0.40275
C	-1.70525	5.44575	-1.62057
O	-2.17508	5.67922	-2.71950
C	-1.59363	-1.57422	5.28027
O	-2.10359	-0.75511	6.02466
C	-1.41457	-3.47550	3.92990
O	-1.73688	-4.50901	3.37555
C	-1.67249	-1.80872	-4.70049
O	-2.02969	-0.83520	-5.33568
C	-1.77492	-3.92810	-3.71492
O	-2.24478	-5.00324	-3.38604
N	-2.48881	-2.90771	-4.36527
N	-2.26262	-2.67148	4.71525
C	-3.78032	5.97586	-0.30718
C	-3.68581	-2.92239	4.89284
C	-3.87179	-3.04584	-4.79664
C	-6.90842	-2.49012	-1.87650
C	-6.83238	-3.72635	-2.51288
C	-5.81211	-3.94268	-3.43892
C	-4.90826	-2.90600	-3.69227
N	-4.95803	-1.72816	-3.05165
C	-5.93686	-1.51628	-2.15747
C	-6.13685	-0.26344	2.64830
C	-6.31509	-0.31045	4.02921
C	-5.51662	-1.16595	4.78859
C	-4.56457	-1.94544	4.12552
N	-4.38272	-1.89389	2.79877
C	-5.15334	-1.07456	2.06710
C	-6.51839	2.72830	0.03846
C	-7.01678	4.03319	0.05220
C	-6.12974	5.09792	-0.06256
C	-4.76300	4.81286	-0.19565
N	-4.28519	3.56905	-0.22485
C	-5.14181	2.53682	-0.10165
C	-4.48789	1.16373	-0.08146
C	-4.93008	-1.14178	0.55987
C	-6.00406	-0.14059	-1.51618
N	-5.40969	0.03302	-0.16428
H	6.75518	-3.31309	0.03228
H	5.01172	-3.34216	0.24284
H	5.89984	-4.47308	-1.87415
H	6.65821	-2.93918	-3.72525
H	7.57284	-2.37981	-2.30179
H	6.66022	1.56437	-3.04536
H	6.25939	-2.67446	2.11013
H	6.67934	1.84440	2.73865
H	4.92449	1.91259	2.69657
H	7.67452	-0.59420	3.05575
H	6.86205	-1.60472	4.27836
H	4.90954	1.44423	-3.12052
H	5.88075	3.81792	-3.07040
H	7.55747	3.10915	-1.05828
H	6.67652	4.64087	-0.82556
H	3.15934	0.62139	5.12880
H	3.50104	-3.41714	2.18069
H	5.96364	0.71024	4.71043
H	3.08169	4.14547	-3.29196
H	3.27233	3.62112	1.68874
H	6.06151	3.28195	1.17036
H	3.08321	-4.80565	-1.95333
H	3.25142	-0.23292	-3.99814
H	6.05502	-0.53059	-3.52821
H	0.66707	-4.98272	-2.54119
H	0.86518	-0.41659	-4.63561
H	1.15336	-4.01070	2.69894
H	0.78181	0.06221	5.62305
H	0.91487	4.37901	1.86795
H	0.69565	4.83684	-3.13352
H	-4.00971	6.56723	-1.19974
H	-3.88741	6.62271	0.57044
H	-3.91733	-2.87770	5.96118
H	-3.86027	-3.94050	4.53223
H	-4.03416	-2.25768	-5.53834
H	-3.98233	-4.02008	-5.28284
H	-7.70557	-2.27496	-1.16949
H	-7.55924	-4.50573	-2.29894
H	-5.71724	-4.89195	-3.95759
H	-6.73039	0.39022	2.01977
H	-7.06041	0.31831	4.51029
H	-5.61083	-1.21273	5.86946
H	-7.17604	1.87228	0.13772
H	-8.08411	4.21359	0.15541
H	-6.48099	6.12692	-0.05000
H	-7.06377	0.15392	-1.47956
H	-5.50544	0.54851	-2.20591

H	-5.46328	-2.02689	0.20112
H	-3.86149	-1.34775	0.38710
H	-3.93835	1.08739	0.86476
H	-3.72561	1.13830	-0.87854
C	-0.03845	0.04744	0.09263
Cl	-0.64910	0.87669	1.56052
Cl	-0.68511	-1.62300	0.04270
Cl	1.75291	-0.00371	0.13590
Cl	-0.57637	0.94061	-1.36360

Frequencies

-45.7303	13.2505	14.7966
16.7706	17.9458	21.3176
22.1837	24.3125	26.0571
27.2111	30.0787	30.8221
34.3047	36.4090	39.1557
46.7184	48.1420	51.3187
52.2543	58.0914	63.6540
71.7288	93.0744	96.4937
102.0775	108.8840	117.7542
119.8383	121.3709	130.0198
139.8112	140.3568	149.6709
150.4380	159.8403	160.7346
168.2310	169.1572	172.9259
173.9305	178.2722	181.8025
189.5313	193.4373	202.4493
211.2688	214.4977	214.9323
224.3652	227.9053	234.0769
235.5717	241.7768	242.5650
247.1101	247.9177	257.7664
260.1031	267.5488	270.9761
277.0912	288.5379	292.7571
299.4771	300.1590	303.9175
306.1536	311.2951	313.5756
313.9666	314.3175	318.4873
324.1793	330.9526	346.6788
348.2043	366.9420	371.3193
372.8149	379.6216	386.6871
396.6234	399.3396	399.9185
404.4796	405.7302	419.5996
419.9238	429.3889	429.9105
436.9815	438.5661	447.2874
449.8803	459.1641	470.3490
477.1359	482.0058	484.6445
484.8963	485.5885	500.4450
502.3549	504.2916	529.2536
533.9820	542.5985	548.5749
549.7005	554.4249	569.3176
572.1576	574.5098	575.9153
577.7927	578.5051	580.6500
594.2425	595.4686	605.6041
606.8795	607.8026	612.0801
623.9362	632.2924	635.0118
650.6391	652.1229	653.3916
654.7429	657.1210	660.7312
660.9217	663.3826	699.3465
715.0723	715.6687	719.8299
722.3261	724.3403	726.5106
733.3289	736.0065	737.7966
738.6841	739.6345	739.9885
741.3639	742.9214	743.0832
747.7087	751.3388	756.5890
762.7671	766.8331	767.7577
768.1590	771.2405	772.2263
775.1019	779.6286	780.4074
783.6526	783.9134	784.4070
788.4623	803.4696	805.5519
813.8882	815.3658	825.6364
826.2262	829.0524	837.9495
839.9143	842.0461	844.0486
859.2052	869.3403	869.4245
877.0725	888.5522	888.6220
895.0501	897.3119	897.4314
900.3930	909.4002	911.9426
914.4975	918.7349	919.5714
920.8401	928.4272	936.4252
937.0163	937.5364	940.6388
941.2267	941.4549	941.8686
945.5765	953.2888	956.9805
961.4058	962.6493	966.4038
967.0469	968.7823	970.5302
988.2414	998.8218	1000.9234
1003.5951	1006.2892	1008.2593
1010.0536	1011.5334	1012.6577
1013.3651	1014.4205	1015.4414
1016.3002	1020.6256	1029.2400
1039.7823	1044.1713	1044.3902
1066.6820	1075.1792	1077.7049
1078.1389	1103.1765	1107.4188
1107.5456	1110.6286	1111.5167
1117.5872	1118.5289	1124.7746
1141.8541	1143.8423	1151.8110
1152.8612	1155.4200	1166.2945
1166.5847	1177.5079	1177.7250
1177.8568	1179.0683	1179.4795
1179.7191	1180.2214	1185.7720
1187.2360	1189.7210	1190.8708
1191.6344	1192.0888	1222.7426
1229.7573	1230.9578	1231.4144
1236.6067	1237.3393	1241.1581
1245.0742	1249.5040	1250.0423
1253.8952	1254.1194	1254.3411
1259.5426	1260.5040	1269.9483
1273.2421	1277.5261	1278.0169
1278.4423	1280.4286	1290.3813
1290.9599	1296.6592	1299.2056
1300.1624	1300.7709	1304.8512
1314.8369	1315.1385	1318.3587

1319.3858	1321.2464	1325.5183
1327.0819	1331.5182	1339.4996
1339.7375	1340.7561	1345.2426
1345.6922	1356.0197	1364.9425
1366.1743	1369.0664	1377.0469
1377.1683	1382.7754	1384.2991
1387.8011	1395.1674	1400.6340
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1451.3328	1468.3613	1470.9104
1471.5902	1474.4339	1474.5038
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1487.3701	1489.6185	1493.3097
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1627.7813	1628.5097	1633.6182
1636.4436	1637.2239	1638.9750
1648.8960	1649.1588	1649.8116
1675.4326	1676.2594	1676.7939
1678.2908	1678.5521	1679.2086
1770.4196	1773.0813	1773.5786
1820.5791	1821.0588	1822.7837
2989.1148	3000.3357	3004.5397
3016.3129	3016.4411	3017.2989
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3064.0605	3066.0200	3068.5836
3070.7764	3074.1810	3076.7911
3078.8938	3079.0804	3079.2350
3081.3101	3086.6539	3103.2349
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3128.2120	3129.4349	3130.5769
3172.4162	3172.8391	3172.9438
3179.7552	3180.5697	3181.4373
3182.1754	3185.8451	3187.4012
3196.9294	3198.1903	3198.4190
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I1⊂CCl_4

E(RB3LYP) = -5602.46198593

E(RB3LYP-D3) = -5602.68237015

H - Sum of electronic and thermal Enthalpies= -5601.281320

G - Sum of electronic and thermal Free Energies= -5601.462818

Number of imaginary frequencies: 0

Cartesian Coordinates

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C	-5.92151	1.21145	-0.51216
C	-5.90844	0.99698	0.88277
C	-5.88772	-0.31846	1.38354
C	-5.90699	-1.41757	0.50004
C	-5.90916	-1.19166	-0.88817
C	-5.83650	0.36518	-2.91330
C	-5.69917	-0.92360	-3.76269
C	-6.64567	-1.98425	-3.16029
C	-5.86179	-2.35787	-1.88082
C	-5.94499	-2.85129	1.03505
C	-5.79759	-2.95780	2.57037
C	-5.80108	-0.60562	2.88829
C	-5.94426	2.17938	1.85487
C	-5.92448	3.56728	1.17012
C	-5.94949	2.65806	-1.02165
C	-6.83617	3.50324	-0.07492
C	-6.65878	-1.85114	3.21677
C	-2.28037	4.55342	0.23417
C	-3.45382	4.44770	1.03649
C	-4.57408	3.83514	0.53175
C	-4.58649	3.30500	-0.79085
C	-3.48143	3.40414	-1.60002
C	-2.29709	4.02745	-1.10946
C	-2.04633	-1.21537	3.78051
C	-2.04636	-2.63900	3.54398
C	-3.25895	-3.27876	3.15470
C	-4.40366	-2.53737	2.99706
C	-4.40009	-1.12809	3.20764
C	-3.25360	-0.47802	3.59610
C	-2.09531	-3.00818	-2.64251
C	-2.00339	-2.15583	-3.80344
C	-3.16204	-1.44454	-4.23585
C	-4.34584	-1.58257	-3.55192
C	-4.44030	-2.45109	-2.42591
C	-3.34614	-3.14715	-1.97594
C	-0.93323	-3.67968	-2.16428
C	0.25071	-3.49681	-2.82873
C	0.33469	-2.69488	-3.99062
C	-0.75788	-2.03026	-4.48670
C	-1.08933	5.14632	0.74538
C	0.02356	5.17884	-0.05410
C	0.00647	4.66745	-1.37286
C	-1.12327	4.11151	-1.91398
C	-0.84084	-3.38236	3.70451
C	0.29609	-2.71746	4.08314
C	0.29500	-1.32473	4.33205
C	-0.84174	-0.57093	4.19133
C	1.66699	-0.93421	4.76683
O	2.08162	0.15220	5.12705
N	2.42701	-2.11529	4.72975
C	1.66917	-3.23294	4.33948

O	2.08742	-4.37438	4.27246
C	1.40174	5.66244	0.23325
O	1.83806	6.19394	1.24014
C	1.37171	4.82408	-1.94987
O	1.76639	4.55341	-3.06752
C	1.60734	-4.03256	-2.53434
O	1.95904	-4.78107	-1.64262
C	1.73916	-2.74997	-4.48317
O	2.21449	-2.27955	-5.50238
N	2.45073	-3.50533	-3.53564
N	2.15259	5.38825	-0.92021
C	3.80719	-2.20172	5.15340
C	3.59033	5.63163	-1.01772
C	3.85450	-3.89224	-3.67653
C	6.74521	-0.78063	-3.50460
C	6.29665	-1.18863	-4.75857
C	5.32892	-2.18696	-4.82860
C	4.84520	-2.73813	-3.63568
N	5.26632	-2.33616	-2.42551
C	6.20075	-1.37074	-2.35474
C	5.85170	2.67147	1.04752
C	5.68788	3.91361	1.65923
C	4.95509	4.90460	1.00585
C	4.40770	4.60548	-0.24650
N	4.55520	3.40936	-0.83224
C	5.26366	2.45775	-0.20485
C	6.73688	-0.83265	2.38324
C	7.13483	-1.17893	3.67614
C	6.17662	-1.62142	4.57993
C	4.84531	-1.71440	4.14740
N	4.46262	-1.40284	2.90853
C	5.38867	-0.95689	2.03620
C	4.86026	-0.57574	0.65674
C	5.42930	1.16758	-0.99590
C	6.69604	-0.94604	-0.97492
N	5.87433	0.01466	-0.22030
H	-6.75522	0.87973	-3.23185
H	-5.00815	1.04363	-3.15265
H	-5.90134	-0.69091	-4.81382
H	-6.73774	-2.85408	-3.82132
H	-7.64806	-1.59623	-2.94689
H	-6.90128	-3.31455	0.74841
H	-6.27479	2.70761	-2.06193
H	-6.85816	2.11423	2.46368
H	-5.10420	2.11665	2.55797
H	-7.80844	3.03860	0.12403
H	-7.00179	4.50290	-0.49363
H	-5.16057	-3.45418	0.56261
H	-6.05778	-3.97103	2.89545
H	-7.67047	-1.79226	2.79965
H	-6.73247	-1.99246	4.30154
H	-3.43908	4.85770	2.04488
H	-3.48064	3.00701	-2.61288
H	-6.21361	4.33683	1.89409
H	-3.25613	-4.35572	2.99495
H	-3.23925	0.59680	3.76478
H	-6.07744	0.26655	3.48191
H	-3.08485	-0.79734	-5.10781
H	-3.40423	-3.80005	-1.10791
H	-6.21209	-3.28640	-1.42828
H	-0.68001	-1.40692	-5.37399
H	-0.98830	-4.30659	-1.27817
H	-1.12295	3.71431	-2.92572
H	-1.06407	5.53978	1.75852
H	-0.83164	0.49902	4.38229
H	-0.82973	-4.45479	3.52649
H	3.99315	-3.25608	5.38529
H	3.91478	-1.62515	6.07912
H	3.78980	6.64002	-0.64367
H	3.83987	5.57796	-2.07985
H	4.05815	-4.57347	-2.84739
H	3.96608	-4.43530	-4.62195
H	7.51480	-0.01872	-3.41292
H	6.69741	-0.74126	-5.66456
H	4.94121	-2.52993	-5.78172
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H	8.17747	-1.09391	3.97320
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H	7.69625	-0.50735	-1.10085
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H	6.18593	1.36666	-1.76524
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H	4.06054	0.15649	0.81120
H	4.38040	-1.45711	0.20478
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Frequencies

12.0163	16.1274	17.3868
18.6296	21.7775	23.8830
25.4311	26.7976	28.1720
29.1450	30.4426	36.9765
37.2842	38.4927	44.1899
47.1199	49.2077	54.3387
57.6646	61.7713	65.4907
74.2247	96.3828	99.1170
100.8124	115.2577	116.6653
121.5693	122.5981	134.7340
139.0434	140.0793	149.0745
150.2855	158.3904	161.2954
164.5527	168.3052	174.2844
177.2916	181.3373	185.4169

189.1409	198.3736	202.4825	959.6812	962.4339	965.7804
207.6322	215.4381	215.7755	966.7768	968.0971	969.7815
223.6500	228.0194	230.6983	985.7346	987.7343	995.7177
236.2554	239.5763	241.3650	1005.5434	1006.7124	1007.0801
243.1188	246.1376	255.0894	1009.2174	1009.9123	1010.8392
261.5052	265.9192	266.4905	1012.7552	1014.2561	1014.8297
271.9804	285.3651	289.3282	1016.5427	1018.4031	1030.1551
297.2168	299.4428	303.4221	1039.6671	1043.5036	1044.8332
304.5278	314.1031	314.4447	1066.6650	1075.0048	1077.5810
314.7859	317.0807	323.4476	1078.4800	1098.1817	1104.1098
329.1913	343.0823	346.7937	1107.4692	1108.4469	1117.0989
348.5678	371.0075	372.1682	1117.4970	1120.3637	1128.0139
383.8339	385.3561	393.4926	1137.6505	1139.4950	1152.5965
393.8085	399.6611	402.7801	1154.8382	1155.6484	1166.2082
404.2098	405.8648	419.8315	1166.5681	1169.6142	1176.4135
426.0801	427.9107	429.4481	1177.0278	1177.1743	1178.7850
436.4353	437.0313	444.3732	1178.9527	1179.3554	1186.1713
449.9454	460.3141	470.0580	1187.9296	1189.9689	1190.7299
478.2187	483.5365	484.4313	1191.0871	1193.2455	1221.7573
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534.5108	538.6246	543.6081	1245.2212	1248.8589	1249.9150
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571.7596	575.1833	575.4788	1255.7843	1259.4438	1269.7854
577.8911	579.3652	581.7798	1275.4196	1276.0413	1277.2611
592.7346	595.0900	601.4594	1278.3270	1278.4073	1290.0334
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648.0951	652.5797	653.4263	1314.0840	1316.0181	1318.2740
655.7974	659.7610	660.4971	1319.5979	1321.8905	1324.3380
661.0319	664.7483	703.5105	1326.7312	1339.2208	1339.8430
714.9954	717.3556	721.2799	1341.2434	1344.5862	1345.1770
721.7284	723.7626	726.7123	1346.1795	1355.0165	1365.1164
733.1439	734.5685	735.9461	1366.5196	1373.2682	1376.1455
737.9915	739.7863	740.9872	1376.4810	1377.5858	1379.1691
741.5134	742.3887	745.0694	1385.6003	1400.4431	1401.4070
747.6641	751.0218	758.1084	1405.2017	1410.0958	1412.1695
762.5078	764.1793	767.3029	1412.7399	1413.2376	1415.9884
767.9632	771.1649	771.5514	1419.6597	1421.2428	1451.0782
776.3912	779.0526	780.1052	1451.8524	1468.4608	1472.7350
782.9639	783.5580	785.4196	1473.3524	1473.8969	1474.5482
788.1883	802.7153	805.4878	1474.7242	1474.9746	1475.5660
813.5082	819.6008	825.0608	1475.6532	1478.6186	1484.1266
825.7209	834.2636	838.0973	1484.3420	1484.4723	1487.3613
839.4889	842.2250	853.5613	1489.1201	1490.2709	1491.1899
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915.7493	918.6501	920.0689	1535.5622	1605.5125	1606.1747
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3182.6485	3186.0017	3190.3203
3195.9658	3198.7103	3198.9090
3199.1428	3201.6254	3201.6830
3201.8914	3202.5857	3217.5201
3227.1230	3229.6887	3234.9464

TS2⊂CCl_4

E(RB3LYP) = -5602.45968353

E(RB3LYP-D3) = -5602.68160909

H - Sum of electronic and thermal Enthalpies= -5601.279679

G - Sum of electronic and thermal Free Energies= -5601.457674

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.80406	1.40646	-0.79667
C	5.97461	0.05951	-1.16910
C	6.04998	-0.94883	-0.18456
C	5.94355	-0.60227	1.17485
C	5.77734	0.74412	1.55949
C	5.72319	1.74351	0.57092
C	5.73402	2.49487	-1.87250
C	5.50014	3.92515	-1.32382
C	6.35121	4.09222	-0.04642
C	5.53916	3.21891	0.94043
C	5.67707	1.12701	3.03930
C	5.63236	-0.08010	4.00797
C	5.94439	-1.67007	2.27477
C	6.27432	-2.41144	-0.57788
C	6.27461	-2.66486	-2.10364
C	6.04708	-0.36444	-2.64242
C	7.06224	-1.52408	-2.78383
C	6.66800	-1.11825	3.52576
C	2.59598	-2.86236	-3.34550
C	3.84193	-3.32652	-2.83263
C	4.88514	-2.44847	-2.67260
C	4.74606	-1.07288	-3.01681
C	3.57045	-0.59485	-3.54274
C	2.46259	-1.47507	-3.71978
C	2.20689	-2.50221	3.02701
C	2.02715	-1.54143	4.08869
C	3.12750	-0.72213	4.47670
C	4.33662	-0.85241	3.83826
C	4.51760	-1.81266	2.80126
C	3.48232	-2.62202	2.40211
C	1.73667	4.07552	0.76980
C	1.72612	4.53802	-0.59721
C	2.93890	4.51745	-1.34675
C	4.09820	4.07203	-0.76020
C	4.11371	3.64550	0.59940
C	2.96352	3.63950	1.34952
C	0.52158	4.04805	1.51453
C	-0.63256	4.46814	0.90634
C	-0.63628	4.95660	-0.42093
C	0.50787	5.00079	-1.17531
C	1.47584	-3.73653	-3.45970
C	0.28628	-3.22425	-3.90784
C	0.15926	-1.86915	-4.29293
C	1.21553	-0.99850	-4.22091
C	0.75294	-1.41240	4.71571
C	-0.28348	-2.18822	4.26494
C	-0.11194	-3.11482	3.20969
C	1.10214	-3.29578	2.60044
C	-1.42680	-3.76131	2.94279
O	-1.70746	-4.62356	2.13051
N	-2.32617	-3.18175	3.85606
C	-1.70632	-2.24919	4.70337
O	-2.26103	-1.65328	5.60921
C	-1.04953	-3.86797	-4.04259
O	-1.37162	-5.02461	-3.82982
C	-1.25517	-1.63381	-4.70198
O	-1.76295	-0.62546	-5.15241
C	-2.02944	4.51077	1.42010
O	-2.45274	4.20380	2.51816
C	-2.02856	5.36133	-0.75658
O	-2.44815	5.90742	-1.76291
N	-2.81102	5.01235	0.35659
N	-1.92000	-2.85799	-4.48000
C	-3.73205	-3.54281	3.93921
C	-3.35759	-3.06172	-4.66255
C	-4.24251	5.29619	0.47204
C	-6.79748	2.93745	-1.98027
C	-6.31460	4.13569	-2.50183
C	-5.46293	4.91282	-1.72029
C	-5.12519	4.45575	-0.44026
N	-5.58839	3.30031	0.06295
C	-6.40889	2.54544	-0.69171
C	-5.53921	-2.72384	-1.01475
C	-5.14945	-3.99806	-1.42787
C	-4.43409	-4.14423	-2.61691
C	-4.13315	-2.99240	-3.35397
N	-4.49586	-1.76726	-2.95316

C	-5.18290	-1.62865	-1.80808
C	-6.43885	-0.42600	2.92483
C	-6.67636	-1.15338	4.08691
C	-5.78564	-2.16391	4.44673
C	-4.69100	-2.40701	3.61477
N	-4.46120	-1.70842	2.49313
C	-5.31225	-0.72898	2.14320
C	-4.96298	0.04055	0.87221
C	-5.58281	-0.19484	-1.50226
C	-6.93048	1.24598	-0.08336
N	-6.04428	0.06790	-0.13911
H	6.67777	2.50220	-2.43751
H	4.94620	2.25691	-2.59838
H	5.72360	4.65751	-2.10713
H	6.36398	5.13732	0.28476
H	7.38446	3.74760	-0.16639
H	6.54464	1.74734	3.31012
H	6.27663	0.48081	-3.29262
H	7.24214	-2.74508	-0.17437
H	5.51355	-3.05055	-0.11340
H	8.02096	-1.31114	-2.29766
H	7.24538	-1.74810	-3.84138
H	4.79110	1.75116	3.20822
H	5.79387	0.26738	5.03418
H	7.64416	-0.67833	3.29229
H	6.80778	-1.91109	4.27007
H	3.94146	-4.37754	-2.56662
H	3.45324	0.45240	-3.81356
H	6.67163	-3.66469	-2.31024
H	2.98580	0.00248	5.27678
H	3.60527	-3.35053	1.60350
H	6.36848	-2.61136	1.92342
H	2.92408	4.86303	-2.37895
H	2.96107	3.30460	2.38454
H	5.80168	3.40593	1.98250
H	0.49161	5.36859	-2.19820
H	0.51528	3.68285	2.53811
H	1.10242	0.04401	-4.50671
H	1.56262	-4.77991	-3.16693
H	1.22211	-4.01202	1.79177
H	0.60889	-0.69772	5.52223
H	-3.94210	-3.92251	4.94483
H	-3.86821	-4.36182	3.22532
H	-3.49456	-4.03546	-5.14116
H	-3.70340	-2.26900	-5.32913
H	-4.50588	5.09593	1.51261
H	-4.39403	6.35965	0.25704
H	-7.47370	2.31398	-2.55892
H	-6.59954	4.46098	-3.49913
H	-5.05191	5.84601	-2.08955
H	-6.09964	-2.56904	-0.09959
H	-5.39599	-4.86930	-0.82626
H	-4.09718	-5.11801	-2.95852
H	-7.11383	0.37197	2.63897
H	-7.53577	-0.92601	4.71273
H	-5.92513	-2.73756	5.35863
H	-7.86447	0.97508	-0.59244
H	-7.17641	1.44426	0.96132
H	-6.40916	0.05089	-2.18237
H	-4.74371	0.45206	-1.80774
H	-4.09292	-0.45926	0.44179
H	-4.64857	1.06095	1.13566
C	-0.50427	-0.05969	-0.15746
Cl	-1.12105	0.61528	1.38278
Cl	-1.05348	-1.75338	-0.32761
Cl	1.29120	-0.00462	-0.15614
Cl	-1.12866	0.91030	-1.52994

Frequencies

-22.7671	15.5663	16.2547
18.0129	20.9402	22.7138
23.6531	26.2722	26.6932
27.8962	30.6574	33.0929
39.2778	41.1450	44.0267
48.9652	50.1945	54.8512
56.2587	63.8275	69.1162
73.9474	95.7693	97.7006
107.4362	111.9745	115.3828
121.6757	123.3168	129.3241
139.6477	140.3854	147.0447
151.4341	158.7352	160.2650
160.8512	167.4716	171.4617
174.7985	184.9206	186.7399
191.9799	198.8029	204.6542
210.2797	215.0368	216.2156
224.6481	229.7630	233.6323
236.5636	240.6963	242.4444
244.8180	250.4755	256.3441
260.7864	262.3245	270.8588
282.1259	289.5694	293.2921
297.4978	299.5473	302.9282
307.7236	314.1323	314.3968
314.8285	316.4825	329.6545
337.4107	344.3540	347.5613
348.3924	371.4091	371.5736
384.7571	389.4269	391.9619
393.8889	399.9694	402.8648
404.1576	410.4342	419.9297
421.5075	427.4389	428.4544
435.5606	436.1777	442.2380
450.0147	461.3478	470.0936
470.5121	483.6544	484.4109
484.6176	486.0233	498.1334
501.2177	501.6176	527.7815
530.3860	536.0842	542.9808
549.3195	550.8151	567.7293
572.3771	574.0706	575.4087
578.5529	580.0068	581.8527

592.4104	593.6990	600.3890
606.4658	607.5185	608.7067
617.3428	624.5430	636.6159
652.6539	653.2733	654.7762
658.4948	659.9108	661.5255
663.7456	668.1233	704.5383
714.8783	718.2697	722.0308
723.0120	724.3747	726.9996
732.5100	734.0001	737.3631
738.7850	739.7722	741.6406
742.1579	742.9437	745.3523
748.5981	755.6895	761.0384
762.4715	767.2373	767.7791
771.4572	772.7590	777.3791
778.1630	779.9342	782.0039
782.7931	783.4086	784.7751
797.9901	801.9529	804.6397
813.1929	819.6825	824.3766
828.5529	834.4458	837.6936
840.1190	840.9433	851.3039
864.9779	869.1043	869.4940
877.0767	888.2507	888.5498
895.2692	897.1196	897.6407
900.3019	904.4596	911.1358
914.5222	917.5549	919.7544
922.4925	930.2625	934.4879
935.7155	936.4673	936.7917
939.7100	941.0882	941.4164
941.7455	947.9735	955.4043
959.2761	961.2128	965.7900
966.4576	968.8160	971.7886
984.1895	986.5019	987.5202
1000.9269	1005.9583	1007.1906
1009.2345	1010.4727	1010.6890
1013.1539	1014.5135	1014.7163
1015.8268	1018.2857	1023.9570
1039.3728	1043.2079	1044.2424
1066.6129	1075.1951	1077.8767
1078.1521	1094.8264	1101.3854
1107.5461	1107.7863	1113.5525
1118.7125	1120.2094	1124.5415
1132.6917	1138.0631	1143.7439
1147.1430	1151.9243	1155.8860
1166.1899	1166.4708	1175.5238
1176.6869	1177.0759	1178.1472
1178.7591	1179.4954	1187.2989
1189.5279	1190.3501	1190.6576
1192.6040	1195.3728	1228.0061
1230.2787	1230.6340	1234.0786
1236.9131	1244.3395	1246.0335
1248.3325	1249.3093	1249.9706
1253.8092	1254.0223	1254.4174
1259.2291	1267.2699	1272.0346
1276.5153	1277.8858	1277.9690
1278.0516	1279.2316	1290.3056
1290.9627	1298.9104	1299.7232
1300.0249	1300.8666	1303.7460
1313.5434	1314.0873	1318.4890
1319.3452	1321.8115	1324.3809
1327.3663	1339.3085	1339.7389
1341.1292	1344.9202	1345.5488
1348.2503	1355.9846	1357.7710
1365.2925	1371.5675	1374.2311
1376.3674	1376.9078	1378.6523
1387.4198	1389.7641	1400.0735
1400.4789	1407.8782	1411.2575
1412.7147	1413.0139	1414.4859
1417.8890	1424.0678	1450.9317
1451.5770	1471.1219	1472.1645
1473.1345	1473.9723	1474.5902
1474.7959	1475.0786	1475.8555
1477.0683	1483.5655	1484.0765
1484.3233	1486.3965	1487.6630
1490.5241	1493.2358	1494.4177
1495.3445	1497.8861	1501.3974
1502.1990	1502.7911	1507.0639
1513.2723	1520.9115	1521.0784
1521.9004	1534.7254	1535.1173
1535.5070	1605.4610	1606.1195
1627.4915	1628.0174	1629.8150
1635.9039	1638.3010	1640.6214
1649.2815	1649.3689	1649.5229
1674.7537	1676.0911	1676.2658
1677.9859	1678.3977	1678.5133
1768.0900	1770.1730	1772.0992
1818.6704	1819.7221	1821.2368
2990.3320	3015.0709	3015.2512
3017.9594	3028.9482	3046.7393
3054.7808	3056.9993	3057.1214
3057.5487	3061.8283	3065.6013
3066.4140	3068.9083	3073.1828
3079.1557	3079.5917	3080.0481
3092.2649	3102.8849	3103.2708
3103.9067	3115.2309	3129.7580
3129.8838	3132.7038	3133.3790
3137.4337	3148.8071	3152.7736
3172.0371	3172.4895	3173.7166
3179.4906	3180.6300	3181.4948
3187.1195	3187.7379	3191.9561
3198.3799	3198.9511	3199.3359
3201.9994	3202.1548	3203.1313
3203.4591	3204.8271	3217.4152
3230.0371	3231.1923	3234.1862

$I_2 \subset CCl_4$

E(RB3LYP) = -5602.46328550

E(RB3LYP-D3) = -5602.68904818

H - Sum of electronic and thermal Enthalpies= -5601.282096

G - Sum of electronic and thermal Free Energies= -5601.461838

Number of imaginary frequencies: 0

Cartesian Coordinates

C	-5.47025	-0.72708	-1.86042
C	-5.76347	0.52743	-1.29306
C	-5.94499	0.65561	0.10067
C	-5.85605	-0.48501	0.91959
C	-5.59891	-1.75314	0.35760
C	-5.39494	-1.86594	-1.03026
C	-5.27714	-0.85176	-3.37472
C	-4.91913	-2.27819	-3.86057
C	-5.77292	-3.28678	-3.06169
C	-5.06814	-3.21311	-1.68492
C	-5.59168	-3.00832	1.23681
C	-5.76555	-2.73374	2.75233
C	-6.01289	-0.39481	2.44140
C	-6.28085	2.01348	0.72397
C	-6.30766	3.18682	-0.28430
C	-5.87460	1.79231	-2.15510
C	-6.99189	2.69539	-1.57854
C	-6.81986	-1.62155	2.93295
C	-2.67564	4.41629	-0.92576
C	-3.95389	4.34849	-0.29919
C	-4.90845	3.49015	-0.78572
C	-4.64666	2.66882	-1.92012
C	-3.43756	2.72832	-2.56862
C	-2.41668	3.59864	-2.08628
C	-2.41972	-0.31659	3.97289
C	-2.30613	-1.73605	4.20803
C	-3.39211	-2.58890	3.85866
C	-4.52596	-2.05497	3.29918
C	-4.65602	-0.65070	3.09888
C	-3.63154	0.20399	3.42908
C	-1.19812	-3.54975	-2.09800
C	-1.12060	-2.99885	-3.42972
C	-2.31560	-2.55743	-4.06938
C	-3.52067	-2.66925	-3.42028
C	-3.60060	-3.22979	-2.11254
C	-2.46940	-3.65650	-1.45991
C	-0.00471	-3.97213	-1.44103
C	1.19204	-3.84161	-2.09781
C	1.26374	-3.32339	-3.41247
C	0.14309	-2.90650	-4.08348
C	-1.64174	5.24448	-0.39992
C	-0.41026	5.21783	-1.00099
C	-0.15825	4.42420	-2.14407
C	-1.13142	3.63683	-2.70212
C	-1.09434	-2.27103	4.73238
C	-0.03965	-1.42201	4.94133
C	-0.13429	-0.03555	4.67839
C	-1.30092	0.53088	4.23155
C	1.21547	0.56637	4.88883
O	1.56168	1.72691	4.78230
N	2.05713	-0.50759	5.25035
C	1.35749	-1.72007	5.35435
O	1.84251	-2.78111	5.70845
C	0.86469	5.87945	-0.61044
O	1.07854	6.65306	0.30787
C	1.27899	4.57876	-2.50855
O	1.88458	4.10156	-3.44822
C	2.57528	-4.17528	-1.65576
O	2.94974	-4.66813	-0.60821
C	2.68950	-3.34852	-3.83982
O	3.17679	-3.05766	-4.91865
N	3.41531	-3.81770	-2.73182
N	1.82872	5.42688	-1.52422
C	3.51929	-0.42176	5.32492
C	3.25706	5.72914	-1.40180
C	4.85743	-4.06357	-2.75416
C	7.27108	-0.55900	-2.70164
C	7.03235	-1.17011	-3.93047
C	6.23008	-2.30940	-3.97122
C	5.70449	-2.79915	-2.77080
N	5.93650	-2.21261	-1.58528
C	6.69840	-1.10275	-1.54245
C	5.12541	3.09818	1.38369
C	4.58392	4.28739	1.86978
C	3.98491	5.18034	0.98003
C	3.94311	4.83645	-0.37662
N	4.46416	3.69467	-0.84757
C	5.04597	2.84196	0.01009
C	5.01135	-2.35495	1.84383
C	5.04418	-3.06070	3.04499
C	4.61663	-2.43096	4.21347
C	4.15870	-1.11170	4.12725
N	4.17113	-0.41345	2.98208
C	4.59469	-1.01519	1.85753
C	4.55330	-0.18195	0.58929
C	5.66217	1.61090	-0.63616
C	6.90299	-0.44395	-0.18109
N	5.83915	0.47201	0.26639
H	-6.20615	-0.54874	-3.87976
H	-4.50311	-0.15249	-3.71518
H	-5.05679	-2.33953	-4.94554
H	-5.68945	-4.29488	-3.48459
H	-6.83257	-3.01232	-3.01069
H	-6.41079	-3.66848	0.91446
H	-6.02947	1.54741	-3.20673
H	-7.27025	1.95260	1.20092
H	-5.56947	2.24896	1.52551
H	-7.92550	2.15181	-1.39483
H	-7.19838	3.53176	-2.25671
H	-4.66498	-3.57546	1.08530
H	-6.00992	-3.66846	3.26852

H	-7.73242	-1.78884	2.34985
H	-7.09212	-1.50777	3.98896
H	-4.14780	4.97738	0.56806
H	-3.22715	2.10833	-3.43755
H	-6.79467	4.05385	0.17508
H	-3.29405	-3.66020	4.02556
H	-3.70975	1.27611	3.26102
H	-6.45919	0.55260	2.74489
H	-2.25137	-2.14444	-5.07455
H	-2.51658	-4.07925	-0.45853
H	-5.32802	-4.04822	-1.03336
H	0.20987	-2.50546	-5.09175
H	-0.04970	-4.37756	-0.43365
H	-0.92258	3.02037	-3.57255
H	-1.82297	5.85465	0.48142
H	-1.36485	1.59674	4.02910
H	-1.00070	-3.33798	4.91883
H	3.84560	-0.88123	6.26245
H	3.76563	0.64184	5.33054
H	3.34790	6.78338	-1.12595
H	3.70128	5.56151	-2.38465
H	5.07857	-4.63910	-1.85252
H	5.08210	-4.67255	-3.63600
H	7.89547	0.32782	-2.63578
H	7.46172	-0.76479	-4.84314
H	5.99919	-2.80346	-4.90920
H	5.58439	2.36783	2.04128
H	4.61915	4.51219	2.93276
H	3.53437	6.10592	1.32434
H	5.28299	-2.82591	0.90408
H	5.36892	-4.09795	3.06499
H	4.58174	-2.96202	5.15904
H	7.83555	0.13286	-0.20109
H	7.01948	-1.22390	0.57564
H	6.65670	1.90046	-1.00235
H	5.06497	1.37136	-1.53199
H	3.82289	0.61312	0.75307
H	4.19695	-0.80169	-0.24860
C	0.24050	0.33484	0.05348
Cl	0.86327	-1.13245	0.87426
Cl	0.62006	1.77433	1.04523
Cl	-1.53607	0.19206	-0.15282
Cl	1.01809	0.49392	-1.55419

Frequencies

16.4114	16.8865	18.6174
19.6431	22.9995	23.6383
24.5093	26.4761	27.8427
28.9301	30.3418	37.0852
38.1280	41.8480	44.5312
50.0628	55.1016	57.8130
62.2283	64.6692	71.9745
81.7243	91.1393	100.6129
106.1797	112.0793	116.7036
122.1316	122.5872	134.0080
140.7291	142.8098	147.0298
152.2305	158.4816	159.5869
162.3417	172.8972	173.8955
177.5849	185.1503	186.7926
197.0891	204.3585	206.5419
211.9965	214.7130	215.4643
225.3973	229.0493	235.9391
240.0600	243.8931	247.3312
248.7802	254.6941	259.8093
261.5088	270.4669	273.4402
289.6859	295.0103	297.5206
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343.0325	347.0075	348.1395
369.4065	371.3498	372.2268
384.6567	391.0223	393.1542
394.1702	402.9462	403.3242
410.2080	415.4066	419.6656
425.4936	426.8698	427.2418
435.4395	438.2480	442.0648
449.9932	461.2225	467.3856
471.7713	484.1332	484.4772
485.2594	489.2084	497.7486
500.2358	500.7940	527.5127
532.2370	537.4399	547.5472
550.5720	556.8388	566.5172
570.8172	573.3821	574.8027
579.2876	582.1410	585.1808
591.4258	592.4590	601.9281
605.1577	605.8034	608.6210
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659.4291	660.6230	661.0669
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737.3603	740.5857	741.9131
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778.2288	780.7901	782.7948
782.9179	784.1397	791.8164
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935.9539	936.3269	936.8518
940.6249	940.9858	941.5353
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958.6096	959.8271	965.5371
966.5726	968.3318	969.6548
985.1471	989.4461	990.9192
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1009.4048	1010.2397	1012.4952
1014.0555	1014.1702	1014.8169
1017.5959	1021.3170	1025.9058
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1115.3010	1119.6370	1125.6364
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1175.5117	1176.1098	1177.2345
1178.9353	1179.5206	1188.2133
1189.4474	1190.2693	1190.5508
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1278.0837	1280.9353	1287.6682
1291.0709	1291.4971	1299.4516
1299.9346	1300.2010	1300.5446
1313.0355	1313.5475	1317.8278
1318.7840	1319.6337	1322.5633
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1365.2014	1365.5117	1369.1126
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1377.1508	1383.6178	1399.6527
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1484.2236	1487.0407	1489.5992
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1497.5205	1499.5193	1501.2516
1502.0304	1502.6206	1510.3307
1511.8719	1520.8348	1521.0206
1521.8417	1534.3738	1535.3951
1535.8291	1604.4132	1605.3946
1625.8579	1626.7932	1627.9696
1636.5957	1637.1301	1637.7727
1647.9126	1648.4008	1650.0228
1672.9465	1675.2841	1676.6362
1676.7523	1678.3487	1679.1142
1767.6934	1769.8356	1770.4675
1817.4999	1819.3974	1820.6081
2987.0761	3007.0184	3015.5942
3017.3871	3017.7815	3046.8859
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3058.8729	3062.7727	3062.9271
3063.8543	3078.3372	3079.3946
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3094.4748	3103.2512	3103.5130
3103.8415	3122.9539	3126.8679
3129.9269	3132.3299	3135.0824
3144.8062	3153.8500	3157.4107
3172.6208	3172.8508	3173.7999
3180.0469	3180.2465	3180.5918
3188.4226	3191.7352	3193.3392
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TS3⊂CCl_4

E(RB3LYP) = -5602.46000886

E(RB3LYP-D3) = -5602.68518331

H - Sum of electronic and thermal Enthalpies= -5601.279992

G - Sum of electronic and thermal Free Energies= -5601.458696

Number of imaginary frequencies: 0

Cartesian Coordinates

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C	5.73558	-0.76292	-0.77739
C	5.51753	-1.73732	0.21898
C	5.34525	-1.33356	1.55616
C	5.23526	0.47149	3.36329
C	4.91244	-0.68090	4.34664
C	5.78529	-1.89532	3.96157
C	5.06601	-2.35099	2.66862
C	5.51000	-3.22760	-0.13557
C	5.65337	-3.52770	-1.64856
C	5.87981	-1.23812	-2.22837
C	6.08146	1.64011	-1.52899
C	6.10861	3.10056	-1.02075
C	5.77968	2.48712	1.24786
C	6.85405	3.12245	0.33207
C	6.69455	-2.55485	-2.24201

C	2.49356	4.49927	-0.69501
C	3.73372	4.18054	-1.32169
C	4.72361	3.55905	-0.60163
C	4.52997	3.22145	0.76914
C	3.36223	3.54284	1.41621
C	2.31163	4.19152	0.70303
C	2.29454	-1.76268	-3.68640
C	2.17802	-3.16084	-3.34830
C	3.26552	-3.81278	-2.69831
C	4.40034	-3.10473	-2.39017
C	4.52460	-1.72876	-2.73758
C	3.50273	-1.06994	-3.37754
C	1.21212	-2.59668	3.24424
C	1.12856	-1.58883	4.27374
C	2.31651	-0.91651	4.68561
C	3.52012	-1.23626	4.10611
C	3.60462	-2.24210	3.10031
C	2.48135	-2.90752	2.67340
C	0.02589	-3.25651	2.80668
C	-1.17144	-2.90804	3.37651
C	-1.25022	-1.93379	4.39975
C	-0.13531	-1.27921	4.85708
C	1.42613	5.08866	-1.43276
C	0.24081	5.33502	-0.78994
C	0.06969	5.05755	0.58650
C	1.07492	4.50742	1.33884
C	0.96547	-3.85611	-3.62514
C	-0.08310	-3.15772	-4.16447
C	0.02034	-1.78218	-4.47723
C	1.18412	-1.08581	-4.27343
C	-1.31626	-1.31383	-4.94737
O	-1.65280	-0.20698	-5.32128
N	-2.15781	-2.44346	-4.88068
C	-1.47762	-3.59258	-4.44901
O	-1.97597	-4.69927	-4.33805
C	-1.05430	5.84243	-1.32143
O	-1.33848	6.18986	-2.45468
C	-1.32851	5.41656	0.96236
O	-1.85837	5.38498	2.05579
C	-2.54982	-3.40038	3.09767
O	-2.91726	-4.25482	2.31346
C	-2.67718	-1.80935	4.80718
O	-3.17167	-1.13129	5.69102
N	-3.39434	-2.67354	3.96266
N	-1.94115	5.84320	-0.23383
C	-3.60967	-2.39240	-5.03581
C	-3.37179	6.09764	-0.37691
C	-4.83987	-2.87367	4.04678
C	-7.07958	0.48120	2.69337
C	-7.01854	0.24671	4.06597
C	-6.28337	-0.84251	4.52948
C	-5.64708	-1.66578	3.59381
N	-5.71817	-1.45075	2.27148
C	-6.41018	-0.38790	1.81956
C	-5.29164	2.63717	-1.95982
C	-5.31783	3.80360	-2.72418
C	-4.70977	4.95989	-2.23126
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C	-4.66045	2.67370	-0.71173
C	-5.33489	-2.99482	-1.19407
C	-5.64585	-3.91265	-2.19569
C	-5.12712	-3.71986	-3.47644
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N	-4.04209	-1.70345	-2.74960
C	-4.54335	-1.88181	-1.51651
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C	-6.42723	-0.14536	0.31289
N	-5.14970	0.23295	-0.30186
H	6.16310	0.95297	3.70562
H	4.45102	1.23565	3.43411
H	5.06033	-0.33468	5.37531
H	5.73253	-2.67755	4.72799
H	6.83677	-1.63646	3.79363
H	6.34265	-3.72005	0.38857
H	5.98430	2.63996	2.30850
H	7.05541	1.42523	-1.99273
H	5.33602	1.55264	-2.32959
H	7.79154	2.55511	0.31826
H	7.06822	4.15024	0.64787
H	4.59299	-3.70233	0.23489
H	5.90029	-4.58549	-1.79017
H	7.61480	-2.49023	-1.65058
H	6.95448	-2.83711	-3.26910
H	3.87301	4.43757	-2.37038
H	3.20887	3.30081	2.46583
H	6.55593	3.74537	-1.78502
H	3.16974	-4.86692	-2.44366
H	3.58119	-0.01642	-3.63766
H	6.31632	-0.46555	-2.86217
H	2.24776	-0.15919	5.46459
H	2.53307	-3.67216	1.90126
H	5.34389	-3.36120	2.36564
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H	1.54649	5.30801	-2.49075
H	1.25242	-0.02739	-4.51084
H	0.86797	-4.90982	-3.37564
H	-3.91756	-3.15290	-5.75950
H	-3.83728	-1.40099	-5.43651
H	-3.50248	6.98397	-1.00330
H	-3.75238	6.30158	0.62740
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Frequencies

-30.7443	11.4685	13.4566
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56.8353	63.9924	65.2304
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334.7019	346.9120	347.9341
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3091.5913	3103.1782	3103.5149
3103.7668	3104.7720	3127.8864
3131.7267	3134.0290	3136.9613
3137.4380	3140.4202	3143.1252
3172.2980	3172.7052	3173.5608
3179.1247	3180.2743	3180.5206
3187.1155	3187.7565	3188.1192
3197.9128	3198.4803	3198.5501
3200.6815	3202.1489	3202.5170
3202.8123	3206.9485	3209.7363
3213.0195	3219.9929	3226.4558

I3⊂CCl_4

E(RB3LYP) = -5602.46405158

E(RB3LYP-D3) = -5602.68977115

H - Sum of electronic and thermal Enthalpies= -5601.283045

G - Sum of electronic and thermal Free Energies= -5601.464556

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.83885	-1.06342	-0.04902
C	5.72359	-0.54143	1.25357
C	5.62970	0.85203	1.45784
C	5.62219	1.71855	0.34930
C	5.70101	1.20439	-0.96169
C	5.82304	-0.18412	-1.15282
C	6.03165	-2.56976	-0.25608
C	6.11277	-3.01173	-1.74039
C	6.93426	-1.96349	-2.51997
C	5.92205	-0.79221	-2.55564
C	5.69202	2.14417	-2.17137
C	5.49759	3.63912	-1.81754
C	5.49044	3.23617	0.52068
C	5.58122	1.43307	2.87382
C	5.51525	0.37132	3.99746
C	5.67471	-1.45280	2.48711
C	6.47220	-0.78446	3.63394
C	6.34051	3.94552	-0.56071
C	1.84704	-0.84634	4.40221
C	3.00361	-0.04532	4.62721
C	4.17490	-0.33672	3.97327
C	4.26063	-1.43705	3.07210
C	3.17015	-2.24117	2.84130
C	1.93243	-1.96687	3.49686
C	1.71468	4.15646	0.17772
C	1.72713	4.41123	-1.24262
C	2.95009	4.26926	-1.96175
C	4.09381	3.89472	-1.29971
C	4.08310	3.65840	0.10533
C	2.92506	3.78471	0.83204
C	2.34400	-1.99310	-3.55122
C	2.49576	-3.35975	-3.11292
C	3.73098	-3.77283	-2.53606
C	4.75563	-2.86965	-2.40025
C	4.62388	-1.53265	-2.87381
C	3.44937	-1.09935	-3.43998
C	1.07595	-1.54183	-4.02405
C	0.02522	-2.42290	-4.03171
C	0.19049	-3.77390	-3.64804
C	1.39400	-4.25805	-3.20690
C	0.60787	-0.54255	5.03763
C	-0.48548	-1.31745	4.75110
C	-0.40469	-2.41913	3.86697

C	0.77266	-2.76129	3.25206
C	0.52017	4.78691	-1.90301
C	-0.63496	4.86517	-1.16859
C	-0.64975	4.59366	0.21978
C	0.49107	4.25963	0.90112
C	-2.05030	4.73302	0.70438
O	-2.49114	4.59215	1.83057
N	-2.80776	5.09274	-0.42440
C	-2.02403	5.21191	-1.58358
O	-2.44120	5.55343	-2.67548
C	-1.89529	-1.19970	5.21544
O	-2.38949	-0.39878	5.98898
C	-1.76410	-3.02371	3.75813
O	-2.12190	-4.00174	3.12807
C	-1.42205	-2.19812	-4.31065
O	-1.98597	-1.18342	-4.67168
C	-1.13544	-4.44099	-3.72142
O	-1.41281	-5.61320	-3.52648
N	-2.05496	-3.43553	-4.05785
N	-2.59460	-2.23600	4.57740
C	-4.23783	5.33671	-0.38387
C	-4.03138	-2.41833	4.69911
C	-3.50870	-3.62770	-4.06490
C	-5.15277	-3.45811	-0.13897
C	-4.40215	-4.58073	-0.48437
C	-3.87925	-4.66909	-1.77157
C	-4.10767	-3.60862	-2.66215
N	-4.84674	-2.53805	-2.33754
C	-5.36912	-2.46204	-1.09794
C	-6.29309	0.34145	2.36928
C	-6.72876	0.06331	3.66216
C	-5.99078	-0.81946	4.45475
C	-4.84246	-1.39812	3.90908
N	-4.42094	-1.13222	2.66521
C	-5.12170	-0.27512	1.90630
C	-6.61235	2.53213	-2.52399
C	-6.98597	3.87302	-2.55225
C	-6.19995	4.80206	-1.87284
C	-5.07183	4.34576	-1.18365
N	-4.70611	3.05714	-1.15974
C	-5.45965	2.15866	-1.81793
C	-5.03701	0.70113	-1.76479
C	-4.54965	0.02406	0.53231
C	-6.22827	-1.24500	-0.77014
N	-5.54312	0.03568	-0.54551
H	6.96394	-2.87720	0.24045
H	5.22556	-3.12843	0.23586
H	6.51640	-4.02838	-1.79809
H	7.15548	-2.31467	-3.53485
H	7.87522	-1.69446	-2.02717
H	6.64683	2.04673	-2.70891
H	6.02758	-2.45890	2.25734
H	6.48026	2.04632	3.03623
H	4.72595	2.11202	2.97706
H	7.46393	-0.44228	3.31730
H	6.59019	-1.47622	4.47639
H	4.91090	1.83985	-2.87937
H	5.75196	4.25636	-2.68600
H	7.36315	3.55615	-0.62035
H	6.38450	5.02408	-0.36883
H	2.93559	0.79320	5.31821
H	3.22084	-3.08328	2.15411
H	5.73366	0.84328	4.96158
H	2.95477	4.46316	-3.03301
H	2.90256	3.59751	1.90351
H	5.74899	3.54998	1.53271
H	3.83273	-4.80023	-2.19085
H	3.32795	-0.07390	-3.78237
H	6.17487	-0.03893	-3.30256
H	1.50047	-5.29251	-2.89006
H	0.94068	-0.50499	-4.31987
H	0.82278	-3.60478	2.56851
H	0.53342	0.30253	5.71756
H	0.46727	4.05696	1.96858
H	0.52097	4.99143	-2.97080
H	-4.43575	6.35244	-0.74271
H	-4.51609	5.28765	0.67466
H	-4.30053	-2.37171	5.75845
H	-4.24202	-3.42714	4.32864
H	-3.93727	-2.81210	-4.64931
H	-3.71120	-4.58275	-4.55980
H	-5.56234	-3.34995	0.86067
H	-4.22349	-5.37052	0.24055
H	-3.29434	-5.52670	-2.08571
H	-6.83319	1.02148	1.71761
H	-7.62513	0.53619	4.05605
H	-6.29241	-1.04380	5.47426
H	-7.19454	1.77983	-3.04886
H	-7.86511	4.19277	-3.10629
H	-6.44320	5.86096	-1.89036
H	-6.81093	-1.47027	0.13089
H	-6.94431	-1.09354	-1.58493
H	-3.73313	-0.69284	0.35041
H	-4.10080	1.02408	0.55864
H	-3.94292	0.63578	-1.83318
H	-5.43276	0.17905	-2.63851
C	-0.11902	-0.05806	-0.10631
Cl	-0.73801	0.81771	-1.54055
Cl	-0.74601	0.71259	1.38249
Cl	1.67453	-0.00494	-0.09949
Cl	-0.66709	-1.76443	-0.16853

Frequencies

9.5645	13.6075	17.4194
17.7655	19.6033	23.1859
24.9485	27.4799	30.1427
31.5648	31.8635	35.2903
35.8262	37.3032	37.9178

48.2603	51.9296	57.8630	865.7539	868.6100	869.3589
60.8669	62.4584	75.2316	877.0900	888.1147	888.7727
76.8465	79.8004	93.7212	895.1306	897.4120	897.6701
100.7337	111.4812	115.3056	900.3093	911.4426	912.8021
122.6377	124.6643	128.3254	916.1987	916.5594	919.9757
140.3381	142.5502	149.0494	921.1248	928.0162	934.4489
151.7516	159.7443	160.4711	936.0687	936.2551	936.5516
165.3581	168.9815	171.9154	941.0585	941.1176	941.2305
174.4631	179.8045	189.2026	945.0665	952.4212	955.5683
192.6398	201.0919	213.0526	957.6735	961.5201	964.6961
214.6734	215.8606	220.5160	966.9492	967.1728	969.3578
227.6143	232.1579	237.6119	980.5104	985.6864	1000.6119
240.5234	242.3258	245.7166	1001.9967	1007.0694	1008.1965
250.2093	253.9289	259.6348	1010.2367	1011.6000	1012.3591
261.2414	263.2033	271.5466	1013.8996	1014.4333	1015.1675
285.8310	294.4150	296.2346	1018.4050	1019.9432	1023.3946
299.1089	301.6324	305.8472	1039.2850	1042.6844	1043.8492
308.5078	313.8052	314.1775	1066.3190	1075.1078	1077.8435
314.4780	316.2024	320.3943	1078.8726	1096.0809	1106.3767
331.7478	346.7729	348.1512	1107.4223	1107.7511	1115.0416
360.6901	371.8854	372.5461	1117.4270	1118.5569	1124.6443
382.9769	385.9308	390.8959	1131.2637	1141.2317	1145.8517
398.8292	401.1436	402.5154	1148.4368	1149.3863	1155.8529
404.4168	406.0841	420.1670	1165.6383	1166.3760	1176.3480
427.0835	428.2254	430.6858	1177.0384	1177.6352	1178.6280
437.4520	440.7945	444.2227	1179.0548	1179.4622	1186.2750
450.0890	464.3854	469.9577	1189.6384	1190.3108	1190.8626
472.2394	477.3938	484.2997	1192.3747	1194.7093	1227.2944
484.7990	485.5662	499.6150	1229.8019	1230.4247	1232.9922
501.0829	503.0224	527.5274	1235.4975	1237.0275	1244.4715
528.7852	544.5827	547.9692	1248.2646	1249.0820	1250.3108
549.9791	558.1904	566.9148	1254.0037	1254.3779	1254.7159
571.8871	573.9720	575.8422	1258.7552	1265.0389	1271.1415
578.0352	579.7384	584.8357	1276.9708	1277.5221	1277.9117
591.6866	594.4554	601.8217	1278.1113	1279.3506	1290.8163
606.0618	606.8277	609.6152	1291.5109	1293.1779	1299.1080
622.3954	625.7507	626.7102	1299.7928	1300.4956	1301.3654
652.7321	653.1244	654.7286	1313.0689	1314.5377	1317.8259
658.5073	660.3178	661.1889	1319.0287	1321.1928	1322.1292
663.1932	669.0994	700.4423	1326.9645	1339.5276	1340.0095
716.8351	718.1737	721.8684	1341.0455	1344.2881	1344.9526
724.1750	726.2579	727.3078	1346.9373	1357.0319	1360.5854
732.1052	735.0677	737.1386	1365.2319	1365.7511	1366.9257
738.7272	739.6548	741.4055	1375.9396	1376.6888	1390.2243
742.5452	743.2690	744.5461	1395.5066	1397.9578	1400.0233
752.0403	759.1760	760.4757	1403.1791	1408.7162	1411.6376
762.3804	767.7929	768.1157	1413.0457	1413.3215	1414.0979
771.9481	775.6590	777.7182	1420.5584	1422.8064	1450.5753
778.0165	779.5885	782.4673	1451.1877	1469.6050	1471.7053
784.4411	785.2348	785.3898	1472.5927	1473.3966	1474.8451
799.2417	801.3975	802.4246	1475.1619	1475.5859	1477.5336
813.1165	817.2062	822.9764	1478.5447	1483.4698	1484.3459
826.3755	828.8815	836.1194	1484.6047	1487.2617	1487.7265
839.6807	842.1130	853.7215	1490.7109	1492.1575	1494.2481

1494.4910	1496.3743	1501.5484
1502.5122	1502.8517	1514.8299
1517.7458	1520.8050	1520.8557
1521.7103	1534.2160	1535.0743
1536.0244	1604.8745	1605.5095
1626.8178	1628.8524	1630.1042
1634.6682	1638.7277	1639.7425
1647.7907	1649.4841	1649.5561
1674.9302	1675.0582	1676.4190
1677.6041	1678.7078	1678.7726
1767.0509	1770.4236	1772.5276
1818.3319	1819.5241	1821.2938
3003.1199	3015.3762	3017.0866
3017.1877	3044.3262	3055.0978
3056.9140	3057.2217	3057.2974
3062.2840	3063.1637	3065.7079
3066.5826	3076.2602	3079.2542
3079.3076	3079.6365	3080.3942
3086.2502	3097.5106	3103.0175
3103.2018	3103.8080	3110.1204
3122.9780	3131.3934	3132.0297
3132.1139	3132.9541	3160.5692
3172.4649	3172.7255	3173.4960
3179.1807	3180.3638	3181.4715
3183.4146	3185.0789	3195.4920
3197.4304	3198.1700	3198.3198
3199.3794	3201.8543	3202.3173
3202.7706	3204.9261	3207.0942
3213.8883	3216.0099	3229.7158

TS4⊂CCl_4

E(RB3LYP) = -5602.46332795

E(RB3LYP-D3) = -5602.68759124

H - Sum of electronic and thermal Enthalpies= -5601.283423

G - Sum of electronic and thermal Free Energies= -5601.462177

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.87520	-1.02475	0.03805
C	5.65773	-0.72633	1.39680
C	5.52252	0.61343	1.82108
C	5.57881	1.65267	0.87383
C	5.77467	1.36327	-0.49262
C	5.93447	0.02693	-0.90072
C	6.09308	-2.47606	-0.40510
C	6.27747	-2.66329	-1.93422
C	7.15175	-1.50781	-2.46450
C	6.14388	-0.33652	-2.37372
C	5.85214	2.48898	-1.52780
C	5.59432	3.90151	-0.95195
C	5.39811	3.12030	1.28037
C	5.36621	0.95055	3.30675
C	5.26405	-0.28326	4.23550
C	5.55026	-1.82950	2.45762
C	6.26633	-1.35039	3.74474
C	6.32041	4.00485	0.40702
C	1.61664	-1.62310	4.23920
C	2.73681	-0.84542	4.65163
C	3.94523	-0.99826	4.01876
C	4.10575	-1.93009	2.95290
C	3.04990	-2.70339	2.53291
C	1.77557	-2.57000	3.16188
C	1.65169	4.09406	0.77525
C	1.77599	4.55051	-0.58808
C	3.05478	4.51745	-1.21716
C	4.14619	4.05379	-0.52460
C	4.02217	3.59794	0.81962
C	2.80730	3.61540	1.45969
C	2.63380	-1.30234	-3.77493
C	2.75913	-2.72687	-3.58046
C	3.95604	-3.24959	-3.01140
C	4.97006	-2.39600	-2.65402
C	4.87123	-0.99649	-2.90018
C	3.73383	-0.45632	-3.44978
C	1.39097	-0.75728	-4.21461
C	0.33852	-1.60981	-4.42778
C	0.48370	-3.01028	-4.29629
C	1.66296	-3.58083	-3.89472
C	0.34476	-1.46731	4.86320
C	-0.70890	-2.21357	4.40416
C	-0.55756	-3.14180	3.34692
C	0.65296	-3.33925	2.73262
C	0.62590	5.03264	-1.27932
C	-0.57909	5.04104	-0.62591
C	-0.70128	4.59276	0.71049
C	0.37857	4.12968	1.41603
C	-2.12188	4.76065	1.12564
O	-2.64360	4.52530	2.20051
N	-2.78056	5.30497	0.01075
C	-1.91924	5.50738	-1.08058
O	-2.24373	6.00080	-2.14520
C	-2.13464	-2.22850	4.83244
O	-2.68378	-1.59196	5.71405
C	-1.88837	-3.76211	3.08472
O	-2.19117	-4.62080	2.27645
C	-1.09709	-1.32114	-4.70741
O	-1.64419	-0.25110	-4.88921
C	-0.83996	-3.63751	-4.54529
O	-1.12558	-4.82306	-4.59237
N	-1.74458	-2.57715	-4.70892
N	-2.77134	-3.16580	4.00403
C	-4.17328	5.69259	0.01475
C	-4.19968	-3.42373	4.04689
C	-3.19949	-2.74383	-4.78197
C	-4.96201	-3.35754	-0.95203
C	-4.14525	-4.36407	-1.46350

C	-3.58180	-4.19344	-2.72468
C	-3.83128	-2.99741	-3.41625
N	-4.62845	-2.03417	-2.93104
C	-5.19603	-2.21277	-1.72231
C	-6.53498	-0.37710	2.19555
C	-7.03033	-0.97347	3.35275
C	-6.27079	-1.95632	3.99108
C	-5.03999	-2.31051	3.43212
N	-4.56158	-1.73915	2.31941
C	-5.28464	-0.78542	1.71132
C	-6.96373	2.74739	-1.27147
C	-7.43122	4.01496	-0.93741
C	-6.51308	4.97818	-0.52373
C	-5.15950	4.63021	-0.46186
N	-4.70433	3.41496	-0.79226
C	-5.58920	2.48461	-1.19281
C	-5.06793	1.10381	-1.56431
C	-4.64705	-0.13996	0.49310
C	-6.14386	-1.12971	-1.21775
N	-5.56505	0.08303	-0.62482
H	6.99207	-2.86741	0.09381
H	5.25934	-3.10514	-0.06884
H	6.68490	-3.66022	-2.13408
H	7.44625	-1.68447	-3.50580
H	8.05432	-1.33651	-1.86727
H	6.85246	2.48711	-1.98569
H	5.93732	-2.77972	2.08759
H	6.23388	1.54658	3.62675
H	4.48552	1.58577	3.46279
H	7.26655	-0.94812	3.54834
H	6.35153	-2.17029	4.46770
H	5.14292	2.30177	-2.34362
H	5.90575	4.65692	-1.68156
H	7.35308	3.63947	0.37417
H	6.32334	5.03770	0.77477
H	2.61282	-0.13821	5.46995
H	3.15733	-3.41729	1.71879
H	5.41754	0.02651	5.27493
H	3.14501	4.87372	-2.24195
H	2.70008	3.26936	2.48557
H	5.56354	3.26461	2.34869
H	4.03390	-4.32249	-2.84440
H	3.63507	0.61458	-3.61381
H	6.44968	0.52911	-2.96212
H	1.75078	-4.65684	-3.76710
H	1.27249	0.31783	-4.31974
H	0.75809	-4.05157	1.91845
H	0.21635	-0.75577	5.67512
H	0.27318	3.79070	2.44326
H	0.71036	5.38514	-2.30431
H	-4.26598	6.57965	-0.62097
H	-4.42378	5.97901	1.04200
H	-4.49561	-3.58332	5.08809
H	-4.35714	-4.35597	3.49374
H	-3.60807	-1.82269	-5.20021
H	-3.40202	-3.57798	-5.46148
H	-5.41259	-3.45465	0.03082
H	-3.95207	-5.26542	-0.88778
H	-2.95493	-4.95818	-3.16953
H	-7.08840	0.39317	1.66709
H	-7.99057	-0.66963	3.76245
H	-6.61988	-2.42893	4.90526
H	-7.64563	1.96391	-1.58908
H	-8.49068	4.25137	-1.00007
H	-6.83629	5.98084	-0.25360
H	-6.80009	-1.58259	-0.46407
H	-6.77981	-0.81380	-2.05099
H	-3.77329	-0.74924	0.21375
H	-4.26305	0.84344	0.79347
H	-3.97146	1.13445	-1.60806
H	-5.41317	0.84720	-2.57044
C	-0.15522	-0.05816	-0.14922
Cl	-0.73755	-1.71335	-0.52089
Cl	-0.70265	1.06537	-1.42921
Cl	1.63740	-0.05734	-0.07329
Cl	-0.81804	0.46194	1.43198

Frequencies

-15.5164	9.0927	15.6896
17.1562	19.5576	22.8759
23.4782	26.0247	28.1600
28.6517	31.9001	32.2023
33.5630	35.5045	37.0813
47.2494	51.4376	58.0052
61.8687	63.1537	75.4793
76.4861	82.5949	96.3015
102.3069	113.1123	116.0818
123.1358	124.0038	127.5401
140.4864	141.9065	149.7832
150.7690	160.1347	160.3002
163.0777	167.0487	170.4913
175.0764	179.6202	185.0671
191.1773	199.5770	212.6802
214.8029	215.4470	218.0547
225.7741	233.7323	234.9135
239.4966	242.0713	245.1392
250.0241	252.3721	257.7830
262.2422	267.5902	271.9149
282.1678	290.7553	296.3838
298.6493	301.7320	306.9513
308.5618	313.3807	314.3800
314.8667	316.5063	321.8842
332.1594	346.5354	347.8267
349.0222	370.4329	372.8271
374.3560	386.1707	390.5242
399.3152	400.0086	402.7371
403.8517	405.6863	419.8398
427.7115	428.2403	429.8808

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3196.4625	3198.3576	3198.3925
3199.5701	3201.1560	3201.8082
3202.3667	3204.4101	3208.0941
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$I4 \subset CCl_4$

E(RB3LYP) = -5602.46443518

E(RB3LYP-D3) = -5602.68601731

H - Sum of electronic and thermal Enthalpies= -5601.283672

G - Sum of electronic and thermal Free Energies= -5601.465032

Number of imaginary frequencies: 0

Cartesian Coordinates

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C	-5.64559	-1.26841	-1.29312
C	-5.59838	0.02594	-1.85483
C	-5.76839	1.15094	-1.02579
C	-5.96680	0.98971	0.36157
C	-5.99254	-0.30382	0.91247
C	-5.90395	-2.84843	0.69014
C	-6.01515	-2.88532	2.23672
C	-6.99887	-1.78100	2.67636
C	-6.13394	-0.52382	2.42126
C	-6.18893	2.20306	1.26808
C	-6.06403	3.56404	0.54591
C	-5.72112	2.57897	-1.58644
C	-5.39763	0.21607	-3.36089
C	-5.18166	-1.09951	-4.14762
C	-5.46017	-2.46862	-2.22959
C	-6.14963	-2.16147	-3.58145
C	-6.75545	3.44778	-0.83015
C	-1.48296	-2.28158	-3.90532
C	-2.61487	-1.58570	-4.42195
C	-3.83827	-1.72155	-3.81326
C	-3.99878	-2.55303	-2.66710
C	-2.93236	-3.24121	-2.14204
C	-1.64541	-3.12459	-2.74545
C	-2.11099	3.99144	-1.11306
C	-2.31607	4.53779	0.20679
C	-3.60503	4.44095	0.80657
C	-4.62609	3.81634	0.13466
C	-4.41662	3.24740	-1.15478
C	-3.19343	3.33816	-1.77332
C	-2.49865	-0.93655	3.77654
C	-2.46515	-2.37892	3.73768
C	-3.60793	-3.08950	3.26887
C	-4.72422	-2.39812	2.86710
C	-4.77937	-0.97781	2.96221
C	-3.69522	-0.25814	3.40311
C	-1.32160	-0.21284	4.13130
C	-0.18133	-0.91543	4.42448
C	-0.16925	-2.32925	4.44566
C	-1.27733	-3.06690	4.12021
C	-0.19873	-2.15365	-4.51114
C	0.85977	-2.82762	-3.95917
C	0.70194	-3.65139	-2.81965
C	-0.51747	-3.81770	-2.21578
C	-1.23241	5.16220	0.89000
C	-0.01388	5.22805	0.26682
C	0.18325	4.71484	-1.03660
C	-0.83072	4.10700	-1.73080
C	1.59739	4.98107	-1.42584
O	2.16411	4.74866	-2.47853
N	2.18588	5.60775	-0.31584
C	1.27427	5.80797	0.73658
O	1.52607	6.36774	1.78775
C	2.29464	-2.86280	-4.35762
O	2.85245	-2.31052	-5.28915
C	2.03436	-4.22049	-2.47201
O	2.33229	-4.98921	-1.57625
C	1.20377	-0.43934	4.70125
O	1.62166	0.69870	4.78701
C	1.20498	-2.77329	4.79718
O	1.60941	-3.90482	5.00891
N	1.98477	-1.60766	4.85405
N	2.92690	-3.70533	-3.42944
C	3.55940	6.07770	-0.27964
C	4.35311	-3.97167	-3.43084
C	3.43070	-1.59145	5.09716
C	5.76464	-2.87055	1.77225
C	5.09954	-3.84305	2.51632
C	4.34085	-3.44433	3.61259
C	4.25489	-2.07524	3.90849
N	4.90219	-1.13844	3.19801
C	5.65375	-1.52740	2.15108
C	6.72237	-0.73105	-2.00816
C	7.23145	-1.51906	-3.03882
C	6.45967	-2.56948	-3.53491
C	5.20280	-2.79598	-2.96447
N	4.71374	-2.04436	-1.97176
C	5.44964	-1.02329	-1.50210
C	6.54873	3.06065	-0.45907
C	6.74061	4.22791	-1.19186
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C	4.61110	4.98450	-0.38771
N	4.42040	3.85976	0.31634
C	5.36719	2.90841	0.28046
C	5.13713	1.66376	1.13374
C	4.78446	-0.17398	-0.43088
C	6.43688	-0.45973	1.39252
N	5.70012	0.45815	0.51733
H	-6.77948	-3.37052	0.27591
H	-5.02746	-3.43235	0.38355
H	-6.30043	-3.89252	2.55922
H	-7.24247	-1.87236	3.74151
H	-7.93140	-1.77711	2.10091

H	-7.19515	2.13984	1.70861
H	-5.82088	-3.39104	-1.77224
H	-6.28234	0.71785	-3.77982
H	-4.54970	0.88759	-3.54582
H	-7.17454	-1.79265	-3.46131
H	-6.16842	-3.05542	-4.21591
H	-5.48567	2.18315	2.10974
H	-6.47138	4.35676	1.18282
H	-7.74564	2.98114	-0.77841
H	-6.85327	4.43076	-1.30581
H	-2.48835	-0.95881	-5.30295
H	-3.04241	-3.87941	-1.26774
H	-5.30743	-0.90934	-5.21905
H	-3.75904	4.87491	1.79310
H	-3.02375	2.91648	-2.76186
H	-5.86872	2.59057	-2.66709
H	-3.56679	-4.17619	3.21879
H	-3.71496	0.82859	3.44923
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H	-1.24658	-4.15357	4.11616
H	-1.32537	0.87390	4.12537
H	-0.62703	-4.45186	-1.33981
H	-0.06660	-1.52201	-5.38609
H	-0.66677	3.70928	-2.72893
H	-1.37466	5.56969	1.88780
H	3.66525	6.60050	0.67718
H	3.70819	6.80562	-1.08485
H	4.65468	-4.26907	-4.44005
H	4.50161	-4.82447	-2.75933
H	3.69588	-0.55661	5.32005
H	3.62916	-2.21752	5.97377
H	6.36718	-3.14423	0.91075
H	5.17216	-4.89380	2.24777
H	3.80664	-4.16429	4.22190
H	7.28316	0.10240	-1.59887
H	8.21196	-1.31031	-3.45994
H	6.81741	-3.19245	-4.35030
H	7.28467	2.26438	-0.45522
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Frequencies

11.5869	15.3625	17.4687
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3198.4714	3199.0085	3199.4889
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3202.2521	3204.0628	3207.0869
3223.3812	3227.7047	3236.6854

TS5⊂CCl_4

E(RB3LYP) = -5602.45566867

E(RB3LYP-D3) = -5602.68025951

H - Sum of electronic and thermal Enthalpies= -5601.276112

G - Sum of electronic and thermal Free Energies= -5601.454519

Number of imaginary frequencies: 0

Cartesian Coordinates

C	-5.43790	0.68154	-2.01030
C	-5.55973	1.63736	-0.98346
C	-5.80192	1.22832	0.34555
C	-5.97103	-0.13939	0.63433
C	-5.87287	-1.10171	-0.39189
C	-5.61272	-0.68536	-1.71074
C	-5.11548	1.13112	-3.43807
C	-4.91292	-0.03123	-4.44176
C	-6.00461	-1.08711	-4.16149
C	-5.46247	-1.70106	-2.84921

C	-6.04763	-2.59117	-0.08578
C	-6.21566	-2.91188	1.41797
C	-6.22719	-0.62944	2.06682
C	-5.88521	2.25651	1.47527
C	-5.61079	3.70965	1.02510
C	-5.40899	3.13911	-1.26906
C	-6.34021	3.92986	-0.31943
C	-7.16755	-1.85719	2.02381
C	-1.79777	4.43488	0.70215
C	-3.06623	4.29790	1.34030
C	-4.16172	3.90703	0.61005
C	-4.04441	3.61281	-0.77967
C	-2.84861	3.76615	-1.43606
C	-1.69426	4.19144	-0.71621
C	-2.77109	-1.54864	3.62293
C	-2.73923	-2.91843	3.17055
C	-3.85897	-3.43977	2.45738
C	-4.93289	-2.62923	2.18120
C	-4.94860	-1.26790	2.60237
C	-3.90568	-0.74018	3.32231
C	-1.67853	-2.58146	-3.16716
C	-1.34351	-1.56479	-4.13483
C	-2.36848	-0.68958	-4.60327
C	-3.65251	-0.82270	-4.13187
C	-3.98114	-1.83696	-3.18613
C	-3.02345	-2.69852	-2.71280
C	-0.66102	-3.44502	-2.66872
C	0.62110	-3.28039	-3.12183
C	0.95008	-2.29789	-4.08525
C	0.00091	-1.45039	-4.59851
C	-0.63481	4.80305	1.43981
C	0.55698	4.92350	0.77252
C	0.64891	4.72930	-0.62578
C	-0.44184	4.37000	-1.37356
C	-1.58119	-3.71452	3.41310
C	-0.51357	-3.14370	4.05692
C	-0.55367	-1.80685	4.51699
C	-1.65316	-1.01186	4.32557
C	0.76125	-1.49447	5.14296
O	1.13178	-0.46877	5.68547
N	1.53733	-2.65441	4.99790
C	0.83533	-3.69794	4.36690
O	1.27591	-4.81118	4.14952
C	1.91653	5.25345	1.28194
O	2.27508	5.48863	2.42199
C	2.05815	4.98648	-1.03677
O	2.54452	5.00513	-2.15223
C	1.86166	-4.02140	-2.76911
O	2.00510	-4.96330	-2.01267
C	2.40745	-2.41479	-4.37797
O	3.08382	-1.80593	-5.18820
N	2.88856	-3.42572	-3.52895
N	2.75381	5.26197	0.15249
C	2.93701	-2.73764	5.38107
C	4.17055	5.54928	0.21458
C	4.24533	-3.95224	-3.57266
C	7.39109	-1.35584	-2.38664
C	7.43156	-1.89703	-3.67052
C	6.38461	-2.71686	-4.08049
C	5.33898	-2.97034	-3.18349
N	5.29224	-2.44051	-1.95351
C	6.29936	-1.64308	-1.55613
C	6.71214	2.30875	-0.85919
C	7.26520	3.58221	-0.73574
C	6.43694	4.64302	-0.38006
C	5.08108	4.38096	-0.14997
N	4.55427	3.15581	-0.24031
C	5.34761	2.12798	-0.59594
C	5.45473	-0.18630	3.08063
C	5.67028	-0.26320	4.45576
C	4.84809	-1.08296	5.22696
C	3.83905	-1.80593	4.58206
N	3.63591	-1.74409	3.26105
C	4.42054	-0.94423	2.51940
C	4.08345	-0.89171	1.03114
C	4.67398	0.76913	-0.75350
C	6.25199	-1.07520	-0.13821
N	5.10150	-0.24741	0.21002
H	-5.93455	1.76101	-3.81570
H	-4.21971	1.76432	-3.43451
H	-4.92646	0.36303	-5.46367
H	-6.03665	-1.84386	-4.95416
H	-7.00456	-0.65354	-4.04741
H	-6.93522	-2.96810	-0.61567
H	-5.58907	3.36277	-2.32188
H	-6.88939	2.22551	1.92325
H	-5.18511	1.98816	2.27626
H	-7.36902	3.55231	-0.31807
H	-6.35416	4.99119	-0.59378
H	-5.19416	-3.15719	-0.47826
H	-6.56278	-3.94421	1.53570
H	-8.06414	-1.68656	1.41715
H	-7.47610	-2.13871	3.03749
H	-3.14408	4.51824	2.40361
H	-2.75529	3.56739	-2.50158
H	-5.91988	4.40153	1.81619
H	-3.83803	-4.47992	2.13640
H	-3.91143	0.29514	3.65642
H	-6.60682	0.17183	2.70236
H	-2.11176	0.07362	-5.33596
H	-3.26295	-3.47319	-1.98771
H	-5.93532	-2.65256	-2.60215
H	0.26250	-0.69697	-5.33747
H	-0.90177	-4.20838	-1.93348
H	-0.35868	4.21030	-2.44557
H	-0.69611	4.97009	2.51233
H	-1.66672	0.01854	4.67134
H	-1.54057	-4.74355	3.06449

H	3.22959	-3.78002	5.21647
H	3.02993	-2.51650	6.44934
H	4.36878	5.87419	1.24185
H	4.39069	6.39061	-0.45319
H	4.25212	-4.79867	-2.87888
H	4.44237	-4.32990	-4.58219
H	8.19522	-0.71836	-2.02861
H	8.25906	-1.67753	-4.34045
H	6.36603	-3.14594	-5.07772
H	7.32438	1.47209	-1.17825
H	8.32086	3.74881	-0.93596
H	6.82532	5.65542	-0.29946
H	6.05404	0.45348	2.44205
H	6.45875	0.32148	4.92365
H	4.97126	-1.14803	6.30450
H	7.18605	-0.51765	0.02729
H	6.27588	-1.91410	0.56642
H	4.83108	0.42034	-1.78683
H	3.60187	0.93709	-0.63933
H	3.14990	-0.32862	0.93359
H	3.85918	-1.91482	0.69496
C	-0.19902	0.01912	0.24022
Cl	0.58826	0.52347	-1.29333
Cl	0.20873	-1.68838	0.58336
Cl	-1.97361	0.19807	0.08114
Cl	0.39488	1.05305	1.57757

Frequencies

-20.6468	11.8133	15.5955
19.7925	21.1718	22.0841
24.2776	27.4993	29.6839
32.3684	34.4535	35.3014
36.5827	37.3340	41.7749
46.4215	50.0451	52.4024
57.4558	61.6153	64.0650
74.2013	82.2570	99.6350
105.1076	111.0411	114.8199
120.5618	122.5931	126.5199
140.1903	141.5617	150.5634
151.1629	159.6241	160.1532
164.1409	171.0058	172.1337
177.6348	178.8289	184.0816
191.0988	198.4340	203.4152
212.6132	214.5582	215.9422
229.4658	233.3744	235.6814
237.8871	241.5737	244.4880
247.1001	248.3037	253.8629
258.2442	262.5469	266.4277
272.3432	288.3684	291.8464
298.0785	299.6237	302.4991
305.5162	311.3117	313.6610
314.0583	315.4698	318.3721
328.8001	341.6620	346.8182
347.4570	358.1137	371.4350
372.4979	372.7567	386.6917
396.7249	399.5949	401.4450
404.6665	405.7455	419.9962
428.5250	429.0557	431.3992
436.0102	438.4900	450.4652
457.2901	468.8874	471.8838
475.6908	483.9477	484.5590
485.0939	493.0841	501.3521
501.9824	503.2026	524.1245
529.9936	532.5901	547.0332
549.2801	549.5369	568.5396
572.4311	574.3892	577.9839
578.1162	579.1862	581.1038
594.3545	595.0926	604.5734
606.9270	607.0725	612.9250
622.3959	625.4254	628.1981
646.9328	652.9202	653.6814
655.9980	658.6455	660.4155
661.2121	664.0429	694.9246
712.3160	716.3372	718.9123
721.4222	724.6219	726.4725
730.2650	733.2029	734.0087
739.9385	740.2207	741.2038
741.7835	743.0948	744.2633
747.7166	750.1080	753.1524
762.7646	764.9690	766.7741
768.1562	769.2645	770.9086
772.4754	779.3417	780.0339
783.7312	785.6288	786.3383
796.2723	802.0841	805.3813
809.8142	817.9148	823.1494
826.0668	827.8412	833.9370
839.5957	842.6715	845.9501
864.1326	869.3546	869.4523
877.1308	888.4246	888.7761
894.8434	897.1870	897.9805
900.4061	904.1452	908.5779
911.8943	914.6457	918.9729
919.9807	922.2503	936.3716
937.0645	937.1779	941.1450
941.5243	941.8936	945.5065
949.6821	957.4329	959.0005
960.9234	964.5945	966.3436
967.3383	970.4757	973.4398
987.9772	989.1255	999.0882
999.8805	1002.0105	1003.7052
1009.3815	1010.9609	1012.2495
1012.9609	1013.9837	1015.5104
1018.7012	1019.2533	1028.8003
1039.5012	1043.8291	1044.5204
1066.5860	1074.9679	1077.5756
1077.7044	1106.6884	1107.0608
1109.3027	1112.7660	1117.0471
1117.3812	1120.2543	1128.4776

1142.9616	1147.4637	1150.4635
1154.2458	1155.3082	1166.2047
1166.5178	1176.6354	1177.5533
1177.8767	1178.0121	1179.1892
1179.5167	1179.8608	1184.0183
1189.6479	1190.7396	1191.0609
1192.1739	1193.2748	1222.0840
1228.3350	1229.9418	1231.2197
1231.6452	1236.3076	1237.8143
1244.9257	1249.3914	1249.6975
1253.6529	1253.9683	1254.1543
1259.4032	1263.6234	1265.4622
1269.5783	1271.7888	1277.5805
1277.7326	1278.0152	1290.2938
1290.5489	1296.6668	1298.7539
1299.5551	1300.3476	1306.2829
1314.4498	1314.9272	1317.9549
1318.7381	1320.8222	1325.6702
1332.2052	1338.9445	1339.5786
1340.6944	1344.9821	1345.5306
1350.2193	1351.4775	1356.4440
1364.6246	1373.0041	1376.6524
1377.3233	1387.1328	1389.0616
1392.6528	1398.9668	1400.3871
1405.4951	1412.5293	1413.1758
1413.4969	1414.8038	1417.4149
1423.7225	1427.4775	1450.4578
1450.9425	1469.6618	1471.0995
1472.4680	1474.3182	1474.5743
1474.7380	1474.9895	1477.3902
1478.1922	1481.8475	1484.1012
1484.1467	1484.2458	1487.6221
1488.7668	1492.3346	1496.7077
1497.6995	1498.4313	1500.6420
1501.2062	1502.2720	1505.3307
1518.5349	1520.9430	1521.0509
1521.8772	1534.6183	1534.8394
1535.1299	1604.3490	1605.2472
1628.5462	1629.3798	1632.6112
1636.4993	1637.3586	1638.5214
1648.4838	1649.3291	1649.4198
1674.7751	1676.1509	1676.5843
1677.9579	1678.6375	1678.7050
1769.9164	1772.8612	1773.5497
1820.0460	1821.1631	1822.7866
2997.9950	3009.4000	3015.6983
3017.1364	3017.4556	3024.1443
3057.2586	3057.4264	3057.5416
3059.7550	3064.6920	3065.9501
3067.0079	3068.1800	3071.9114
3078.5415	3078.8113	3079.5023
3083.1207	3099.7868	3103.0922
3103.3978	3103.6228	3106.0398
3116.8217	3119.0865	3124.4832
3128.3396	3129.0986	3139.1526
3171.8853	3172.6311	3172.7679
3179.8207	3180.4855	3180.7307
3181.2856	3184.1121	3184.2823
3196.7508	3197.5841	3197.9767
3198.4973	3198.7085	3200.1065
3201.0456	3202.2949	3202.3520
3212.1753	3221.7089	3224.5913

I5⊂CCl_4

E(RB3LYP) = -5602.45628027

E(RB3LYP-D3) = -5602.68375817

H - Sum of electronic and thermal Enthalpies= -5601.275722

G - Sum of electronic and thermal Free Energies= -5601.456980

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.29239	1.32768	1.84702
C	5.51069	1.84207	0.55428
C	5.79991	0.97121	-0.51850
C	5.94759	-0.40854	-0.27662
C	5.77076	-0.92629	1.02327
C	5.44084	-0.05523	2.07828
C	4.88651	2.26820	2.98474
C	4.57432	1.55245	4.32284
C	5.65172	0.46536	4.53032
C	5.18528	-0.58442	3.49439
C	5.93506	-2.42291	1.29780
C	6.18781	-3.27374	0.03127
C	6.27445	-1.39122	-1.41118
C	5.95060	1.51205	-1.94154
C	5.70709	3.03381	-2.06365
C	5.41950	3.34975	0.26984
C	6.40773	3.71202	-0.86404
C	7.19067	-2.51067	-0.86187
C	1.91487	3.92939	-2.17311
C	3.19164	3.52729	-2.66836
C	4.25455	3.40703	-1.80635
C	4.09254	3.65813	-0.41249
C	2.89395	4.09381	0.09363
C	1.77460	4.25094	-0.77365
C	2.89641	-2.83773	-2.71717
C	2.81268	-3.93961	-1.78945
C	3.88419	-4.15829	-0.87400
C	4.95625	-3.29998	-0.85724
C	5.01963	-2.19115	-1.75009
C	4.02940	-1.97397	-2.67558
C	1.36846	-1.29377	3.84934
C	0.99431	0.00679	4.34994
C	2.00681	0.99645	4.53091
C	3.31575	0.70314	4.23018
C	3.68119	-0.58747	3.74811

C	2.73665	-1.56522	3.56022
C	0.36717	-2.28552	3.64153
C	-0.93690	-1.97240	3.92026
C	-1.30680	-0.70490	4.42859
C	-0.37442	0.27761	4.65062
C	0.77596	4.00128	-3.02853
C	-0.42761	4.38229	-2.49206
C	-0.54940	4.75054	-1.13189
C	0.51665	4.69550	-0.27332
C	1.64779	-4.76213	-1.77379
C	0.62092	-4.46433	-2.63235
C	0.71363	-3.39753	-3.55613
C	1.82375	-2.59711	-3.62423
C	-0.57166	-3.32227	-4.30450
O	-0.89437	-2.56869	-5.20559
N	-1.38810	-4.32688	-3.76294
C	-0.73378	-5.07369	-2.76521
O	-1.21145	-6.01867	-2.16622
C	-1.78064	4.46225	-3.11146
O	-2.11972	4.21113	-4.25356
C	-1.96688	5.12911	-0.87919
O	-2.47732	5.56325	0.13760
C	-2.16489	-2.80192	3.79703
O	-2.27752	-3.95870	3.43696
C	-2.78117	-0.71740	4.65830
O	-3.49458	0.14376	5.14159
N	-3.22585	-1.97771	4.22296
N	-2.64190	4.90347	-2.08966
C	-2.78823	-4.50388	-4.12154
C	-4.08066	5.02908	-2.25098
C	-4.58179	-2.47544	4.39628
C	-7.68007	-0.52401	2.23950
C	-7.86635	-0.76099	3.59932
C	-6.83781	-1.36452	4.31839
C	-5.66666	-1.72389	3.64109
N	-5.48689	-1.50053	2.33147
C	-6.47154	-0.90459	1.63819
C	-6.21374	2.72173	0.61788
C	-6.73729	3.95882	0.24517
C	-6.05466	4.72164	-0.69971
C	-4.87283	4.20640	-1.24293
N	-4.38898	3.00343	-0.91431
C	-5.03749	2.26781	0.00532
C	-5.13839	-1.11824	-3.04962
C	-5.25616	-1.61803	-4.34553
C	-4.49623	-2.72572	-4.71819
C	-3.64520	-3.29616	-3.76651
N	-3.54318	-2.83139	-2.51525
C	-4.26901	-1.75870	-2.15854
C	-4.05339	-1.27165	-0.72780
C	-4.40227	0.93834	0.38560
C	-6.27886	-0.66400	0.13753
N	-4.97364	-0.21290	-0.32009
H	5.69724	2.98777	3.17230
H	4.01572	2.86145	2.67996
H	4.52750	2.29251	5.12909
H	5.60608	0.04989	5.54387
H	6.66939	0.82605	4.34267
H	6.78153	-2.57311	1.98458
H	5.58298	3.93337	1.17765
H	6.96643	1.30391	-2.30818
H	5.26774	0.97918	-2.61528
H	7.42040	3.33240	-0.68685
H	6.45623	4.79939	-0.99471
H	5.04899	-2.80935	1.81573
H	6.52434	-4.27452	0.32320
H	8.05295	-2.12261	-0.30791
H	7.55321	-3.14436	-1.67980
H	3.30079	3.32707	-3.73290
H	2.77075	4.31793	1.15103
H	6.06223	3.38236	-3.03958
H	3.82626	-5.00451	-0.19140
H	4.07260	-1.13682	-3.36905
H	6.70307	-0.87837	-2.27342
H	1.72077	1.97472	4.91357
H	3.00517	-2.55212	3.18980
H	5.64756	-1.56068	3.64661
H	-0.66622	1.24925	5.04178
H	0.63811	-3.26610	3.25895
H	0.40640	4.95989	0.77530
H	0.86182	3.73215	-4.07833
H	1.87553	-1.76963	-4.32712
H	1.56714	-5.58477	-1.06747
H	-3.12742	-5.38740	-3.57171
H	-2.86021	-4.71028	-5.19422
H	-4.29455	4.69904	-3.27349
H	-4.36862	6.08328	-2.16896
H	-4.55393	-3.51565	4.05464
H	-4.82390	-2.47414	5.46516
H	-8.45597	-0.04638	1.64640
H	-8.78913	-0.46718	4.09347
H	-6.93140	-1.54350	5.38551
H	-6.68972	2.12701	1.39206
H	-7.64608	4.33692	0.70708
H	-6.40869	5.70897	-0.98401
H	-5.68358	-0.23975	-2.72286
H	-5.91690	-1.13762	-5.06318
H	-4.53889	-3.12272	-5.72844
H	-7.04748	0.05521	-0.17988
H	-6.50903	-1.59729	-0.39196
H	-4.45504	0.81492	1.47999
H	-3.34856	1.00711	0.11492
H	-3.03025	-0.88797	-0.66949
H	-4.08463	-2.14157	-0.05609
C	0.30816	-0.01653	-0.37333
Cl	-0.32040	0.42886	-1.98961
Cl	-0.46249	1.02224	0.87284
Cl	2.08113	0.22182	-0.32105

Cl	-0.08104	-1.73161	-0.04037

Frequencies

11.9488	14.8023	17.2514
19.8760	21.4425	22.6190
25.2945	25.6813	28.1713
32.5416	33.9474	35.8219
38.1365	40.1505	45.7694
46.9500	50.6366	53.2099
56.3790	63.3101	64.7883
75.6730	83.6104	98.5150
104.9817	114.6829	116.4770
120.0301	121.8623	130.3914
140.4413	142.4070	150.3509
151.9751	159.1023	160.4451
165.9402	170.4435	176.5240
179.0223	184.4191	185.7532
190.7584	199.0340	204.7375
213.3608	213.9356	216.7545
228.3200	231.0030	236.6686
240.3245	245.1290	245.6166
246.9015	250.1668	257.1255
259.7026	263.9860	265.0589
272.5301	287.8664	292.1881
298.9162	300.3031	303.2167
305.8619	309.7023	313.2320
314.0470	316.2294	318.4305
328.5760	344.2082	346.6792
347.4920	354.8469	371.2466
371.8123	380.5800	386.6108
397.5923	399.3140	402.0922
405.1693	406.3058	420.1253
428.5119	428.9967	431.5980
436.3188	437.9946	450.6109
454.9377	469.1131	471.7814
475.1463	484.0020	484.6478
485.1937	493.8336	500.6559
501.4883	502.1802	526.6622
530.4211	533.6909	547.8971
549.9360	550.5986	567.7095
572.3082	574.1307	577.7037
577.9063	580.6465	582.3181
594.3662	594.7312	601.2832
606.5960	607.2436	613.9276
620.0042	625.3866	629.4941
645.4346	653.1640	654.7261
657.0340	660.2803	660.9039
663.2503	668.0815	686.2690
710.3239	715.6647	718.0144
721.1308	724.1837	726.0391
732.1046	732.8698	737.5050
739.9094	740.6862	741.1500
742.3466	743.2923	744.4088
746.6171	749.6248	759.1042
762.8136	764.5417	768.3357
768.4523	770.0256	772.4654
778.8106	779.1429	781.6189
783.3917	785.2283	786.0092
803.2475	805.2760	806.7383
809.7203	814.1661	818.8908
826.2785	827.6419	830.1083
840.1769	842.7227	847.7640
869.3126	869.4174	874.8795
877.2798	888.7652	888.8738
894.8679	897.4508	897.8784
900.2940	906.4837	911.4989
915.1380	918.7882	919.3537
920.3015	930.4528	936.2692
936.9399	937.3877	941.1018
941.7304	941.8338	948.8945
950.7624	959.1010	960.3146
961.0937	965.2994	966.4191
967.9331	970.7018	976.9777
988.2172	991.1707	998.0943
1002.7508	1004.7206	1009.0367
1009.6359	1011.9422	1012.8492
1013.4820	1014.1341	1015.3130
1016.0239	1020.1043	1020.8019
1039.1594	1043.6848	1044.5484
1066.4894	1074.7079	1077.2358
1077.7178	1105.7568	1106.6656
1108.0946	1114.0517	1114.5208
1117.5341	1122.7986	1128.7365
1144.2260	1145.7848	1147.0598
1153.8551	1155.1567	1165.8434
1166.1220	1175.9224	1177.1524
1177.5689	1178.3093	1178.7178
1179.4172	1180.0154	1184.0173
1189.6480	1190.5858	1190.7648
1192.2768	1193.3279	1222.9415
1229.0560	1230.1093	1230.8526
1232.5229	1235.7987	1236.8773
1244.9054	1249.1376	1249.6601
1253.4993	1253.7638	1254.0974
1259.0999	1261.2329	1265.5917
1266.9418	1276.0627	1277.5117
1277.5878	1277.6253	1290.3005
1290.4899	1294.8524	1298.0987
1298.9224	1300.0024	1303.6823
1308.9801	1314.6583	1317.4288
1318.4045	1320.3161	1325.2481
1327.9450	1337.7731	1339.1935
1339.6469	1340.9483	1344.7024
1345.6347	1350.6932	1350.9951
1363.5932	1364.2884	1376.4491
1377.0606	1385.9263	1390.1454
1392.0574	1395.0862	1399.9664
1400.1217	1412.3669	1412.8433

1413.1484	1415.6630	1417.7351
1424.9663	1430.6823	1449.8529
1450.3202	1469.3981	1471.9495
1472.1319	1473.4411	1474.4098
1474.6081	1474.8416	1478.2792
1479.0566	1483.2859	1484.1020
1484.3845	1485.2947	1486.9541
1494.2892	1494.8187	1497.7902
1498.8026	1500.6446	1501.0944
1501.9141	1503.1966	1507.1208
1517.6713	1520.9263	1521.2378
1522.0420	1534.1561	1535.0115
1535.2660	1603.4811	1604.5131
1628.0781	1629.5817	1631.2457
1635.8450	1638.3761	1639.0451
1647.4970	1649.2842	1649.4098
1673.7910	1675.9718	1676.5795
1677.1177	1678.6436	1678.7393
1769.5415	1772.2593	1773.4111
1819.9551	1820.4181	1822.5791
2991.0141	3015.4951	3017.2847
3018.7177	3021.0555	3031.7537
3057.2372	3057.3868	3057.8070
3062.1250	3063.0155	3063.3154
3066.8316	3067.7503	3069.0362
3075.0586	3078.3232	3078.8398
3079.4966	3102.3197	3103.1538
3103.3555	3103.8474	3106.9069
3110.2230	3121.4111	3122.3560
3127.9536	3129.0631	3150.9581
3171.6938	3172.7094	3172.7546
3179.9619	3180.1078	3181.7558
3182.1129	3183.3539	3185.0564
3195.9834	3197.2066	3197.8881
3198.6022	3198.7862	3199.8949
3200.9817	3202.1414	3204.4327
3208.7002	3208.9764	3227.6339

TS6⊂CCl_4

E(RB3LYP) = -5602.45485624

E(RB3LYP-D3) = -5602.68389571

H - Sum of electronic and thermal Enthalpies= -5601.275427

G - Sum of electronic and thermal Free Energies= -5601.452970

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.27885	1.36091	1.82248
C	5.56370	1.72766	0.49320
C	5.83292	0.73716	-0.47565
C	5.92347	-0.61343	-0.08461
C	5.68125	-0.98431	1.25468
C	5.34584	0.00396	2.19921
C	4.88305	2.43363	2.83965
C	4.46448	1.87469	4.22127
C	5.46768	0.76139	4.59570
C	4.99535	-0.36467	3.64621
C	5.77974	-2.44799	1.69085
C	6.06216	-3.43470	0.53387
C	6.26477	-1.72011	-1.09464
C	6.00969	1.11802	-1.94665
C	5.82159	2.62675	-2.22943
C	5.55659	3.20144	0.05610
C	6.55707	3.39512	-1.10712
C	7.12412	-2.79613	-0.38852
C	2.06881	3.67759	-2.42828
C	3.32284	3.16524	-2.88034
C	4.38665	3.09088	-2.01358
C	4.24580	3.50428	-0.65638
C	3.07534	4.05488	-0.20009
C	1.95679	4.16364	-1.07466
C	2.90339	-3.21111	-2.38889
C	2.74316	-4.19917	-1.34977
C	3.77097	-4.34982	-0.37251
C	4.86907	-3.52539	-0.40168
C	5.00440	-2.52203	-1.40442
C	4.06311	-2.38294	-2.39344
C	1.13244	-0.84602	3.89537
C	0.80733	0.52239	4.21742
C	1.86280	1.47597	4.33526
C	3.16648	1.08539	4.14238
C	3.48233	-0.26679	3.82029
C	2.49529	-1.21294	3.69809
C	0.09069	-1.81240	3.78764
C	-1.20402	-1.41126	3.98890
C	-1.52701	-0.07043	4.30535
C	-0.55546	0.89170	4.42513
C	0.92204	3.69480	-3.27663
C	-0.26095	4.17774	-2.77651
C	-0.35119	4.70479	-1.46715
C	0.72381	4.71233	-0.61870
C	1.54327	-4.96738	-1.28520
C	0.55508	-4.72150	-2.20374
C	0.72495	-3.77081	-3.23671
C	1.87258	-3.03199	-3.35610
C	-0.53961	-3.70840	-4.01945
O	-0.80148	-3.04253	-5.00563
N	-1.42488	-4.59443	-3.38687
C	-0.83075	-5.26501	-2.30027
O	-1.37302	-6.10835	-1.61171
C	-1.62181	4.22576	-3.38349
O	-1.98643	3.85585	-4.48454
C	-1.75350	5.14889	-1.24055
O	-2.23593	5.70758	-0.27180
C	-2.46192	-2.20599	3.99365
O	-2.61775	-3.40145	3.82734
C	-3.00130	0.00759	4.51891

O	-3.68228	0.95742	4.86099
N	-3.49070	-1.29162	4.29153
N	-2.45442	4.80463	-2.40681
C	-2.83652	-4.70169	-3.73599
C	-3.89377	4.94658	-2.55525
C	-4.83838	-1.70989	4.61665
C	-7.90648	-1.22407	1.70874
C	-8.24193	-1.68329	2.97899
C	-7.22875	-1.83109	3.92238
C	-5.91444	-1.52275	3.55107
N	-5.58560	-1.09088	2.32676
C	-6.56531	-0.93627	1.41883
C	-6.01483	2.99230	0.57401
C	-6.49018	4.22424	0.12539
C	-5.81072	4.87249	-0.90340
C	-4.68114	4.25309	-1.45045
N	-4.24413	3.05598	-1.04511
C	-4.89015	2.43029	-0.04532
C	-4.85843	-1.02056	-3.03402
C	-4.93095	-1.57639	-4.30982
C	-4.28429	-2.78595	-4.56178
C	-3.58710	-3.39537	-3.51473
N	-3.53282	-2.87553	-2.28107
C	-4.15088	-1.70803	-2.03973
C	-3.99836	-1.16507	-0.62036
C	-4.32395	1.09522	0.41086
C	-6.24256	-0.41502	0.00970
N	-4.88517	-0.04591	-0.32298
H	5.72867	3.11969	2.99728
H	4.06653	3.04280	2.43427
H	4.41786	2.69395	4.94695
H	5.34881	0.45534	5.64172
H	6.51192	1.04922	4.42910
H	6.58728	-2.54941	2.43127
H	5.75382	3.86410	0.90102
H	7.01802	0.83809	-2.28484
H	5.30952	0.54008	-2.56318
H	7.55155	2.98913	-0.88978
H	6.65581	4.45937	-1.35074
H	4.85751	-2.75169	2.20107
H	6.35658	-4.40664	0.94460
H	7.97283	-2.37197	0.15983
H	7.50256	-3.52250	-1.11734
H	3.41255	2.84119	-3.91581
H	2.97241	4.40469	0.82474
H	6.18679	2.85588	-3.23649
H	3.65706	-5.11338	0.39521
H	4.16218	-1.62888	-3.17129
H	6.74438	-1.31208	-1.98574
H	1.61325	2.50422	4.59156
H	2.72668	-2.24791	3.45581
H	5.39566	-1.34185	3.91951
H	-0.81132	1.91738	4.67959
H	0.32596	-2.84745	3.55367
H	0.63682	5.09898	0.39356
H	0.98395	3.30179	-4.28834
H	1.98144	-2.28937	-4.14224
H	1.40367	-5.70002	-0.49407
H	-3.24360	-5.49082	-3.09694
H	-2.92388	-5.01328	-4.78161
H	-4.13556	4.51419	-3.53219
H	-4.15624	6.01014	-2.58045
H	-4.77657	-2.77410	4.86967
H	-5.14410	-1.16359	5.51623
H	-8.66881	-1.08687	0.94517
H	-9.27317	-1.91720	3.23190
H	-7.44808	-2.17715	4.92958
H	-6.48902	2.48159	1.40781
H	-7.35853	4.68502	0.58979
H	-6.12580	5.85231	-1.25203
H	-5.31639	-0.06647	-2.79705
H	-5.46683	-1.06301	-5.10455
H	-4.29128	-3.23188	-5.55209
H	-6.89817	0.44874	-0.17324
H	-6.56931	-1.17988	-0.70789
H	-4.46307	0.99188	1.49684
H	-3.25169	1.11807	0.21263
H	-2.96330	-0.82681	-0.50976
H	-4.11395	-2.00433	0.08220
C	0.39953	-0.06276	-0.50677
Cl	-0.16582	0.18271	-2.18764
Cl	-0.36907	1.15413	0.56578
Cl	2.17697	0.12585	-0.42471
Cl	-0.05866	-1.70682	0.03523

Frequencies

-25.6988	13.8816	17.0536
18.4005	19.5544	22.6222
24.3262	26.0179	30.3538
33.8438	35.8705	37.2421
39.4209	41.8697	45.3849
48.6192	50.3105	54.3545
57.3810	65.1576	66.4845
77.1729	84.7306	97.9596
104.4768	116.3758	116.7777
119.7836	122.8142	131.1933
141.5003	143.5911	150.3083
152.6983	153.1889	159.3254
161.8488	170.1570	173.9044
179.4001	182.8811	188.2562
191.5671	198.8309	206.5050
212.0373	214.1027	218.0340
227.9762	232.0732	234.7469
239.0359	243.0446	246.3871
246.6357	250.9362	253.7126
263.2656	264.4437	266.3019
273.2079	289.0883	292.3166
299.0040	300.6098	302.0085

307.1993	310.4886	313.6265	1066.4817	1074.3314	1076.7718
314.4698	316.8842	317.8555	1078.0422	1104.4944	1106.3999
321.5960	328.7115	346.9858	1107.4869	1113.8528	1117.3101
347.2867	359.3063	370.6691	1117.8491	1121.9403	1124.1866
372.1099	379.8491	386.8152	1143.7364	1146.4135	1150.7954
396.9985	399.4675	402.1801	1153.7704	1161.0303	1165.9534
405.9599	406.7631	420.1702	1166.1570	1176.0581	1176.8416
428.4345	429.0491	431.2155	1177.7515	1178.4407	1179.2440
433.7108	436.9472	451.1943	1179.8664	1180.1349	1184.2576
451.4816	467.9207	472.5590	1189.1957	1190.3969	1190.7203
478.0684	484.0226	484.5649	1191.8942	1193.2106	1214.5858
485.7611	488.4959	500.1764	1229.1237	1230.2967	1230.4089
502.0952	504.2290	530.5682	1233.6200	1234.7885	1236.1009
534.7733	536.5648	547.9341	1244.6529	1248.7398	1249.6719
550.1914	552.0276	567.5149	1253.4616	1253.7822	1253.9033
572.1525	573.6881	576.5828	1258.7829	1259.6229	1260.4760
577.6947	580.7228	583.3262	1267.9105	1275.0777	1277.1795
594.4346	595.5568	602.7311	1277.5870	1277.8595	1289.7438
606.0787	607.4183	616.2827	1290.4494	1294.8134	1297.9074
622.5253	625.3946	634.5850	1298.8054	1300.0162	1302.9927
646.5089	653.0797	654.1738	1307.7839	1314.7364	1317.3878
655.5193	660.3355	660.9194	1318.1353	1319.9325	1325.0186
662.8260	664.0054	669.3884	1329.1395	1337.3705	1338.7923
714.4157	715.6009	718.6278	1339.3231	1340.7294	1344.5721
720.8551	723.4508	724.9208	1345.7806	1351.7549	1361.2781
732.6891	733.2980	737.7634	1363.9682	1375.9174	1376.6238
737.9500	740.3159	741.0514	1377.0301	1383.5364	1388.6969
741.6851	743.3545	744.5016	1391.1374	1399.8384	1401.9922
745.2681	750.2250	754.3390	1404.1033	1412.1523	1412.7317
760.2650	762.8795	767.9403	1413.0686	1415.0706	1416.9814
768.4157	770.6864	772.2569	1420.4672	1430.9491	1449.6896
778.0885	778.9062	780.1852	1449.9232	1467.4154	1469.8045
782.4108	785.0646	785.2025	1471.5802	1472.7592	1474.0723
785.9280	804.1324	806.2505	1474.5089	1474.8980	1475.9983
809.7262	810.7394	818.0912	1477.6096	1479.5842	1483.3384
826.3498	827.1639	828.4409	1484.1906	1484.3147	1486.1864
841.1798	842.5765	847.4139	1488.2649	1493.3880	1494.6109
869.0873	869.4465	877.2083	1498.3419	1501.3327	1501.6341
881.0915	888.6043	888.9309	1502.2497	1502.9042	1503.5465
894.7174	897.3356	897.4003	1521.0064	1521.3666	1521.9246
900.0689	902.8928	911.1684	1522.1572	1533.6598	1535.0459
916.6542	918.4351	919.0711	1535.3980	1603.1832	1603.9615
919.6776	934.2260	936.1869	1627.4154	1629.9872	1632.1704
936.8063	937.6489	941.2010	1634.8598	1637.6409	1638.7083
941.5533	942.0010	949.5398	1647.1443	1648.8455	1649.4869
951.8706	954.8755	959.5051	1673.0652	1675.8051	1676.2844
960.4639	963.7802	966.0781	1676.5786	1678.7967	1678.8722
966.6629	968.6056	970.9706	1769.6913	1772.4274	1773.5793
988.5485	991.3943	999.5630	1820.1897	1820.7280	1822.8569
1002.3036	1002.9668	1009.1641	3015.1996	3015.7258	3016.2981
1009.8479	1010.6423	1012.1543	3019.3355	3020.9866	3027.9517
1013.3902	1014.8257	1015.1656	3055.2521	3057.2527	3057.5029
1015.5682	1020.0964	1031.0610	3057.9106	3062.0039	3063.0355
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3079.3613	3099.7973	3103.1286
3103.5343	3103.8554	3106.5688
3108.9888	3118.6597	3125.9790
3127.9038	3130.0971	3146.5460
3171.5585	3172.4656	3172.7831
3177.5148	3180.7177	3180.9266
3180.9833	3183.2581	3186.1071
3186.6342	3196.4997	3197.2024
3197.7511	3198.5642	3199.8562
3201.2736	3201.3196	3201.7665
3206.3507	3206.5233	3226.5960

I6⊂CCl_4

E(RB3LYP) = -5602.46082192

E(RB3LYP-D3) = -5602.68790399

H - Sum of electronic and thermal Enthalpies= -5601.279949

G - Sum of electronic and thermal Free Energies= -5601.461382

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.58343	0.96546	1.26031
C	5.63842	1.47351	-0.05181
C	5.67752	0.59471	-1.15441
C	5.71621	-0.79592	-0.93530
C	5.67317	-1.31307	0.37643
C	5.62694	-0.42860	1.47152
C	5.45376	1.92921	2.44096
C	5.29261	1.22769	3.80951
C	6.29876	0.05506	3.84777
C	5.58305	-0.95067	2.91600
C	5.66012	-2.82391	0.61797
C	5.61469	-3.66994	-0.67662
C	5.77569	-1.78546	-2.10839
C	5.66125	1.13777	-2.58423
C	5.52852	2.67585	-2.67065
C	5.62874	2.98617	-0.32107
C	6.45723	3.28135	-1.59367
C	6.59371	-3.02855	-1.68546
C	1.85059	3.87967	-2.19825
C	3.00023	3.38373	-2.88359
C	4.16778	3.16262	-2.19399
C	4.24062	3.40441	-0.79105
C	3.16985	3.92008	-0.10509
C	1.94824	4.18068	-0.79065
C	2.13460	-2.79112	-3.06995
C	2.00728	-3.88610	-2.13914
C	3.12537	-4.23693	-1.32416
C	4.29101	-3.51441	-1.41019
C	4.39868	-2.40967	-2.30449
C	3.35808	-2.06338	-3.12916
C	1.85036	-1.36872	3.95056
C	1.63970	-0.00947	4.38638
C	2.74065	0.89920	4.37811
C	3.96811	0.48596	3.91844
C	4.15432	-0.84194	3.43440
C	3.13311	-1.75750	3.46884
C	0.76896	-2.29542	3.97829
C	-0.46623	-1.85091	4.36913
C	-0.68823	-0.50764	4.75232
C	0.33595	0.40488	4.79195
C	0.60878	4.07085	-2.87326
C	-0.46356	4.54228	-2.15946
C	-0.35191	4.88138	-0.79081
C	0.82045	4.71437	-0.10199
C	0.76526	-4.58027	-2.03515
C	-0.28489	-4.17418	-2.81905
C	-0.14930	-3.11549	-3.74733
C	1.02851	-2.43119	-3.89284
C	-1.46381	-2.91482	-4.41624
O	-1.77236	-2.12163	-5.28764
N	-2.33207	-3.85529	-3.84093
C	-1.69731	-4.65115	-2.86932
O	-2.23064	-5.54150	-2.23333
C	-1.87585	4.77427	-2.57576
O	-2.39537	4.59758	-3.66266
C	-1.67611	5.38202	-0.32793
O	-1.99280	5.82683	0.76036
C	-1.76276	-2.57488	4.44549
O	-1.99256	-3.75938	4.27072
C	-2.14431	-0.34465	5.03238
O	-2.75009	0.64374	5.40023
N	-2.72220	-1.60931	4.78741
N	-2.53345	5.26617	-1.43348
C	-3.75811	-3.89437	-4.11634
C	-3.95474	5.55928	-1.38789
C	-4.14908	-1.90113	4.93265
C	-5.98818	-2.91884	1.23217
C	-5.62005	-3.95712	2.08615
C	-5.02271	-3.64424	3.30498
C	-4.81367	-2.29640	3.62110
N	-5.18128	-1.29573	2.80695
C	-5.75724	-1.59454	1.62744
C	-6.04894	3.20987	1.47838
C	-6.49566	4.50747	1.23282
C	-5.81795	5.28673	0.29766
C	-4.71896	4.72783	-0.36463
N	-4.30384	3.47549	-0.14875
C	-4.94990	2.72206	0.75909
C	-5.77568	-0.43126	-2.66384
C	-6.19327	-0.97783	-3.87630
C	-5.54140	-2.10580	-4.37586
C	-4.49403	-2.65199	-3.62766
N	-4.10259	-2.14128	-2.45481
C	-4.71952	-1.04638	-1.98094
C	-4.13842	-0.48246	-0.69390

C	-4.41904	1.31677	0.98185
C	-6.15805	-0.43433	0.71966
N	-5.06605	0.32355	0.09525
H	6.34607	2.57029	2.49459
H	4.60316	2.60170	2.27539
H	5.43215	1.95894	4.61313
H	6.38898	-0.35933	4.85872
H	7.29659	0.33387	3.49063
H	6.56170	-3.11323	1.17804
H	5.97560	3.54596	0.54922
H	6.59097	0.85100	-3.09743
H	4.84428	0.67075	-3.14806
H	7.45097	2.81965	-1.57398
H	6.57322	4.36278	-1.73093
H	4.80677	-3.09015	1.25362
H	5.84403	-4.71415	-0.43772
H	7.56231	-2.77202	-1.24157
H	6.76317	-3.68529	-2.54676
H	2.93071	3.19546	-3.95365
H	3.22630	4.13402	0.96007
H	5.75800	3.00463	-3.69011
H	3.03237	-5.08141	-0.64331
H	3.43725	-1.23222	-3.82651
H	6.16457	-1.30995	-3.01024
H	2.58490	1.91361	4.74138
H	3.27318	-2.77973	3.12432
H	5.99259	-1.95974	2.98691
H	0.15950	1.43266	5.09953
H	0.92183	-3.32601	3.66833
H	0.89045	4.96256	0.95406
H	0.51558	3.82581	-3.92839
H	1.11584	-1.60999	-4.59960
H	0.65251	-5.39709	-1.32651
H	-4.13871	-4.78630	-3.60728
H	-3.91178	-4.01838	-5.19300
H	-4.33122	5.36299	-2.39790
H	-4.09925	6.62412	-1.17368
H	-4.26299	-2.70371	5.66896
H	-4.60568	-0.98786	5.32035
H	-6.44404	-3.12659	0.26808
H	-5.78376	-4.99308	1.80087
H	-4.69499	-4.42145	3.98708
H	-6.52729	2.58939	2.23105
H	-7.34189	4.91459	1.78078
H	-6.11417	6.31462	0.10536
H	-6.23285	0.46051	-2.24710
H	-7.00447	-0.51924	-4.43662
H	-5.82421	-2.54025	-5.33096
H	-6.76622	0.27283	1.29321
H	-6.80003	-0.83076	-0.07637
H	-4.53624	1.03151	2.03303
H	-3.34789	1.33626	0.77066
H	-3.30612	0.16843	-0.98358
H	-3.69641	-1.32317	-0.13425
C	0.22417	-0.01046	-0.11512
Cl	-0.34068	0.49675	-1.73841
Cl	-0.35237	1.16896	1.10735
Cl	2.01195	-0.06749	-0.09093
Cl	-0.43526	-1.63168	0.26545

Frequencies

9.2553	14.3724	15.1204
17.7626	18.9277	21.2503
23.9959	28.9124	30.4471
32.1614	33.8444	37.3016
38.3654	39.1046	44.2425
49.6479	51.7585	54.6959
61.0878	64.3514	68.0784
78.9875	80.1351	97.9984
100.5281	112.1875	113.4125
120.7614	124.2118	127.0673
140.7677	141.2547	150.2856
152.6281	159.7670	160.3157
164.2756	172.5633	175.7901
176.2146	182.2567	188.6046
192.2371	199.0972	210.0948
215.3398	215.4666	223.4754
230.8906	234.4138	237.0247
240.3279	242.7820	245.5924
246.6802	250.8661	253.8792
261.5344	263.9821	270.2034
274.2298	293.0830	298.2183
298.7636	301.8987	306.0257
307.2858	313.3753	313.8079
314.4093	315.8945	319.4294
328.3791	345.7505	346.5425
353.0011	369.7424	371.7650
378.0353	385.4576	390.9405
396.5451	401.0491	402.1873
406.0999	406.6171	420.1840
426.7813	428.0416	429.7983
436.4459	439.6107	449.0683
450.9989	469.9602	471.4201
474.5702	483.7168	484.2780
485.3318	487.1414	499.2266
502.2063	502.8467	529.8199
533.3450	541.8231	548.6477
549.5083	551.4893	567.6038
571.5062	572.8869	576.6261
579.8091	579.9748	581.8935
593.8949	595.2941	602.1620
605.4469	606.7410	611.2196
619.2102	624.3076	629.3552
649.7446	653.6832	654.2386
657.7905	659.5455	660.2856
663.4440	666.2454	701.4665
714.9346	716.4647	718.7482
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734.5590 735.2825 737.2012
738.7093 740.0135 740.4211
742.4500 743.8476 745.4154
751.5150 755.7000 758.1365
762.9595 767.3401 767.9975
768.6222 771.4410 771.9422
779.2165 779.4704 780.1003
782.5736 786.0687 786.9020
800.6419 801.4716 804.0702
809.2443 816.7165 822.5144
825.7661 826.5501 838.2202
842.9022 846.0957 851.9713
866.3926 869.2313 869.4390
877.0482 888.4485 888.7010
894.5775 897.0109 897.7450
899.8695 910.4845 913.3282
913.7833 916.9231 918.7927
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941.1615 941.5316 941.9064
944.0707 956.1252 959.0627
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967.4986 970.7774 971.3086
988.7311 989.9340 1001.2660
1003.5803 1004.4024 1007.7879
1010.0644 1010.4637 1012.9280
1013.6683 1013.9446 1014.4692
1017.1475 1020.0306 1022.2363
1039.2648 1044.2372 1044.5862
1066.5101 1074.6410 1077.0993
1077.1590 1101.6674 1106.2510
1107.0541 1108.3668 1114.6549
1116.5366 1120.6713 1121.2936
1133.1471 1142.4599 1147.1577
1148.5392 1153.0492 1153.4926
1165.9750 1166.0248 1176.2280
1177.8789 1178.0666 1178.3900
1179.6312 1179.8527 1184.9850
1189.3663 1190.2394 1190.8867
1191.6841 1192.4347 1229.0261
1229.0936 1230.5200 1232.1005
1232.6486 1236.1819 1243.1272
1244.8867 1249.1982 1249.4447
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1259.3866 1262.2772 1270.4187
1271.4806 1276.1299 1277.2766
1277.5118 1277.6004 1290.0173
1290.2524 1297.7703 1298.7056
1298.8945 1299.3763 1302.5579
1313.8370 1315.3816 1317.5797
1318.0921 1319.2504 1325.0783
1327.2365 1338.3521 1338.7938
1340.2729 1343.8723 1345.1077
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1363.9335 1372.9298 1374.6981
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1449.8822 1470.7794 1471.6750
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1492.4359 1494.7673 1497.1395
1499.0626 1500.5713 1500.6561
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1627.4213 1628.5565 1630.8795
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1768.7132 1771.7166 1772.7423
1818.6494 1820.3498 1821.9073
2993.7278 3017.2063 3017.6346
3017.7815 3052.7950 3057.5548
3057.7424 3057.8913 3064.0798
3067.0545 3068.2404 3068.3599
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3103.6173 3103.9596 3107.1973
3117.4207 3123.0335 3124.0679
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3179.8831 3181.0526 3181.5919
3182.6247 3184.5163 3190.6083
3196.1259 3197.7770 3197.9467
3198.2273 3199.3791 3200.5843
3200.6378 3201.0981 3206.0744
3206.7084 3219.8457 3225.3142

TS7⊂CCl_4

E(RB3LYP) = -5602.46040459

E(RB3LYP-D3) = -5602.68552331

H - Sum of electronic and thermal Enthalpies= -5601.280643

G - Sum of electronic and thermal Free Energies= -5601.459578

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.76067	0.91081	1.06168
C	5.68419	1.60570	-0.16022

C	5.64663	0.90037	-1.38052
C	5.72223	-0.50549	-1.37318
C	5.80119	-1.20993	-0.15375
C	5.85188	-0.49695	1.05997
C	5.71593	1.68841	2.37779
C	5.68207	0.78772	3.63278
C	6.72119	-0.33661	3.41818
C	5.95856	-1.22621	2.40949
C	5.80490	-2.73972	-0.13795
C	5.62934	-3.38478	-1.53329
C	5.67880	-1.30955	-2.68060
C	5.50413	1.64702	-2.70803
C	5.32515	3.17545	-2.55459
C	5.60427	3.13852	-0.19924
C	6.31797	3.65362	-1.47135
C	6.52030	-2.59721	-2.52025
C	1.66327	4.14285	-1.63531
C	2.77051	3.80804	-2.47106
C	3.99335	3.52964	-1.91050
C	4.16802	3.55422	-0.49597
C	3.13450	3.89783	0.33901
C	1.85573	4.20897	-0.20698
C	1.96637	-2.18875	-3.47710
C	1.90892	-3.40658	-2.70567
C	3.08683	-3.86196	-2.03949
C	4.24637	-3.12812	-2.11561
C	4.28566	-1.90489	-2.84676
C	3.18317	-1.44947	-3.52491
C	2.33714	-1.93605	3.64810
C	2.10948	-0.64772	4.25651
C	3.18230	0.29311	4.30715
C	4.38968	-0.01164	3.72584
C	4.57908	-1.25452	3.05331
C	3.59543	-2.21019	3.04102
C	1.28975	-2.89986	3.62014
C	0.06142	-2.54497	4.11006
C	-0.18601	-1.26107	4.64767
C	0.81321	-0.32691	4.75900
C	0.37559	4.41419	-2.18423
C	-0.64967	4.73517	-1.33165
C	-0.45153	4.83050	0.06580
C	0.76801	4.57812	0.63684
C	0.67858	-4.12332	-2.61530
C	-0.42381	-3.62694	-3.26426
C	-0.35639	-2.44700	-4.04173
C	0.80484	-1.73077	-4.16364
C	-1.70856	-2.18614	-4.60712
O	-2.07546	-1.29279	-5.34919
N	-2.52902	-3.21607	-4.12179
C	-1.82999	-4.12205	-3.30325
O	-2.31522	-5.10281	-2.76898
C	-2.07727	5.05173	-1.61599
O	-2.65809	5.09322	-2.68575
C	-1.73975	5.24503	0.68943
O	-1.98399	5.50401	1.85323
C	-1.20984	-3.31303	4.13875
O	-1.40156	-4.48326	3.85347
C	-1.64068	-1.17097	4.96554
O	-2.26557	-0.24631	5.44788
N	-2.19136	-2.41609	4.58592
N	-2.65972	5.33436	-0.36814
C	-3.95767	-3.28220	-4.36815
C	-4.03560	5.74906	-0.20480
C	-3.61361	-2.75124	4.69824
C	-5.48473	-3.34400	0.92013
C	-4.88641	-4.44340	1.53291
C	-4.28237	-4.27101	2.77542
C	-4.28185	-2.99252	3.35021
N	-4.86850	-1.93580	2.76708
C	-5.46780	-2.10551	1.57356
C	-6.68522	2.86106	1.45613
C	-7.15812	4.14892	1.21832
C	-6.28821	5.09099	0.67420
C	-4.97569	4.70104	0.38410
N	-4.51968	3.46255	0.60496
C	-5.35634	2.55200	1.13631
C	-6.16541	-0.19753	-2.42429
C	-6.62638	-0.66860	-3.65201
C	-5.90495	-1.66360	-4.31268
C	-4.74786	-2.16003	-3.70442
N	-4.30750	-1.71717	-2.52109
C	-4.99125	-0.74612	-1.89325
C	-4.37645	-0.23261	-0.60152
C	-4.81706	1.15183	1.38740
C	-6.17528	-0.90202	0.95604
N	-5.34605	0.17754	0.41155
H	6.59822	2.34106	2.45396
H	4.84280	2.35220	2.38402
H	5.86460	1.39647	4.52505
H	6.90896	-0.88892	4.34637
H	7.67656	0.03210	3.02799
H	6.75436	-3.10238	0.28313
H	6.00033	3.58116	0.71615
H	6.39789	1.47216	-3.32523
H	4.65751	1.23927	-3.27367
H	7.32385	3.23664	-1.59538
H	6.38928	4.74742	-1.45281
H	5.01528	-3.10297	0.53094
H	5.86866	-4.45212	-1.47366
H	7.52657	-2.40472	-2.13111
H	6.60720	-3.11841	-3.48079
H	2.62545	3.79076	-3.54993
H	3.26503	3.94031	1.41818
H	5.46350	3.65846	-3.52804
H	3.04491	-4.79711	-1.48355
H	3.21040	-0.52710	-4.10089
H	5.99233	-0.70250	-3.53150
H	3.01924	1.24646	4.80693

H	3.74382	-3.17429	2.55972
H	6.40458	-2.21559	2.29270
H	0.61948	0.65378	5.18629
H	1.45791	-3.88140	3.18444
H	0.90850	4.64756	1.71253
H	0.21455	4.35791	-3.25798
H	0.84153	-0.81869	-4.75382
H	0.61829	-5.03451	-2.02524
H	-4.28478	-4.25310	-3.98016
H	-4.13431	-3.26753	-5.44866
H	-4.38903	6.04320	-1.19876
H	-4.05020	6.63698	0.43783
H	-3.70518	-3.64185	5.32928
H	-4.08723	-1.90311	5.19625
H	-5.96101	-3.43966	-0.05147
H	-4.88618	-5.41615	1.04804
H	-3.79205	-5.09427	3.28231
H	-7.33040	2.10228	1.88991
H	-8.18263	4.41850	1.46308
H	-6.61400	6.11123	0.48536
H	-6.68443	0.58379	-1.87781
H	-7.52802	-0.25569	-4.09791
H	-6.22461	-2.03808	-5.28163
H	-6.83307	-0.46257	1.71315
H	-6.82182	-1.27049	0.14973
H	-5.08424	0.83191	2.39909
H	-3.72344	1.18977	1.35203
H	-3.77841	0.65170	-0.85298
H	-3.67109	-0.99890	-0.24163
C	0.01114	0.01330	0.06613
Cl	-0.57290	0.70728	-1.47850
Cl	-0.64053	0.97341	1.43158
Cl	1.80234	0.05589	0.10272
Cl	-0.55125	-1.68218	0.20834

Frequencies

-17.0091	9.4368	16.4175
16.8632	17.7651	21.8603
23.2308	24.9587	26.1805
30.3557	32.8321	34.7317
36.3121	36.4789	39.4159
48.2486	51.1109	54.8417
59.9985	63.4971	69.7572
76.9653	81.4220	97.5467
102.0610	110.6772	111.6631
121.0061	122.9263	126.4553
140.5501	141.9082	150.5483
151.6523	158.9758	160.1025
164.0181	167.5306	172.0111
177.1021	179.5302	186.7642
189.4048	199.7275	210.6664
214.9097	215.5245	221.8027
229.9308	233.0825	234.3377
236.9364	241.9173	244.0054
246.2032	248.7026	253.6516
261.7742	264.5121	270.2285
273.6638	285.2737	295.6968
298.1169	301.2209	306.0829
307.5344	313.5761	313.9918
314.5235	315.2940	319.5582
327.6308	345.4444	346.0266
349.5572	368.9950	371.8606
376.1022	385.8216	392.5093
394.4031	400.1116	401.3076
406.0063	406.5804	420.1041
427.3702	427.9905	429.4342
435.3032	440.2804	447.6745
450.7239	469.6956	471.2838
476.5324	480.9537	483.2632
484.1667	485.1216	498.9869
502.3937	504.2778	528.1796
532.5225	546.2177	548.1772
548.6218	551.9713	567.8517
572.2374	573.2327	576.9214
577.8977	579.5455	582.8450
594.1269	595.8430	604.8716
606.4280	607.1071	609.7837
622.0971	626.5771	633.1772
648.9532	653.1567	653.9080
655.7401	659.1787	659.7602
660.4088	664.1452	701.0189
715.4149	716.6214	718.6960
721.8285	724.4585	726.7498
729.9778	734.9234	737.8689
738.3652	738.9883	739.6888
740.6133	743.3314	745.0225
751.2222	753.5086	757.6035
762.9766	766.8790	767.5523
768.2015	771.2027	771.4851
777.5420	779.3261	780.6369
783.1750	786.0023	786.9206
795.9311	797.6814	803.1458
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843.3275	844.2231	854.8508
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877.1282	888.3793	888.7483
894.6856	897.1116	897.5557
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914.4570	916.5337	918.9224
919.4943	921.0942	933.6527
936.0970	937.0557	937.3816
941.2566	941.3672	941.8591
943.0701	955.8864	958.1150
961.4427	963.7671	965.8835
967.1394	967.9551	970.6938
980.8771	989.8397	998.9756
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1009.4742	1009.9999	1011.3730
1012.1441	1014.2127	1014.7738
1016.0755	1022.3111	1030.2656
1039.3793	1044.3316	1044.9931
1066.5916	1074.6924	1077.0341
1077.3322	1098.6195	1106.6214
1106.8563	1109.6383	1116.8012
1117.6646	1120.2414	1124.6291
1133.3816	1143.3910	1148.6179
1151.2806	1153.2841	1154.2953
1165.8623	1166.0708	1176.4241
1178.0206	1178.4899	1179.1637
1179.5512	1179.7792	1185.5733
1189.8272	1190.5834	1191.1195
1192.4544	1193.7894	1226.9246
1227.9092	1231.1418	1231.3425
1232.2041	1236.1084	1244.9196
1245.1932	1248.8313	1249.6150
1253.4656	1253.9358	1254.0339
1259.9192	1264.4628	1270.9631
1272.1545	1274.7474	1277.3890
1277.7581	1277.8063	1289.4656
1290.2420	1297.4481	1298.0901
1298.9675	1299.6323	1300.2326
1314.9181	1315.6931	1318.1410
1318.2471	1319.4756	1325.0138
1325.2323	1338.4383	1338.8235
1340.4115	1344.7498	1345.4454
1346.3322	1355.6528	1363.7175
1365.1009	1371.4728	1373.3724
1376.7061	1377.0976	1388.5190
1393.6260	1399.8347	1402.6479
1404.9739	1411.1974	1411.6787
1413.3166	1413.7671	1415.7327
1417.5578	1422.9086	1450.2521
1450.4246	1469.8223	1470.7139
1472.7610	1473.7365	1474.6183
1475.7142	1475.9962	1477.9970
1478.8467	1483.5229	1483.8359
1484.1254	1484.9302	1487.7688
1490.3107	1493.5463	1494.2659
1494.9942	1496.7048	1500.7946
1501.1555	1501.2356	1510.7748
1520.0266	1521.1187	1521.4134
1522.2251	1534.3389	1534.8115
1535.8347	1604.0324	1604.8720
1628.1946	1629.0548	1631.4933
1635.9269	1637.9380	1638.7910
1648.3649	1649.0994	1649.3063
1675.2101	1675.5370	1676.3299
1678.0569	1678.7969	1679.2141
1768.3125	1771.3937	1773.2631
1819.0968	1820.1775	1822.5518
3000.5284	3016.8628	3017.1611
3017.3847	3047.2377	3057.5175
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3068.4872	3068.7454	3068.8480
3069.8464	3070.4792	3075.4934
3077.3385	3078.5720	3078.6934
3078.8148	3095.7780	3103.3405
3103.4985	3103.9734	3109.8490
3112.9454	3120.1146	3121.4807
3124.4582	3124.9437	3152.4123
3172.2830	3172.3746	3173.0185
3178.8879	3180.1922	3181.2336
3181.2927	3183.6173	3192.3221
3192.6373	3197.8307	3198.0409
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3208.1991	3216.6548	3234.6370

I7⊂CCl_4

E(RB3LYP) = -5602.46276382

E(RB3LYP-D3) = -5602.68502822

H - Sum of electronic and thermal Enthalpies= -5601.282095

G - Sum of electronic and thermal Free Energies= -5601.464399

Number of imaginary frequencies: 0

Cartesian Coordinates

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C	5.92205	1.16796	-0.52416
C	5.70972	0.36471	-1.66277
C	5.65872	-1.03543	-1.52225
C	5.78235	-1.63077	-0.24912
C	5.97263	-0.81801	0.88519
C	6.13324	1.48321	1.98542
C	6.04494	0.71455	3.32192
C	6.94955	-0.53219	3.19331
C	6.06331	-1.42447	2.29532
C	5.69615	-3.14966	-0.08725
C	5.38046	-3.90834	-1.39757
C	5.43739	-1.94962	-2.73511
C	5.51760	1.00376	-3.04034
C	5.51130	2.55198	-3.02446
C	5.99721	2.68914	-0.70721
C	6.64189	3.00956	-2.07608
C	6.22025	-3.26783	-2.52540
C	2.06456	3.99245	-1.90593
C	3.05756	3.48588	-2.79761
C	4.28750	3.11037	-2.31327
C	4.58827	3.22573	-0.92463
C	3.66629	3.72382	-0.03918
C	2.37859	4.11549	-0.50326
C	1.62783	-2.68715	-3.13894
C	1.58286	-3.83491	-2.26574
C	2.78891	-4.28896	-1.65313

C	3.96882	-3.62519	-1.88633
C	4.00331	-2.47010	-2.72092
C	2.86716	-2.01242	-3.34088
C	2.41938	-1.59962	3.65625
C	2.34967	-0.23826	4.12959
C	3.52209	0.57476	4.07274
C	4.67569	0.07728	3.51555
C	4.70912	-1.23892	2.96800
C	3.62416	-2.07282	3.06279
C	1.27526	-2.44120	3.75401
C	0.10923	-1.90660	4.23315
C	0.01567	-0.55361	4.63125
C	1.11033	0.27428	4.61683
C	0.76983	4.36892	-2.37115
C	-0.15228	4.81926	-1.46067
C	0.15889	4.93424	-0.08564
C	1.39547	4.60668	0.40270
C	0.34100	-4.49815	-2.03818
C	-0.78344	-4.02562	-2.66556
C	-0.73299	-2.91651	-3.54245
C	0.43724	-2.24675	-3.78753
C	-2.10407	-2.68807	-4.07833
O	-2.48917	-1.86532	-4.88921
N	-2.91466	-3.66296	-3.47497
C	-2.19339	-4.50417	-2.60914
O	-2.66624	-5.43365	-1.98001
C	-1.56782	5.24903	-1.64552
O	-2.22071	5.33578	-2.67044
C	-1.04944	5.43203	0.62687
O	-1.18838	5.69738	1.80615
C	-1.22550	-2.53534	4.40808
O	-1.53519	-3.70851	4.28448
C	-1.40464	-0.28263	4.99695
O	-1.91006	0.74501	5.40414
N	-2.09409	-1.49945	4.78276
N	-2.03975	5.57102	-0.36250
C	-4.33866	-3.78579	-3.71235
C	-3.38839	6.04293	-0.08868
C	-3.51939	-1.68127	5.07429
C	-5.88983	-2.88657	1.75026
C	-5.27260	-3.87948	2.50830
C	-4.49746	-3.50058	3.60002
C	-4.34901	-2.13468	3.87919
N	-4.94904	-1.17736	3.15411
C	-5.71566	-1.54455	2.11057
C	-6.43001	3.09762	-0.47586
C	-6.57776	4.29051	-1.17649
C	-5.57603	5.25688	-1.08142
C	-4.46734	4.98756	-0.27535
N	-4.31698	3.83412	0.39381
C	-5.27688	2.90159	0.29850
C	-6.69683	-0.64637	-2.06055
C	-7.20272	-1.36148	-3.14563
C	-6.43019	-2.37516	-3.70799
C	-5.17729	-2.64633	-3.14477
N	-4.69479	-1.97181	-2.09738
C	-5.43002	-0.97783	-1.56772
C	-4.76204	-0.19690	-0.44727
C	-5.09602	1.63544	1.13203
C	-6.45442	-0.45377	1.33942
N	-5.67647	0.45252	0.48965
H	7.09208	2.02261	1.96562
H	5.35021	2.24990	1.95781
H	6.32073	1.38013	4.14714
H	7.10954	-1.01182	4.16606
H	7.92485	-0.30823	2.74652
H	6.65280	-3.52912	0.30180
H	6.51689	3.16502	0.12610
H	6.32585	0.67905	-3.71214
H	4.58388	0.64238	-3.48909
H	7.58422	2.47462	-2.23984
H	6.82665	4.08620	-2.16857
H	4.93923	-3.40198	0.66519
H	5.57054	-4.97775	-1.25511
H	7.26605	-3.10221	-2.24284
H	6.19296	-3.87850	-3.43547
H	2.81992	3.41038	-3.85737
H	3.89081	3.82560	1.02017
H	5.61135	2.92677	-4.04890
H	2.75324	-5.17289	-1.01855
H	2.88694	-1.14254	-3.99393
H	5.70009	-1.44547	-3.66649
H	3.47749	1.58583	4.47404
H	3.65176	-3.08979	2.67780
H	6.39784	-2.46280	2.26461
H	1.03568	1.30890	4.94211
H	1.32531	-3.47672	3.42733
H	1.62250	4.69874	1.46171
H	0.52038	4.28265	-3.42580
H	0.46343	-1.39062	-4.45671
H	0.29291	-5.35785	-1.37438
H	-4.63937	-4.73379	-3.25239
H	-4.51264	-3.86097	-4.79130
H	-3.59686	6.90227	-0.73396
H	-3.37862	6.37995	0.95273
H	-3.61157	-2.41140	5.88667
H	-3.88008	-0.71111	5.42133
H	-6.50434	-3.14323	0.89182
H	-5.39203	-4.92900	2.25215
H	-3.98938	-4.23709	4.21143
H	-7.17956	2.31553	-0.52093
H	-7.45598	4.46558	-1.79331
H	-5.64302	6.19157	-1.63052
H	-7.25561	0.16190	-1.60164
H	-8.18065	-1.12210	-3.55637
H	-6.78429	-2.93988	-4.56668
H	-7.00625	0.16423	2.05568
H	-7.20101	-0.95252	0.70741

H	-5.59631	1.78660	2.09560
H	-4.02864	1.52055	1.36567
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Cl	-0.86737	1.34619	1.25803
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Frequencies

10.0830	13.1754	15.7073
16.4978	19.1726	20.4651
22.6939	25.2125	27.2586
30.7215	32.9338	34.0061
35.6601	39.1312	39.9255
46.8321	49.8040	51.8765
59.6289	63.6163	68.2946
82.2719	88.0032	98.3563
101.0828	110.8342	117.2283
120.5563	125.6231	130.1008
139.4883	140.4723	149.9263
150.9172	159.9761	161.4611
168.7882	170.5464	175.7938
178.2546	180.4977	182.9586
188.8008	202.0629	207.3714
214.7511	216.0026	220.5781
227.5759	229.5727	234.6760
236.6468	240.2631	242.8804
245.6603	246.8540	257.7348
262.2715	264.3062	267.0152
272.5983	286.9420	293.1643
296.9383	300.4062	304.2628
306.7896	313.4486	314.2660
314.8435	318.1045	326.8906
327.2363	345.2815	346.3843
349.5988	368.7919	371.6080
373.8770	385.6340	392.9064
394.2441	398.6965	400.8448
404.5561	406.3671	420.2740
428.6267	429.0773	433.8774
435.7374	439.0903	450.0362
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762.8936	766.8154	767.4968
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773.7264	779.0984	780.3828
783.3090	783.9275	786.4333
791.7113	803.1579	805.8791
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894.7040	896.6877	897.3930
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1179.1592	1179.8994	1184.5417
1187.1440	1189.7530	1191.2052
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1259.9803	1265.9088	1269.3348
1271.9132	1273.5172	1277.2968
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3079.2490	3083.4872	3094.9675
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3124.3265	3125.4633	3150.3957
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3198.2641	3198.4686	3198.7819
3199.6555	3200.7050	3200.9261
3200.9898	3206.2909	3206.4330
3224.5325	3229.3949	3237.6451

TS8⊂CCl_4

E(RB3LYP) = -5602.46024621

E(RB3LYP-D3) = -5602.68151918

H - Sum of electronic and thermal Enthalpies= -5601.280607

G - Sum of electronic and thermal Free Energies= -5601.459851

Number of imaginary frequencies: 0

Cartesian Coordinates

C	-5.82464	-1.15665	0.68661
C	-5.83646	-1.04887	-0.71637
C	-5.74963	0.21449	-1.33658
C	-5.72660	1.37654	-0.54160
C	-5.71196	1.27917	0.86584
C	-5.75910	0.01073	1.47545
C	-5.87554	-2.53960	1.33878
C	-5.69902	-2.51671	2.87385
C	-6.55563	-1.35767	3.43004
C	-5.69370	-0.14697	3.00156
C	-5.64953	2.53834	1.73366
C	-5.55856	3.85848	0.93135
C	-5.70312	2.77461	-1.17422
C	-5.66889	0.32915	-2.86061
C	-5.60642	-1.03284	-3.59326
C	-5.88993	-2.29731	-1.60694
C	-6.63772	-1.96510	-2.91898
C	-6.51290	3.74302	-0.27828
C	-2.03212	-2.59219	-3.51331
C	-3.11049	-1.78437	-3.98521
C	-4.30874	-1.77712	-3.31228
C	-4.48899	-2.56937	-2.14100
C	-3.48280	-3.37260	-1.66686
C	-2.22733	-3.40596	-2.33809
C	-2.01596	3.99308	-1.52195
C	-1.91280	4.60338	-0.21861
C	-3.05021	4.59678	0.64248
C	-4.21635	3.99778	0.23258
C	-4.30701	3.37421	-1.04579
C	-3.24141	3.37835	-1.91055
C	-1.95479	-0.68409	3.97553
C	-1.93917	-2.11700	3.80444
C	-3.14873	-2.78728	3.45525
C	-4.29956	-2.06439	3.25604
C	-4.30032	-0.64415	3.37644
C	-3.16396	0.03371	3.74268
C	-0.76156	-0.00734	4.36270
C	0.38642	-0.73829	4.52362
C	0.41242	-2.13692	4.31469
C	-0.71948	-2.83483	3.97898
C	-0.76801	-2.60538	-4.17437
C	0.23668	-3.38604	-3.66109
C	0.03904	-4.18688	-2.51174
C	-1.16176	-4.21822	-1.85400
C	-0.67906	5.19169	0.18846
C	0.38712	5.14863	-0.67306
C	0.27937	4.56209	-1.95579
C	-0.88935	3.99731	-2.39430
C	1.60447	4.66873	-2.62531
O	1.93685	4.30654	-3.74016
N	2.44881	5.30229	-1.70118
C	1.78812	5.62981	-0.50213

O	2.29312	6.20300	0.44496
C	1.64508	-3.57515	-4.11308
O	2.22297	-3.08483	-5.06654
C	1.31134	-4.90136	-2.21669
O	1.55416	-5.70460	-1.33522
C	1.75303	-0.30582	4.92611
O	2.13658	0.79518	5.28046
C	1.80730	-2.60986	4.53648
O	2.25284	-3.74060	4.48632
N	2.55594	-1.45584	4.85264
N	2.21696	-4.48287	-3.20669
C	3.87124	5.50183	-1.92684
C	3.60114	-4.90934	-3.25610
C	3.95542	-1.51000	5.26719
C	6.63503	1.09151	3.23766
C	6.32236	1.37572	4.56597
C	5.42649	0.54447	5.23097
C	4.87519	-0.54190	4.54005
N	5.16806	-0.81239	3.25978
C	6.03358	-0.00996	2.61379
C	6.38035	-2.05247	-1.75986
C	6.79917	-2.92682	-2.76330
C	5.89364	-3.84956	-3.27958
C	4.59594	-3.86964	-2.75386
N	4.19311	-3.03686	-1.79021
C	5.06117	-2.13316	-1.30131
C	6.03353	1.83320	-1.96044
C	6.29673	2.76114	-2.96798
C	5.59601	3.96613	-2.98294
C	4.65328	4.19624	-1.97540
N	4.40225	3.31040	-1.00541
C	5.07491	2.14783	-0.99248
C	4.72312	1.22411	0.17093
C	4.49780	-1.22645	-0.21028
C	6.37722	-0.34551	1.16541
N	5.34423	-0.09462	0.15651
H	-6.84283	-3.01349	1.11350
H	-5.10813	-3.18817	0.90039
H	-5.95611	-3.49787	3.28768
H	-6.62898	-1.40779	4.52281
H	-7.56743	-1.33089	3.00994
H	-6.54962	2.58819	2.36392
H	-6.32366	-3.14701	-1.07727
H	-6.54861	0.87128	-3.23769
H	-4.79581	0.93227	-3.13937
H	-7.60668	-1.48235	-2.74821
H	-6.79638	-2.87553	-3.50871
H	-4.79756	2.47665	2.42242
H	-5.77993	4.70319	1.59277
H	-7.50151	3.35188	-0.01265
H	-6.63858	4.71141	-0.77661
H	-2.96272	-1.18729	-4.88349
H	-3.61598	-3.98888	-0.78052
H	-5.78010	-0.87834	-4.66375
H	-2.97380	5.07892	1.61561
H	-3.30498	2.91731	-2.89386
H	-6.06385	2.74963	-2.20382
H	-3.13738	-3.87144	3.35678
H	-3.15820	1.11594	3.85360
H	-5.97387	0.77488	3.51314
H	-0.69207	-3.91220	3.83584
H	-0.76682	1.06901	4.51382
H	-1.30075	-4.83530	-0.96997
H	-0.60661	-1.99463	-5.05919
H	-0.95690	3.54173	-3.37886
H	-0.58753	5.64734	1.17134
H	4.22360	6.12163	-1.09596
H	4.00957	6.05625	-2.86031
H	3.84518	-5.18588	-4.28646
H	3.66501	-5.80780	-2.63207
H	4.00917	-1.32005	6.34564
H	4.27740	-2.53763	5.07919
H	7.33588	1.71258	2.68597
H	6.76467	2.23097	5.07033
H	5.14106	0.73725	6.26020
H	7.05516	-1.31224	-1.34591
H	7.81642	-2.88036	-3.14479
H	6.17826	-4.53179	-4.07618
H	6.53806	0.87525	-1.92150
H	7.02794	2.54076	-3.74202
H	5.75595	4.70007	-3.76769
H	6.64079	-1.40667	1.11272
H	7.28212	0.22105	0.89896
H	4.25621	-1.85241	0.66294
H	3.54033	-0.84823	-0.57983
H	3.62968	1.14008	0.20254
H	4.98604	1.75898	1.09308
C	0.00784	0.12208	-0.16104
Cl	0.55598	-1.45553	0.48325
Cl	0.57661	1.43802	0.91685
Cl	-1.78124	0.14804	-0.24437
Cl	0.69181	0.36491	-1.80090

Frequencies

-25.4445	11.7924	16.6404
17.9970	19.9074	22.5429
23.1626	26.2821	28.5828
29.1802	30.7742	32.3140
35.1510	37.9935	44.4315
44.6039	47.6392	49.2652
51.5823	60.8223	63.7217
66.7848	89.6531	98.2801
101.6354	113.4036	116.5552
119.3496	121.3052	134.1385
139.7779	140.1746	149.8370
150.8162	155.7394	159.4240
160.5934	163.7067	174.1844
178.7796	180.1314	181.2242

184.2846	194.3462	202.6950	961.1057	963.7556	966.6455
210.3772	215.0880	215.5885	966.7330	970.4218	972.7850
224.4706	226.1786	230.0350	986.4510	988.8123	993.6699
236.6457	238.2786	242.5925	1003.3237	1003.7779	1005.3826
246.3716	248.6293	255.3280	1007.0021	1010.3727	1012.8128
261.2778	262.3817	270.6431	1013.4966	1014.1584	1015.1395
272.2267	286.1690	290.7466	1015.7308	1018.4151	1024.7395
299.7722	301.1899	307.1958	1039.5597	1043.8928	1045.1586
310.0394	313.5477	314.2680	1066.6726	1074.8353	1077.1758
315.5739	318.6917	328.1346	1078.2103	1104.5854	1106.7468
330.4624	342.9163	346.4337	1107.1782	1109.9653	1113.9303
348.5449	357.4411	370.8524	1116.4084	1120.2253	1129.2258
372.4730	385.3216	387.9820	1140.3959	1145.9649	1149.7685
395.7737	400.1564	401.7150	1154.4507	1164.5699	1166.1412
404.9933	406.7302	419.8921	1166.4646	1176.2007	1177.3555
427.7953	428.6603	432.4487	1177.7106	1178.0327	1178.7198
436.5024	437.1411	450.3797	1179.5491	1180.0677	1183.1073
458.8540	466.2832	470.9878	1187.5846	1189.8292	1191.0063
481.1340	484.0207	484.6045	1191.6519	1192.7840	1228.0792
485.8524	492.8788	500.0510	1229.5383	1230.3699	1231.9373
502.0174	505.5688	529.2573	1232.9987	1236.4942	1240.1732
530.8843	533.7997	539.0568	1244.8316	1249.2039	1249.9475
548.5092	550.6366	568.6560	1253.6776	1254.1021	1254.1891
571.5361	574.3918	576.7286	1259.5504	1262.7816	1266.7458
578.8181	578.9947	580.4672	1269.9351	1274.5962	1277.6493
594.2815	595.7012	603.9985	1277.9662	1277.9903	1289.8113
606.8643	607.4415	610.1685	1290.7671	1298.5941	1299.2063
620.1273	623.5441	631.0117	1299.9537	1300.4707	1312.3521
644.6987	650.2545	652.8851	1315.0568	1315.2855	1318.1294
654.9432	658.1262	660.4666	1318.9026	1320.6174	1325.6150
661.1833	662.7129	700.0152	1338.2848	1338.6992	1339.8515
714.0351	714.9860	717.5033	1340.7140	1343.6602	1344.9815
720.8144	723.9143	725.1695	1345.8474	1349.7792	1361.0502
729.5177	734.4723	736.2922	1364.6677	1376.7871	1377.0936
737.9367	739.2507	740.6327	1378.6878	1380.0350	1383.7038
740.8946	742.1790	742.6847	1393.0520	1395.5371	1400.4268
746.5100	748.5840	752.2345	1404.1645	1409.9159	1412.8136
762.7990	766.2035	767.5490	1413.0617	1414.0059	1417.0653
767.8952	769.0051	771.5794	1421.9943	1424.9609	1450.6385
771.9403	779.1417	779.6350	1451.1074	1468.6680	1469.9743
783.8375	785.1460	785.9502	1472.9430	1474.0246	1474.1929
795.2535	803.0351	805.4307	1474.4448	1475.1392	1475.7305
806.7291	814.2759	822.3182	1476.3197	1478.8676	1482.6280
825.6865	827.0939	835.3041	1483.9386	1484.4832	1485.2056
840.5701	842.6169	849.8257	1489.1162	1490.6222	1494.1659
861.5521	869.0362	869.7099	1497.3043	1499.6021	1501.3824
877.1353	888.4371	888.7217	1501.7109	1502.6170	1504.0548
894.8443	897.3266	897.5693	1511.9872	1521.1709	1521.3819
900.1088	904.6014	909.6527	1522.1958	1534.6088	1534.8512
911.5597	915.1602	919.2150	1535.2594	1604.7378	1605.2428
919.9746	930.4034	936.4262	1628.2447	1628.7957	1631.5213
936.9928	937.6723	940.8223	1637.2921	1637.4303	1640.6155
941.2463	941.6953	942.9584	1648.8908	1648.9848	1649.5665
952.0477	953.6530	959.9357	1674.6089	1676.3539	1676.5505

1677.7288	1679.0429	1679.1063
1769.7676	1772.4018	1773.5784
1819.6384	1820.7688	1822.6350
3007.7533	3013.5977	3015.2027
3017.6408	3017.9088	3039.2438
3057.2686	3057.6190	3057.7198
3061.8614	3063.1080	3065.9102
3071.0853	3074.0435	3074.0761
3075.5634	3078.7727	3079.0325
3079.2279	3098.0958	3103.2183
3103.3726	3103.9206	3108.9908
3116.8651	3121.5146	3124.3793
3125.3775	3129.2190	3130.4160
3172.6124	3172.7513	3172.8294
3180.4444	3181.1516	3181.5298
3183.1231	3185.8663	3186.6319
3198.1554	3198.3273	3199.1727
3200.3044	3200.4488	3200.9431
3201.3326	3201.4642	3204.8429
3217.1879	3229.5222	3240.8935

I8⊂CCl_4

E(RB3LYP) = -5602.46130358

E(RB3LYP-D3) = -5602.68235649

H - Sum of electronic and thermal Enthalpies= -5601.280623

G - Sum of electronic and thermal Free Energies= -5601.461947

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.92432	-1.43237	-0.14458
C	5.92409	-0.81978	1.12216
C	5.86828	0.58396	1.23696
C	5.88349	1.37516	0.07258
C	5.85894	0.77099	-1.20198
C	5.88133	-0.63314	-1.30587
C	5.96046	-2.95839	-0.24590
C	5.78120	-3.49581	-1.68335
C	6.65008	-2.63225	-2.62435
C	5.80624	-1.33682	-2.66879
C	5.80239	1.62784	-2.46889
C	5.72974	3.15005	-2.20050
C	5.89712	2.90775	0.15349
C	5.76649	1.24928	2.61141
C	5.61806	0.25061	3.78464
C	5.90638	-1.65811	2.40681
C	6.62657	-0.89419	3.54114
C	6.70241	3.46895	-1.04282
C	1.97433	-1.11034	4.09470
C	3.07539	-0.22426	4.29840
C	4.29604	-0.50281	3.73086
C	4.47726	-1.67202	2.93559
C	3.44754	-2.55445	2.72785
C	2.16908	-2.29848	3.29976
C	2.23066	4.22484	0.07900
C	2.10581	4.30607	-1.35603
C	3.22846	3.96963	-2.17007
C	4.39894	3.55188	-1.58467
C	4.50736	3.44387	-0.16747
C	3.45900	3.78413	0.64976
C	2.05242	-2.13766	-3.36872
C	2.01942	-3.40637	-2.68159
C	3.22349	-3.92091	-2.11647
C	4.38569	-3.19428	-2.20271
C	4.40384	-1.91662	-2.83431
C	3.27295	-1.40298	-3.41958
C	0.86524	-1.63433	-3.97618
C	-0.29296	-2.35692	-3.85425
C	-0.33562	-3.57782	-3.14208
C	0.78921	-4.11901	-2.57432
C	0.69041	-0.84579	4.65855
C	-0.33181	-1.72864	4.41606
C	-0.13470	-2.89247	3.63636
C	1.08264	-3.19461	3.08716
C	0.86438	4.70589	-1.93319
C	-0.18751	4.99083	-1.10038
C	-0.05597	4.92702	0.30651
C	1.12085	4.56282	0.90526
C	-1.36999	5.27611	0.91025
O	-1.67625	5.37312	2.08623
N	-2.24001	5.49457	-0.16775
C	-1.59482	5.37120	-1.41514
O	-2.11466	5.56120	-2.49805
C	-1.75474	-1.71518	4.86435
O	-2.33337	-0.91335	5.57508
C	-1.42251	-3.63494	3.57228
O	-1.67088	-4.69549	3.02867
C	-1.65492	-2.08899	-4.39311
O	-2.02107	-1.19827	-5.13982
C	-1.73661	-4.08090	-3.17428
O	-2.19443	-5.10902	-2.71314
N	-2.47417	-3.11500	-3.89365
N	-2.33674	-2.87108	4.31715
C	-3.65813	5.79410	-0.00318
C	-3.71200	-3.26871	4.53535
C	-3.86747	-3.32663	-4.28311
C	-6.62784	-0.17425	-3.58299
C	-6.18300	-0.38035	-4.88648
C	-5.25137	-1.38746	-5.11964
C	-4.79970	-2.15103	-4.03699
N	-5.21501	-1.94342	-2.77737
C	-6.11371	-0.96834	-2.54739
C	-6.63406	-1.21978	2.21538
C	-7.02244	-1.80479	3.42136
C	-6.06594	-2.45141	4.19695
C	-4.74859	-2.50326	3.72146
N	-4.37347	-1.95147	2.56494

C	-5.29429	-1.30745	1.82330
C	-5.86387	2.46278	1.46806
C	-5.75517	3.58798	2.28353
C	-5.03634	4.69216	1.82665
C	-4.44662	4.62154	0.56082
N	-4.53941	3.53742	-0.22076
C	-5.23658	2.47692	0.21644
C	-5.35229	1.33269	-0.78205
C	-4.76982	-0.66481	0.54297
C	-6.61071	-0.76488	-1.11862
N	-5.78973	0.06027	-0.21695
H	6.92343	-3.32534	0.14049
H	5.18743	-3.39615	0.39593
H	6.02360	-4.56379	-1.70970
H	6.71779	-3.07970	-3.62299
H	7.66405	-2.46760	-2.24267
H	6.69708	1.43558	-3.07916
H	6.31846	-2.65476	2.24127
H	6.66548	1.85522	2.79872
H	4.92041	1.94720	2.61987
H	7.62089	-0.53596	3.25115
H	6.72633	-1.53232	4.42698
H	4.94376	1.32893	-3.08337
H	5.94712	3.69426	-3.12602
H	7.68209	2.99188	-1.15901
H	6.84699	4.55014	-0.93320
H	2.92663	0.66221	4.91267
H	3.57909	-3.45277	2.12898
H	5.76496	0.77848	4.73320
H	3.13666	4.05732	-3.25133
H	3.53808	3.72226	1.73291
H	6.27729	3.24980	1.11773
H	3.19886	-4.89292	-1.62670
H	3.28021	-0.43685	-3.91971
H	6.09560	-0.66997	-3.48223
H	0.74864	-5.06677	-2.04328
H	0.88324	-0.69045	-4.51487
H	1.22109	-4.09272	2.49070
H	0.53034	0.04503	5.26087
H	1.20589	4.50736	1.98748
H	0.75479	4.76015	-3.01345
H	-4.02956	6.05016	-0.99907
H	-3.75749	6.66520	0.65202
H	-3.93821	-3.16274	5.60138
H	-3.76377	-4.33269	4.27768
H	-3.89482	-3.59027	-5.34731
H	-4.20516	-4.18938	-3.70361
H	-7.37246	0.58717	-3.36676
H	-6.55833	0.22867	-5.70482
H	-4.86904	-1.57766	-6.11721
H	-7.34438	-0.68993	1.59097
H	-8.05588	-1.74594	3.75465
H	-6.32654	-2.90268	5.15086
H	-6.41369	1.58440	1.78478
H	-6.21827	3.60111	3.26709
H	-4.90983	5.57662	2.44341
H	-6.72933	-1.74766	-0.65290
H	-7.60867	-0.30744	-1.17563
H	-4.26914	-1.43785	-0.05964
H	-3.98679	0.04259	0.83729
H	-4.39720	1.26177	-1.32762
H	-6.09420	1.64345	-1.52792
C	-0.36818	0.25406	-0.02426
Cl	-0.89286	-1.45380	0.05960
Cl	-1.00594	1.00371	-1.52292
Cl	1.42444	0.33219	-0.03156
Cl	-0.99885	1.14335	1.39918

Frequencies

13.5143	14.7312	17.6957
18.2058	21.5586	23.3202
26.3107	27.8667	28.5599
30.9133	32.4151	34.7457
38.8816	42.7334	43.8684
47.0103	47.4957	52.1069
56.6754	60.6155	65.0280
73.3218	97.2423	97.8152
103.7227	112.9583	116.7191
120.2426	121.4192	135.7898
139.2139	139.7302	149.8537
150.5273	159.2487	161.5000
166.3196	170.2365	175.8552
181.2562	183.4225	184.5091
185.7232	198.3457	200.5731
211.0359	215.1461	216.3000
223.0728	225.3489	229.3947
237.2313	238.6785	241.3776
245.3270	245.5636	256.8309
261.1546	262.5184	268.6362
271.2967	284.2013	287.2278
298.1720	298.7831	305.0325
305.6966	313.9740	314.4910
315.0717	318.0347	321.3457
327.4843	341.2147	346.5621
348.5718	370.2069	371.3905
378.4666	385.7877	392.0786
395.5817	399.9744	403.1406
405.9367	407.3204	420.0905
424.9692	427.8245	428.9994
436.7592	437.4035	447.6590
450.2452	461.2129	469.9089
477.6448	483.8594	484.3109
484.8663	487.0193	498.6618
502.0992	504.6270	530.3353
532.7924	539.0771	542.1155
548.6127	550.9875	568.2380
572.2205	574.9948	576.1500
578.1354	578.9240	581.1045

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730.9510	734.5989	736.1203
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768.7051	770.4714	771.5491
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783.8960	784.4227	785.6522
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988.0988	989.4075	996.6432
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1012.9027	1014.4814	1014.7551
1016.2425	1018.7598	1027.1619
1039.3772	1043.9115	1045.3527
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1177.1983	1177.6508	1179.0039
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1259.5379	1260.0059	1268.8947
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1278.1621	1278.3572	1289.3271
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1319.0145	1320.7768	1321.6745
1325.7837	1338.4663	1339.3142
1340.6161	1341.7012	1345.0752
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1472.9925	1473.9921	1474.3357
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1476.6146	1479.8205	1484.0546
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1489.5159	1491.1122	1494.0748
1497.2239	1500.9902	1502.0105
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1648.6023	1649.2472	1649.8364
1674.8852	1676.1207	1676.7773
1677.8782	1679.1248	1679.3984
1769.1467	1771.5975	1773.5676
1819.6213	1820.2426	1822.5767
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3018.0946	3019.1757	3024.9317
3057.1702	3057.4766	3057.8722
3058.4217	3062.4999	3067.2539
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3078.9550	3079.1134	3079.4510
3080.3947	3090.7428	3103.0563
3103.2524	3104.1239	3109.8385
3111.4792	3121.8172	3125.9493
3129.0426	3133.9920	3135.2668
3172.4187	3172.7369	3172.8941
3180.4024	3181.2079	3181.8836
3182.2492	3186.4725	3189.8229
3198.4318	3198.5932	3198.8592
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3201.4840	3201.6872	3212.9303
3219.3703	3228.0586	3238.7367

TS9⊂CCl_4

E(RB3LYP) = -5602.45887407

E(RB3LYP-D3) = -5602.67915846

H - Sum of electronic and thermal Enthalpies= -5601.279351

G - Sum of electronic and thermal Free Energies= -5601.458851

Number of imaginary frequencies: 0

Cartesian Coordinates

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C	5.79702	-0.67948	-1.19067
C	5.78920	-1.43454	0.00105
C	5.77606	-0.77220	1.24291
C	5.74878	1.36289	2.64812
C	5.60294	0.42503	3.86965
C	6.52488	-0.79322	3.64256
C	5.71790	-1.55205	2.56276
C	5.80432	-2.96447	-0.04321
C	5.73766	-3.55772	-1.47025
C	5.80283	-1.43403	-2.52703
C	5.73393	1.53426	-2.44328
C	5.64055	3.06523	-2.23645
C	5.79243	2.91494	0.12599
C	6.59991	3.43977	-1.08485
C	6.65909	-2.71470	-2.37934
C	2.00054	4.22316	-1.46470
C	3.13293	3.86674	-2.25647
C	4.30056	3.47623	-1.64683
C	4.39630	3.41683	-0.22600
C	3.33281	3.76249	0.56960
C	2.10682	4.17649	-0.02656
C	2.12254	-2.32060	-3.46485
C	2.07059	-3.58685	-2.77491
C	3.23693	-4.06071	-2.10512
C	4.38206	-3.30258	-2.10571
C	4.42332	-2.04043	-2.76600
C	3.32829	-1.56127	-3.44103
C	1.96950	-1.88022	3.59239
C	1.89315	-0.65477	4.35062
C	3.06171	0.15112	4.48805
C	4.23636	-0.23846	3.89223
C	4.30538	-1.44082	3.13020
C	3.20501	-2.24907	2.98517
C	0.81069	-2.69951	3.45695
C	-0.35876	-2.28764	4.04103
C	-0.43668	-1.08077	4.77560
C	0.65642	-0.27087	4.94709
C	0.77127	4.62404	-2.06664
C	-0.28592	4.94687	-1.25463
C	-0.17691	4.90673	0.15543
C	0.98681	4.53788	0.77702
C	0.85619	-4.33392	-2.76190
C	-0.24087	-3.81722	-3.40154
C	-0.18413	-2.58348	-4.09148
C	0.96446	-1.83800	-4.14103
C	-1.53112	-2.31372	-4.66556
O	-1.90420	-1.37968	-5.35309
N	-2.33768	-3.39028	-4.26636
C	-1.62968	-4.34608	-3.51400
O	-2.09406	-5.38404	-3.08067
C	-1.67161	5.37770	-1.59540
O	-2.18087	5.54774	-2.68863
C	-1.48500	5.31972	0.73454
O	-1.80483	5.44442	1.90237
C	-1.69869	-2.93689	4.07685
O	-2.05124	-4.00914	3.61838
C	-1.82967	-0.93716	5.28274
O	-2.30473	-0.06950	5.99093
N	-2.52651	-2.06303	4.79964
N	-2.31712	5.58699	-0.36576
C	-3.75536	-3.48835	-4.57226
C	-3.70719	5.96749	-0.24200
C	-3.89639	-2.37607	5.17008
C	-6.86971	-2.25270	2.13942
C	-6.78415	-3.39498	2.93122
C	-5.77771	-3.46813	3.89231
C	-4.89837	-2.38810	4.02613
N	-4.95686	-1.30311	3.24036
C	-5.92208	-1.23123	2.30823
C	-6.45135	2.71272	-0.40481
C	-6.93921	4.00973	-0.57608
C	-6.04870	5.07810	-0.54437
C	-4.69082	4.80426	-0.33012
N	-4.22158	3.56699	-0.16262
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C	-4.43803	1.15919	-0.05502
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H	4.93552	2.09852	2.66173
H	5.82010	0.98251	4.78727
H	6.61193	-1.39881	4.55235
H	7.53039	-0.51597	3.30632
H	6.72581	-3.33007	0.43383
H	6.16027	3.30118	1.07784
H	6.64253	1.32984	-3.02863
H	4.89101	1.20091	-3.06156
H	7.58612	2.97049	-1.17551
H	6.73106	4.52599	-1.01547
H	4.97344	-3.36591	0.55002
H	5.99796	-4.62128	-1.43704

H	7.64244	-2.52079	-1.93623
H	6.80019	-3.19618	-3.35416
H	3.05215	3.92190	-3.34076
H	3.39956	3.72946	1.65489
H	5.86000	3.57444	-3.18120
H	3.19793	-5.02616	-1.60346
H	3.35211	-0.60357	-3.95653
H	6.13656	-0.79404	-3.34517
H	3.00129	1.06627	5.07462
H	3.24861	-3.17122	2.40965
H	6.04921	-2.58342	2.43481
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H	0.85945	-3.62783	2.89367
H	1.05814	4.50868	1.86127
H	0.67841	4.66155	-3.14923
H	0.99336	-0.88696	-4.66648
H	0.80330	-5.28485	-2.23756
H	-4.06728	-4.47903	-4.22584
H	-3.88978	-3.44059	-5.65777
H	-3.93111	6.69879	-1.02489
H	-3.81428	6.45981	0.73105
H	-3.90855	-3.34952	5.67195
H	-4.18846	-1.60862	5.89463
H	-7.65625	-2.14709	1.39667
H	-7.49146	-4.21092	2.80688
H	-5.67519	-4.34130	4.52996
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Cl	1.78961	-0.00708	-0.13325
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Frequencies

-41.9926	14.0813	15.8147
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33.5658	37.8735	40.7424
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52.0175	58.5454	63.7006
69.7269	92.9424	98.1028
102.9355	109.8491	115.5018
119.8603	121.4055	131.0318
139.3951	139.9243	149.1369
151.0538	159.2229	160.6805
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177.1949	179.9040	181.5208
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236.4396	238.9834	242.6573
245.6410	248.2290	257.6633
261.3317	267.8473	270.8616
272.7585	282.6295	290.3286
297.8626	299.7597	302.3703
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322.5611	329.3518	346.7349
347.3571	359.2316	370.3916
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1178.0844	1178.8853	1179.2556
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1187.2255	1189.7361	1191.0193
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1253.8148	1254.0866	1254.1682
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3125.6596	3127.1723	3129.8064
3172.4706	3172.7310	3172.9615
3179.9132	3180.6595	3180.6946
3181.7732	3185.6062	3186.2709
3197.9818	3198.0187	3198.4388
3198.8574	3198.8900	3200.6132
3201.3059	3201.3140	3205.3851
3210.8861	3229.2550	3237.7260

B(–)⊂CCl_4

E(RB3LYP) = -5602.47269242

E(RB3LYP-D3) = -5602.69671341

H - Sum of electronic and thermal Enthalpies= -5601.292208

G - Sum of electronic and thermal Free Energies= -5601.473361

Number of imaginary frequencies: 0

Cartesian Coordinates

C	-5.61723	1.34654	0.43689
C	-5.62603	0.29715	1.37541
C	-5.61964	-1.04650	0.94487
C	-5.62764	-1.33451	-0.43313
C	-5.61895	-0.28985	-1.38156
C	-5.62493	1.04755	-0.94191
C	-5.61739	2.79897	0.92028
C	-5.54948	3.84778	-0.21572
C	-6.47424	3.37125	-1.35753
C	-5.62212	2.21593	-1.93652
C	-5.62087	-0.59731	-2.88110
C	-5.55558	-2.10565	-3.22146
C	-5.62782	-2.78002	-0.94786
C	-5.62174	-2.19136	1.96100
C	-5.55393	-1.73192	3.43724
C	-5.62432	0.57437	2.88451
C	-6.47774	-0.50405	3.59503
C	-6.48090	-2.85478	-2.23730

C	-1.90292	-0.90038	4.50221
C	-3.06251	-1.69915	4.27614
C	-4.20140	-1.12456	3.76712
C	-4.24328	0.26558	3.45672
C	-3.15092	1.06933	3.67089
C	-1.95092	0.50968	4.19944
C	-1.95550	-3.89110	-1.65982
C	-1.90644	-3.44852	-3.03239
C	-3.06510	-2.85213	-3.61172
C	-4.20409	-2.69706	-2.86003
C	-4.24706	-3.12319	-1.50097
C	-3.15563	-3.71172	-0.91142
C	-1.94795	3.38410	-2.53973
C	-1.89881	4.35161	-1.47027
C	-3.05783	4.55612	-0.66490
C	-4.19733	3.82872	-0.90728
C	-4.24048	2.86471	-1.95577
C	-3.14854	2.64717	-2.75923
C	-0.79531	3.17180	-3.35166
C	0.34257	3.88617	-3.08022
C	0.39271	4.83118	-2.02823
C	-0.69656	5.08089	-1.23366
C	-0.70121	-1.47099	5.01553
C	0.38865	-0.65889	5.19689
C	0.33962	0.72478	4.90488
C	-0.79773	1.31805	4.42196
C	-0.70447	-3.60892	-3.78258
C	0.38464	-4.17280	-3.16933
C	0.33464	-4.61130	-1.82491
C	-0.80303	-4.48871	-1.07029
C	1.67159	-5.16399	-1.46975
O	2.05281	-5.65036	-0.42036
N	2.45433	-5.03795	-2.62875
C	1.75524	-4.43737	-3.69049
O	2.21444	-4.21968	-4.79669
C	1.75909	-0.97907	5.68631
O	2.21758	-2.04636	6.05046
C	1.67698	1.30768	5.20607
O	2.05891	2.45948	5.10317
C	1.67942	3.85489	-3.73659
O	2.06047	3.18933	-4.68259
C	1.76350	5.41441	-1.99661
O	2.22296	6.26325	-1.25481
N	2.46231	4.79548	-3.04795
N	2.45884	0.24034	5.67653
C	3.86268	-5.36521	-2.68032
C	3.86745	0.35815	5.98504
C	3.87090	5.00270	-3.30514
C	6.38373	2.05631	-1.52107
C	6.92358	2.88577	-2.50439
C	6.11061	3.84486	-3.10454
C	4.77631	3.93851	-2.69034
N	4.25429	3.14018	-1.75575
C	5.03724	2.21370	-1.17564
C	6.38162	0.28725	2.54236
C	6.92067	0.72489	3.75242
C	6.10715	0.76510	4.88270
C	4.77323	0.35848	4.75631
N	4.25189	-0.05230	3.59752
C	5.03530	-0.09122	2.50543
C	6.37982	-2.35013	-1.02158
C	6.91762	-3.61747	-1.24734
C	6.10307	-4.61573	-1.77736
C	4.76936	-4.30180	-2.06606
N	4.24925	-3.09227	-1.84279
C	5.03373	-2.12765	-1.33092
C	4.37505	-0.77133	-1.16321
C	4.37503	-0.62304	1.24734
C	4.37617	1.39031	-0.08633
N	4.84566	-0.00162	-0.00069
H	-6.53481	2.98687	1.49741
H	-4.78207	2.96354	1.61238
H	-5.80784	4.83481	0.18304
H	-6.61360	4.15865	-2.10757
H	-7.45827	3.04002	-1.00685
H	-6.53801	-0.18995	-3.33158
H	-5.95884	1.58927	3.10380
H	-6.53984	-2.78396	1.83475
H	-4.78718	-2.87408	1.75793
H	-7.46165	-0.64128	3.13232
H	-6.61742	-0.24811	4.65188
H	-4.78518	-0.08155	-3.37046
H	-5.81489	-2.25341	-4.27545
H	-7.46412	-2.38394	-2.12511
H	-6.62211	-3.89779	-2.54415
H	-3.02509	-2.75917	4.52152
H	-3.17432	2.13287	3.44295
H	-5.81330	-2.57044	4.09269
H	-3.02679	-2.53475	-4.65242
H	-3.17985	-4.04577	0.12368
H	-5.96356	-3.47700	-0.17877
H	-3.01946	5.29875	0.13026
H	-3.17279	1.91756	-3.56590
H	-5.95724	1.89882	-2.92503
H	-0.64797	5.81082	-0.42937
H	-0.82147	2.44556	-4.15999
H	-0.82301	2.38126	4.19733
H	-0.65341	-2.53262	5.24510
H	-0.82908	-4.82539	-0.03710
H	-0.65589	-3.27715	-4.81681
H	4.11673	-5.49816	-3.73764
H	4.01432	-6.32001	-2.16689
H	4.12129	-0.49162	6.62816
H	4.02007	1.27973	6.55568
H	4.02293	5.03463	-4.38871
H	4.12558	5.98491	-2.89218
H	6.97881	1.29127	-1.03341
H	7.96403	2.78206	-2.80256

H	6.49590	4.50038	-3.88164
H	6.97719	0.24738	1.63630
H	7.96089	1.03567	3.81202
H	6.49173	1.11117	5.83892
H	6.97621	-1.54600	-0.60333
H	7.95769	-3.82540	-1.00814
H	6.48671	-5.61725	-1.95574
H	3.28578	1.44873	-0.23530
H	4.58424	1.87250	0.87720
H	3.28461	-0.52288	1.37147
H	4.58271	-1.69869	1.18362
H	3.28438	-0.92751	-1.13958
H	4.58440	-0.17865	-2.06271
C	-0.31223	-0.00375	0.00080
Cl	0.28342	-0.29984	-1.66425
Cl	0.29383	-1.29460	1.08753
Cl	-2.09930	-0.00639	0.00655
Cl	0.28749	1.58618	0.57310

Frequencies

14.0248	15.3780	15.7960
19.9485	20.7123	23.4705
26.6457	28.6170	29.2749
29.6990	32.1539	32.3778
34.2065	34.5288	42.8953
47.3940	47.6857	52.2864
59.4784	62.6744	62.7491
87.9099	95.0726	95.2885
107.0370	119.1690	119.2190
123.3069	128.1298	128.3369
139.8912	140.1321	148.9166
151.9931	159.6969	160.1244
167.5144	172.4182	172.4830
178.7061	178.7525	179.1844
191.7233	191.7784	208.8680
214.7141	215.2586	225.2304
225.4815	232.5458	235.4499
241.0400	241.1032	250.5051
250.5762	251.6615	259.7960
260.1056	265.1703	270.4313
270.5479	272.7303	300.5762
300.7170	307.4022	313.7261
313.9201	315.3366	315.5189
315.9137	321.0883	323.7493
324.0330	330.4551	341.7417
347.0317	347.2771	373.6386
373.7729	380.4966	388.8972
398.1295	400.7823	400.8383
405.4851	405.6208	419.2712
429.0425	429.2629	436.1669
436.2235	439.6075	451.0800
460.4701	460.6747	469.0238
479.3510	479.3556	484.7021
484.9872	485.7383	502.7201
503.4553	503.5552	528.7019
532.6526	549.8032	549.8511
556.6467	556.6574	569.4772
571.5546	571.5804	576.0416
578.1576	578.1876	579.2611
595.6547	595.6957	605.8208
606.0168	606.0330	624.5460
630.2502	647.0471	647.0651
651.6787	652.8268	652.8513
654.4920	655.5433	655.5516
660.6185	660.8339	660.8841
716.9952	717.0473	719.1837
721.8827	721.9371	729.7958
735.4795	736.2402	736.4073
738.5920	738.6356	741.2530
743.5456	743.5935	745.5720
751.4236	752.9219	753.0032
762.7465	767.3063	767.4513
768.0629	772.1810	775.1714
775.2335	780.0065	780.0928
787.3403	787.7020	787.7179
795.7045	799.0134	799.0416
808.9928	809.0752	816.4760
826.5450	826.5630	827.7079
841.4271	841.4398	843.0022
869.3839	869.4283	877.3149
883.1779	888.7143	888.7744
894.6372	897.7963	897.9583
900.8371	911.1242	913.3818
913.4781	913.9500	919.5270
919.7816	935.2989	935.4031
936.6941	937.2027	937.3192
941.3817	941.4203	941.6391
957.0587	957.0753	957.8004
963.1010	963.1426	967.3866
967.5243	970.7800	973.8345
986.9372	1004.7596	1005.5155
1005.6319	1010.3365	1010.3792
1011.8201	1014.1213	1014.2661
1014.8289	1014.9385	1027.4083
1027.5391	1027.5591	1033.5176
1039.2374	1043.5898	1043.6424
1066.4170	1075.0800	1077.8070
1077.8514	1107.0217	1107.1843
1108.9204	1108.9606	1112.6835
1117.2030	1117.3872	1117.3997
1148.4589	1148.5587	1149.8338
1152.0663	1152.1008	1154.9327
1165.8969	1165.9429	1177.6359
1178.8797	1178.9553	1179.3006
1179.8880	1179.9591	1185.3665
1185.3998	1186.8974	1191.0684
1191.8197	1191.8622	1224.0167
1224.0323	1227.7582	1231.0177

1231.3486	1231.3859	1237.1297
1245.1703	1249.9446	1249.9703
1253.9951	1254.2664	1254.3041
1258.9636	1268.5247	1269.5844
1269.6611	1277.4434	1277.5176
1277.5339	1287.6420	1287.9201
1290.8696	1291.1624	1291.2090
1299.5820	1299.6648	1300.1343
1314.6860	1318.2376	1318.3638
1320.8081	1321.9988	1323.8422
1324.0973	1326.1645	1339.3105
1339.3577	1340.3788	1345.2490
1345.3635	1361.3906	1362.4693
1362.5792	1365.4924	1376.7013
1376.9039	1385.0296	1390.4481
1390.4794	1400.1996	1408.7842
1408.8721	1411.1394	1412.6048
1412.6293	1413.5908	1415.9895
1416.0582	1421.2039	1450.2979
1450.4476	1468.7520	1468.7896
1469.9707	1474.1664	1474.4052
1474.4456	1476.6177	1476.6528
1478.1864	1481.8415	1481.9555
1483.0987	1484.4970	1484.5987
1484.6761	1492.2885	1492.3354
1495.9641	1500.7810	1501.4222
1501.7612	1511.2619	1511.5792
1512.2718	1520.8491	1521.0235
1521.8308	1534.4809	1534.5054
1534.8281	1604.3381	1604.4966
1631.5710	1631.5900	1633.3652
1636.9331	1636.9366	1638.0970
1648.8191	1648.8502	1648.9467
1675.6384	1675.7703	1675.8179
1678.1318	1678.2379	1678.2879
1771.1831	1773.7406	1773.7592
1821.2966	1821.3023	1823.1253
3002.6696	3003.2450	3008.1960
3017.2887	3017.4039	3017.5520
3057.2644	3057.2812	3057.3759
3063.6383	3063.7214	3063.9242
3066.5009	3067.5650	3067.6572
3073.1148	3073.1341	3073.1980
3078.9840	3079.0293	3079.1841
3103.1513	3103.1713	3103.4608
3117.2788	3117.2818	3117.3148
3128.4371	3128.8085	3128.9206
3172.5587	3172.6384	3172.6636
3179.8489	3179.9464	3179.9998
3182.4062	3182.4156	3182.4848
3198.0638	3198.0688	3198.1191
3198.1483	3198.1653	3198.3125
3200.7801	3200.8250	3200.8604
3219.8739	3219.9834	3221.7436

B(+)⊂CBr_4

E(RB3LYP) = -14058.1817938

E(RB3LYP-D3) = -14058.4195355

H - Sum of electronic and thermal Enthalpies= -14057.002235

G - Sum of electronic and thermal Free Energies= -14057.187099

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.62517	0.12349	-1.41125
C	5.63550	-1.15217	-0.81375
C	5.62677	-1.28234	0.59158
C	5.63835	-0.12710	1.39761
C	5.62775	1.15502	0.80768
C	5.63645	1.27542	-0.59583
C	5.60849	0.24789	-2.93649
C	5.53655	1.70466	-3.45340
C	6.47967	2.56137	-2.57926
C	5.64334	2.65000	-1.27975
C	5.61348	2.41370	1.67804
C	5.54336	2.13301	3.19816
C	5.64790	-0.22218	2.93000
C	5.61161	-2.66541	1.24650
C	5.53783	-3.84148	0.24354
C	5.64133	-2.43176	-1.66218
C	6.47895	-3.51275	-0.93705
C	6.48604	0.94692	3.50160
C	1.89766	-4.47403	-0.98996
C	3.04208	-4.57769	-0.14437
C	4.19225	-3.89622	-0.46107
C	4.25841	-3.07616	-1.62484
C	3.18485	-2.96734	-2.47388
C	1.97623	-3.66510	-2.18221
C	1.98522	-0.05825	4.26511
C	1.90576	1.37873	4.36907
C	3.04919	2.16354	4.03433
C	4.19906	1.54923	3.60077
C	4.26601	0.13135	3.47273
C	3.19369	-0.65906	3.80536
C	1.97867	3.72124	-2.08435
C	1.89819	3.09344	-3.38104
C	3.04139	2.41183	-3.89474
C	4.19215	2.34404	-3.14728
C	4.26026	2.94175	-1.85525
C	3.18794	3.62377	-1.33543
C	0.84674	4.41569	-1.56513
C	-0.30647	4.44297	-2.30564
C	-0.39308	3.80924	-3.56789
C	0.67958	3.15572	-4.11959
C	0.67976	-5.14529	-0.67296
C	-0.39401	-4.99503	-1.51350
C	-0.30921	-4.21908	-2.69382

C	0.84323	-3.56356	-3.04195
C	0.68777	1.98825	4.79249
C	-0.38544	1.18461	5.08308
C	-0.29984	-0.22551	5.00154
C	0.85292	-0.85417	4.60793
C	-1.62142	-0.79414	5.38920
O	-1.95677	-1.95893	5.49620
N	-2.44446	0.31526	5.65965
C	-1.77388	1.53762	5.49395
O	-2.27202	2.63596	5.67008
C	-1.78217	-5.52809	-1.41286
O	-2.27970	-6.23006	-0.54961
C	-1.63096	-4.27117	-3.37973
O	-1.96693	-3.78146	-4.44179
C	-1.62756	5.06354	-2.00599
O	-1.96211	5.73808	-1.05010
C	-1.78173	3.98952	-4.07818
O	-2.28070	3.59351	-5.11727
N	-2.45124	4.74441	-3.10187
N	-2.45320	-5.06097	-2.55427
C	-3.85310	0.21148	5.98489
C	-3.86193	-5.29082	-2.80602
C	-3.85992	5.07797	-3.17318
C	-6.42913	2.04514	-1.63033
C	-6.92246	2.88595	-2.62819
C	-6.09012	3.86901	-3.16335
C	-4.78319	3.97130	-2.67269
N	-4.30208	3.15365	-1.73119
C	-5.10363	2.20959	-1.21029
C	-6.43150	-2.43738	-0.95267
C	-6.92439	-3.72241	-1.18028
C	-6.09196	-4.67768	-1.76352
C	-4.78534	-4.30372	-2.09850
N	-4.30468	-3.07906	-1.86272
C	-5.10636	-2.15564	-1.30625
C	-6.42567	0.39684	2.58987
C	-6.91571	0.84448	3.81683
C	-6.08201	0.81500	4.93473
C	-4.77717	0.33357	4.77713
N	-4.29905	-0.07662	3.59826
C	-5.10194	-0.05429	2.52126
C	-4.48799	-0.61180	1.25109
C	-4.48893	-0.77862	-1.15265
C	-4.48589	1.38653	-0.09578
N	-4.96851	-0.00065	0.00120
H	6.52025	-0.21007	-3.34747
H	4.76705	-0.32362	-3.34786
H	5.78036	1.72477	-4.52119
H	6.62240	3.55875	-3.01143
H	7.46161	2.10016	-2.42381
H	6.52557	2.99773	1.48576
H	5.99275	-2.23460	-2.67603
H	6.52468	-2.79227	1.84667
H	4.77172	-2.73598	1.94897
H	7.46138	-3.14742	-0.61696
H	6.62071	-4.38569	-1.58496
H	4.77229	3.05652	1.38989
H	5.78862	3.04751	3.74913
H	7.46729	1.04212	3.02289
H	6.63039	0.82242	4.58122
H	2.98373	-5.20763	0.74161
H	3.22931	-2.35362	-3.37101
H	5.78253	-4.77624	0.75965
H	2.99029	3.24578	4.13664
H	3.23884	-1.74286	3.72270
H	6.00092	-1.19853	3.26521
H	2.98163	1.95956	-4.88321
H	3.23361	4.09359	-0.35531
H	5.99641	3.42898	-0.60239
H	0.60486	2.67798	-5.09338
H	0.89917	4.89733	-0.59220
H	0.89423	-2.96191	-3.94569
H	0.60644	-5.74958	0.22790
H	0.90461	-1.93765	4.53919
H	0.61382	3.07054	4.86509
H	-4.09351	0.98383	6.72116
H	-3.99592	-0.77043	6.45031
H	-4.10258	-6.31379	-2.50266
H	-4.00509	-5.20559	-3.88926
H	-4.00205	5.97265	-2.55634
H	-4.10163	5.32829	-4.21016
H	-7.04214	1.26640	-1.18811
H	-7.94217	2.77382	-2.98841
H	-6.44013	4.53347	-3.94900
H	-7.04466	-1.66485	-0.49984
H	-7.94383	-3.97848	-0.90221
H	-6.44167	-5.69063	-1.94485
H	-7.03984	0.40412	1.69514
H	-7.93386	1.21664	3.90053
H	-6.42939	1.16619	5.90284
H	-4.71180	1.88655	0.85458
H	-3.39176	1.43163	-0.21695
H	-4.71739	-0.20587	-2.06041
H	-3.39473	-0.90587	-1.13406
H	-4.71942	-1.68372	1.20961
H	-3.39338	-0.53510	1.34976
C	0.17355	0.00188	0.00145
Br	-0.48011	1.52759	1.05009
Br	-0.48226	-1.66785	0.79939
Br	-0.48418	0.14719	-1.84275
Br	2.12843	0.00055	-0.00085

Frequencies

13.1448	13.9718	15.9469
17.4963	17.7939	21.0661
24.6221	24.9771	25.8689
31.8705	32.3741	32.4621
35.6580	35.9575	41.2821

48.5424	49.0124	52.9829	869.2270	869.3323	876.9936
60.5220	64.3476	64.3945	883.6221	888.6023	888.8070
91.4293	93.8034	94.2011	894.6601	897.5560	897.7119
107.0000	120.3832	120.5333	900.5756	910.9832	914.5612
121.9515	125.4005	125.5424	914.7640	916.5583	919.5932
128.5853	128.8943	141.0663	919.7431	935.9833	936.0868
141.1308	150.1792	152.1313	936.6174	937.1187	937.5971
159.8383	160.2564	168.4818	941.2838	941.4700	941.8410
171.8685	171.9954	176.0680	954.3553	956.2676	956.2976
176.1112	178.4009	181.1138	962.9673	963.0422	967.2404
181.1956	183.6145	195.8377	967.4004	970.7579	978.2486
195.9293	208.5577	221.2548	987.9787	1005.7933	1006.1249
221.5870	231.2858	236.2631	1006.1803	1010.8469	1010.8766
243.1239	243.3473	250.4609	1011.9826	1014.0309	1014.1468
250.8254	250.9184	258.2414	1016.4280	1016.5164	1024.7457
258.4752	261.1411	269.3457	1025.1019	1025.1261	1037.5157
275.3178	275.8614	276.2099	1039.5244	1044.0625	1044.2382
300.3519	300.7479	305.1098	1066.2419	1075.0841	1077.7640
312.7478	312.8556	319.2323	1077.8257	1106.5446	1106.7868
322.9214	323.5460	331.0801	1107.6232	1107.9586	1110.0096
341.5454	346.8399	346.8468	1117.7022	1117.7661	1117.9796
372.4249	372.7098	383.7636	1148.0628	1148.1030	1148.1888
387.9871	398.3798	399.3456	1151.2925	1151.3785	1154.4800
399.4080	405.2473	405.4796	1165.9782	1166.3797	1177.9257
419.4440	429.5572	429.6425	1178.6425	1178.7542	1179.1671
437.2084	437.2788	439.4995	1180.3149	1180.3626	1185.0640
459.2192	459.3702	468.0880	1185.1787	1186.3498	1191.2317
479.7285	479.8370	484.7038	1192.0885	1192.1353	1228.6515
485.1449	485.8450	501.2449	1228.7398	1230.1074	1232.4588
503.2986	503.4904	528.9183	1232.5777	1234.6540	1237.4882
530.3425	548.8262	548.8813	1245.7052	1250.2447	1250.4144
552.6427	552.6855	568.9387	1253.7291	1254.0636	1254.1436
571.9923	572.0181	575.3718	1258.8015	1272.2814	1273.3034
578.1919	578.2533	579.9386	1273.5750	1277.4937	1277.5357
594.8742	594.9164	606.1293	1277.5451	1288.3278	1288.8696
606.9013	606.9171	620.7094	1291.1787	1291.2129	1294.3610
621.1723	623.4988	628.8473	1299.7538	1300.1200	1300.3950
635.2693	645.3627	645.4441	1315.3547	1318.1513	1318.2139
653.0289	653.1302	653.4977	1320.3457	1321.0439	1323.2887
658.0603	659.7677	659.8705	1323.5676	1325.8972	1339.4905
660.1617	661.9973	662.1308	1339.6486	1340.6767	1345.7535
715.7764	715.9191	717.9091	1345.8301	1361.6744	1362.9490
723.3529	723.4822	726.8068	1363.1412	1365.4486	1377.3327
734.4153	734.4332	737.2957	1377.7148	1386.6826	1390.7014
739.9907	744.8916	744.9478	1390.8035	1400.6624	1407.8831
749.8020	752.6602	752.7472	1407.9527	1409.5123	1413.7946
762.9590	767.6160	767.8281	1413.8446	1414.7390	1418.1654
770.2601	772.0742	776.2817	1418.3178	1423.2249	1449.9325
776.4262	779.7789	779.8310	1450.0318	1468.8810	1468.9256
787.0418	787.2715	787.3611	1470.1845	1474.4121	1474.6478
800.3916	800.4559	801.5102	1474.7253	1476.5494	1476.5953
813.2531	813.3347	817.3459	1478.0143	1482.4492	1482.5262
825.4357	825.4901	827.7913	1483.9648	1484.6284	1484.6545
840.8446	840.9659	841.9490	1484.7456	1492.3522	1492.4521

1496.1298	1500.6032	1501.0008
1501.7428	1511.1100	1511.4511
1512.8036	1520.9998	1521.1536
1521.9711	1534.9353	1534.9786
1535.2963	1603.1387	1603.2258
1630.4965	1630.5181	1631.9933
1637.0435	1637.0854	1638.3428
1648.8701	1648.9012	1649.0131
1675.5344	1675.6603	1675.6758
1678.0568	1678.1667	1678.2145
1771.8037	1774.2685	1774.2955
1822.2541	1822.2696	1823.9570
3007.2736	3007.9161	3013.1226
3018.9386	3018.9568	3019.0918
3058.4599	3058.4896	3058.5921
3065.6098	3065.9157	3066.1964
3067.6190	3068.4165	3068.5976
3073.2779	3073.3059	3073.3447
3080.3476	3080.3792	3080.5275
3104.2669	3104.3060	3104.5833
3124.4205	3124.4499	3124.5173
3128.9227	3129.2000	3129.2645
3174.6775	3174.7356	3174.7642
3182.5955	3182.6795	3182.7167
3186.3209	3186.3478	3186.4148
3199.6177	3199.6541	3199.6661
3202.2581	3202.2677	3202.4650
3203.4447	3203.4544	3203.5378
3219.6444	3219.6537	3220.7096

TS1⊂CBr_4

E(RB3LYP) = -14058.1699850

E(RB3LYP-D3) = -14058.4036929

H - Sum of electronic and thermal Enthalpies= -14056.991282

G - Sum of electronic and thermal Free Energies= -14057.174094

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.81420	-1.36209	-0.24256
C	5.83984	-0.78551	1.04168
C	5.78402	0.61603	1.19765
C	5.75138	1.44103	0.05649
C	5.74697	0.87300	-1.23532
C	5.78168	-0.52721	-1.37929
C	5.82760	-2.88541	-0.39262
C	5.69045	-3.37885	-1.85284
C	6.58876	-2.48456	-2.73600
C	5.74456	-1.18836	-2.76343
C	5.72178	1.76366	-2.47999
C	5.62180	3.27750	-2.17626
C	5.70927	2.97058	0.17536
C	5.77137	1.24469	2.59347
C	5.74772	0.21744	3.75135
C	5.90006	-1.65614	2.30396
C	6.72516	-0.92245	3.38810
C	6.54372	3.58474	-0.97526
C	2.14224	-1.12654	4.35598
C	3.26873	-0.26172	4.49199
C	4.42689	-0.53256	3.80449
C	4.52307	-1.67589	2.95877
C	3.46910	-2.54457	2.82126
C	2.24837	-2.29143	3.51110
C	2.00844	4.19787	-0.01280
C	1.94866	4.34034	-1.44752
C	3.11094	4.05341	-2.22278
C	4.26254	3.63575	-1.60140
C	4.31442	3.47588	-0.18615
C	3.22011	3.75510	0.59518
C	2.02139	-1.96442	-3.62229
C	1.97675	-3.27811	-3.02670
C	3.15927	-3.81017	-2.43121
C	4.31444	-3.06594	-2.41786
C	4.34955	-1.76182	-2.99208
C	3.23702	-1.22188	-3.58799
C	0.84851	-1.42050	-4.22152
C	-0.30609	-2.15774	-4.19508
C	-0.35474	-3.44312	-3.60543
C	0.75544	-4.01524	-3.03721
C	0.90992	-0.84558	5.01616
C	-0.15539	-1.68339	4.80528
C	-0.04838	-2.82720	3.97961
C	1.12370	-3.15148	3.34826
C	0.73475	4.76365	-2.06470
C	-0.35398	5.01826	-1.27047
C	-0.29168	4.89072	0.13730
C	0.85630	4.49433	0.77328
C	-1.62519	5.25417	0.69378
O	-1.98789	5.30959	1.85508
N	-2.42421	5.57466	-0.41670
C	-1.73268	5.45117	-1.63361
O	-2.20367	5.68391	-2.73274
C	-1.56094	-1.59976	5.29168
O	-2.07315	-0.78313	6.03802
C	-1.37996	-3.49316	3.93079
O	-1.70332	-4.52112	3.36566
C	-1.65874	-1.83610	-4.72658
O	-2.02500	-0.86129	-5.35558
C	-1.74625	-3.95792	-3.74506
O	-2.21094	-5.03478	-3.41273
N	-2.47007	-2.93678	-4.38387
N	-2.23184	-2.68835	4.71163
C	-3.81498	5.95897	-0.32126
C	-3.65709	-2.93775	4.88146
C	-3.85688	-3.07703	-4.80337
C	-6.88543	-2.52842	-1.87173
C	-6.80049	-3.76851	-2.49980

C	-5.78088	-3.98280	-3.42783
C	-4.88736	-2.93971	-3.69231
N	-4.94536	-1.75805	-3.05862
C	-5.92223	-1.54826	-2.16156
C	-6.10524	-0.24768	2.66811
C	-6.25474	-0.28147	4.05322
C	-5.45597	-1.14629	4.80232
C	-4.53310	-1.94918	4.12515
N	-4.37904	-1.91044	2.79426
C	-5.14893	-1.08107	2.07251
C	-6.55494	2.70898	0.00558
C	-7.05482	4.01378	-0.00066
C	-6.16682	5.07865	-0.11140
C	-4.79731	4.79408	-0.21988
N	-4.31817	3.55043	-0.23053
C	-5.17592	2.51800	-0.11170
C	-4.52087	1.14636	-0.06880
C	-4.95347	-1.16098	0.56222
C	-5.99754	-0.16775	-1.53023
N	-5.43879	0.01222	-0.16242
H	6.77127	-3.28256	0.01014
H	5.02715	-3.32701	0.21349
H	5.93750	-4.44490	-1.90287
H	6.68824	-2.89803	-3.74654
H	7.58997	-2.33254	-2.31705
H	6.64070	1.59493	-3.06091
H	6.28470	-2.65280	2.08224
H	6.66731	1.87063	2.71798
H	4.91137	1.91914	2.69129
H	7.69084	-0.56082	3.01702
H	6.90120	-1.58156	4.24634
H	4.88992	1.47375	-3.13376
H	5.86390	3.84797	-3.07957
H	7.53835	3.13387	-1.06740
H	6.65790	4.66568	-0.83194
H	3.18686	0.60748	5.14233
H	3.53459	-3.42252	2.18238
H	5.98564	0.72405	4.69301
H	3.06595	4.18226	-3.30287
H	3.25097	3.64544	1.67713
H	6.03971	3.30267	1.16060
H	3.12441	-4.80817	-1.99768
H	3.25477	-0.22957	-4.03320
H	6.05772	-0.49639	-3.54645
H	0.70993	-5.00526	-2.59030
H	0.87269	-0.43295	-4.67447
H	1.19251	-4.02783	2.70907
H	0.81605	0.03270	5.64994
H	0.89158	4.39396	1.85486
H	0.67817	4.87118	-3.14508
H	-4.04463	6.55713	-1.20924
H	-3.92517	6.59846	0.56156
H	-3.89113	-2.90612	5.94986
H	-3.83284	-3.95047	4.50685
H	-4.02662	-2.28890	-5.54352
H	-3.96940	-4.05147	-5.28892
H	-7.68304	-2.31491	-1.16473
H	-7.52027	-4.55241	-2.27861
H	-5.67971	-4.93482	-3.94022
H	-6.70075	0.41165	2.04725
H	-6.97810	0.36428	4.54513
H	-5.52758	-1.18313	5.88524
H	-7.21274	1.85262	0.10274
H	-8.12379	4.19407	0.08377
H	-6.51941	6.10725	-0.11448
H	-7.05578	0.13379	-1.52286
H	-5.47685	0.51258	-2.21237
H	-5.49943	-2.04474	0.22005
H	-3.88937	-1.37503	0.37301
H	-3.98845	1.07788	0.88760
H	-3.74309	1.11640	-0.84995
C	-0.04156	0.03532	0.09381
Br	-0.74305	-1.79634	0.06527
Br	-0.63602	0.99061	-1.51249
Br	-0.71455	0.96183	1.68987
Br	1.91902	-0.01144	0.14011

Frequencies

-46.3583	12.4342	15.3152
16.4285	17.1234	20.7797
21.6410	23.0766	24.8358
26.8325	31.5697	32.5719
35.5953	37.4548	40.4706
47.8479	48.9175	52.1334
53.8842	61.0172	65.6077
74.1612	93.8129	96.7819
102.6565	108.7551	118.2146
120.2951	121.6543	125.9042
126.1360	130.1981	141.0163
141.4222	150.6621	150.9890
159.7005	161.2996	168.5802
169.5423	172.9932	174.0839
178.1665	181.1752	181.6946
182.3361	182.4404	190.0222
193.9070	202.5866	211.2144
223.9895	227.6014	233.9070
235.7316	241.6092	242.4837
246.4705	247.4148	257.8145
260.2801	260.4479	267.4245
271.2525	276.1800	287.3109
292.3813	298.7841	300.6340
303.8660	306.2782	310.8973
318.1115	324.4373	331.0690
346.6924	347.7974	368.6865
371.5408	372.7767	379.6234
386.5020	396.4732	399.0166
399.5992	404.4685	405.6937
419.7150	419.8593	429.4093

429.6121	437.3388	438.7581	1180.0035	1180.3536	1185.5547
447.0382	458.7777	470.2030	1187.3146	1189.9091	1191.4521
477.1328	481.5488	484.4110	1192.2798	1192.5287	1223.2106
485.0570	485.7452	500.1638	1230.4902	1231.7380	1232.1846
502.1955	504.2242	529.0596	1237.3252	1238.5254	1241.7775
534.3802	542.8281	548.7385	1245.7756	1250.0746	1250.6750
549.9344	554.6688	568.9131	1253.9246	1254.1928	1254.4384
572.1701	574.5058	575.8191	1259.5693	1261.2172	1270.2790
577.8011	578.4451	580.6828	1273.9489	1277.6207	1278.2217
593.8850	595.1649	605.5336	1278.6118	1281.0734	1290.8108
606.7546	607.6584	611.7256	1291.3886	1295.9505	1299.6009
621.1507	623.8731	625.1339	1300.5143	1301.2551	1305.2507
627.5459	632.7397	635.2837	1314.7770	1315.3629	1318.4155
650.5635	651.8931	653.1959	1319.4990	1321.2885	1325.7459
654.5060	657.1964	660.5936	1327.5303	1330.8442	1339.9775
660.8147	663.4560	699.5400	1340.1483	1341.1096	1345.6173
715.0192	715.6815	719.7337	1346.0846	1355.9390	1365.3137
722.2626	724.3711	726.3518	1366.8915	1369.5175	1377.5480
733.7240	738.2877	738.9346	1377.7560	1383.5949	1384.8003
741.0403	743.3699	743.9272	1388.4776	1395.8335	1401.1029
748.3996	751.6789	757.4214	1412.4238	1414.0039	1414.3375
762.8774	767.4471	768.1640	1414.7278	1418.4428	1420.9610
768.7489	771.8357	772.9615	1423.3132	1428.9862	1450.9692
775.6661	779.8172	780.8410	1451.1863	1468.7087	1471.5463
784.5932	784.9848	785.3941	1472.0126	1474.9538	1475.0743
789.6334	803.2416	805.4499	1475.2359	1475.8906	1476.5773
813.6436	816.3393	825.8423	1477.0075	1478.3028	1484.4340
826.4314	829.8344	838.0008	1484.8762	1485.0343	1486.9804
839.7926	842.0129	845.8366	1487.4672	1489.8831	1493.6015
859.8383	869.4331	869.4994	1494.8668	1499.3896	1500.7916
877.1609	888.6147	888.9500	1501.8900	1502.5510	1509.2611
895.1528	897.5509	897.6722	1521.0908	1521.2309	1522.0437
900.6870	910.0310	911.9563	1528.1173	1535.1777	1535.3674
915.3602	919.2595	919.7974	1535.8673	1604.6921	1604.7380
921.2608	928.6664	936.4987	1627.8501	1628.6138	1633.8268
937.0681	937.2008	940.0846	1636.5724	1637.1888	1639.0332
941.3627	941.6415	941.8328	1649.2454	1649.3668	1650.1734
945.4637	953.4566	957.1886	1675.7084	1676.2671	1676.9507
961.6183	962.8196	966.4332	1678.5643	1678.6438	1679.3786
967.1544	969.1329	970.7383	1770.5980	1773.1173	1773.7206
988.2159	999.9807	1001.2005	1820.7462	1821.3564	1823.0053
1004.0537	1006.6598	1008.9950	2995.2524	3003.0697	3007.2936
1009.9667	1011.4499	1012.9860	3017.5840	3017.7555	3018.7459
1013.6374	1014.3346	1015.4316	3058.2610	3058.3118	3058.4116
1016.5788	1021.2848	1029.8165	3064.8250	3067.2092	3068.8944
1039.9931	1044.4160	1044.6066	3071.0340	3076.9330	3077.5836
1066.4605	1075.6156	1078.1478	3080.3985	3080.5836	3080.7205
1078.5768	1103.1196	1107.6626	3082.3251	3087.5732	3104.0832
1107.8830	1110.6849	1111.2212	3104.1472	3104.4189	3106.7851
1117.8851	1118.8215	1124.7217	3115.9898	3127.8325	3128.2689
1142.3147	1144.2983	1151.3433	3129.9127	3130.9335	3132.3502
1153.1893	1155.6781	1166.4430	3174.4260	3174.7691	3174.9852
1166.8159	1178.0224	1178.1222	3182.2180	3182.4486	3183.9447
1178.3798	1179.5766	1179.8641	3184.5193	3187.6831	3189.6064

3198.9350	3200.1631	3200.5969
3200.6208	3201.9702	3203.6797
3204.2248	3205.1100	3211.6834
3215.1106	3229.2318	3235.3819

I1⊂CBr_4

E(RB3LYP) = -14058.1733980

E(RB3LYP-D3) = -14058.4076390

H - Sum of electronic and thermal Enthalpies= -14056.993726

G - Sum of electronic and thermal Free Energies= -14057.178712

Number of imaginary frequencies: 0

Cartesian Coordinates

C	-5.92320	0.01573	-1.38582
C	-5.95113	1.16159	-0.56774
C	-5.93309	1.03714	0.83846
C	-5.90945	-0.24372	1.42300
C	-5.93126	-1.39766	0.61198
C	-5.94298	-1.26160	-0.78826
C	-5.88292	0.16162	-2.91027
C	-5.76409	-1.18039	-3.67656
C	-6.71087	-2.19278	-2.99590
C	-5.91352	-2.48959	-1.70432
C	-5.96390	-2.79421	1.23829
C	-5.81867	-2.80144	2.77777
C	-5.82396	-0.43344	2.94334
C	-5.97062	2.27938	1.73292
C	-5.96172	3.62073	0.96038
C	-5.98700	2.57271	-1.16880
C	-6.87662	3.47149	-0.27517
C	-6.68213	-1.65584	3.34956
C	-2.32583	4.56675	-0.04738
C	-3.49720	4.50681	0.76309
C	-4.61482	3.85586	0.30186
C	-4.62762	3.24229	-0.98441
C	-3.52567	3.29760	-1.80236
C	-2.34315	3.95652	-1.35491
C	-2.07220	-0.98210	3.88654
C	-2.07039	-2.41813	3.74327
C	-3.28164	-3.08293	3.39210
C	-4.42597	-2.35373	3.18086
C	-4.42384	-0.93354	3.30018
C	-3.27937	-0.25889	3.65135
C	-2.16322	-3.22173	-2.46968
C	-2.07805	-2.44476	-3.68294
C	-3.23685	-1.75312	-4.14678
C	-4.41300	-1.83595	-3.44043
C	-4.50033	-2.63027	-2.26005
C	-3.40697	-3.30798	-1.78096
C	-0.99949	-3.86512	-1.95859
C	0.18072	-3.72509	-2.64014
C	0.25840	-2.99899	-3.85116
C	-0.83740	-2.36689	-4.38254
C	-1.13453	5.19098	0.42504
C	-0.02044	5.16874	-0.37367
C	-0.03798	4.57400	-1.65707
C	-1.16915	3.98792	-2.16299
C	-0.86369	-3.14795	3.95278
C	0.27357	-2.45745	4.28322
C	0.27064	-1.05116	4.43901
C	-0.86819	-0.31021	4.25255
C	1.64550	-0.62863	4.83192
O	2.06073	0.48106	5.11375
N	2.41004	-1.80732	4.86444
C	1.65100	-2.95080	4.55964
O	2.07320	-4.09328	4.56404
C	1.36164	5.65611	-0.11239
O	1.80037	6.24658	0.86062
C	1.33109	4.67825	-2.23648
O	1.72821	4.32957	-3.33209
C	1.54206	-4.22507	-2.30919
O	1.90078	-4.90494	-1.36570
C	1.66373	-3.07457	-4.33892
O	2.13601	-2.66776	-5.38699
N	2.38224	-3.75756	-3.34211
N	2.11456	5.29907	-1.24187
C	3.79257	-1.86240	5.28662
C	3.55496	5.52389	-1.35046
C	3.79178	-4.13578	-3.45127
C	6.66177	-0.99853	-3.47929
C	6.19193	-1.46712	-4.70420
C	5.22945	-2.47341	-4.70911
C	4.77203	-2.97145	-3.48245
N	5.21375	-2.51050	-2.30051
C	6.14278	-1.53687	-2.29249
C	5.80147	2.68755	0.89975
C	5.61765	3.95772	1.44569
C	4.88789	4.90869	0.73157
C	4.36451	4.54295	-0.51393
N	4.53133	3.32011	-1.03603
C	5.23543	2.40626	-0.34957
C	6.72568	-0.73409	2.41113
C	7.12631	-0.99960	3.72257
C	6.16661	-1.36514	4.65910
C	4.83071	-1.46465	4.24096
N	4.44546	-1.23071	2.98574
C	5.37335	-0.85972	2.08006
C	4.84408	-0.56521	0.67950
C	5.41946	1.07879	-1.07152
C	6.66111	-1.04327	-0.94361
N	5.85874	-0.03257	-0.23384
H	-6.80051	0.66216	-3.25331
H	-5.05157	0.81671	-3.19949
H	-5.97766	-1.01402	-4.73797
H	-6.81705	-3.10258	-3.59846
H	-7.70781	-1.78397	-2.79600

H	-6.91783	-3.27919	0.98133
H	-6.31510	2.55367	-2.20919
H	-6.88160	2.24842	2.34877
H	-5.12714	2.26604	2.43468
H	-7.84546	3.01464	-0.04390
H	-7.04944	4.44133	-0.75647
H	-5.17610	-3.42226	0.80566
H	-6.07932	-3.79179	3.16674
H	-7.69290	-1.62462	2.92717
H	-6.75805	-1.72693	4.44105
H	-3.48227	4.97993	1.74344
H	-3.52480	2.83653	-2.78775
H	-6.25389	4.43317	1.63458
H	-3.27782	-4.16796	3.30269
H	-3.26603	0.82449	3.75070
H	-6.10193	0.47511	3.47885
H	-3.16525	-1.16298	-5.05876
H	-3.45959	-3.90448	-0.87297
H	-6.26467	-3.38424	-1.18851
H	-0.76457	-1.79945	-5.30693
H	-1.04892	-4.43099	-1.03211
H	-1.16837	3.52422	-3.14589
H	-1.10896	5.64663	1.41172
H	-0.85930	0.77011	4.37004
H	-0.85131	-4.22966	3.84491
H	3.97755	-2.89380	5.60615
H	3.90494	-1.20979	6.15992
H	3.76120	6.55256	-1.04041
H	3.80684	5.40066	-2.40621
H	3.99933	-4.75864	-2.57839
H	3.91383	-4.73836	-4.35871
H	7.42868	-0.22960	-3.43835
H	6.57308	-1.06092	-5.63760
H	4.82658	-2.86337	-5.63743
H	6.36411	1.92245	1.42225
H	6.03410	4.20230	2.41975
H	4.70425	5.89983	1.13401
H	7.43805	-0.41869	1.65745
H	8.17201	-0.91214	4.00786
H	6.43684	-1.56527	5.69317
H	7.66407	-0.62313	-1.10597
H	6.77246	-1.90634	-0.28054
H	6.18690	1.24287	-1.83866
H	4.48860	0.86769	-1.62284
H	4.04295	0.17349	0.78729
H	4.36461	-1.47289	0.28336
C	0.38593	0.19258	-0.05894
Br	1.01695	-1.58655	0.45814
Br	1.01407	1.51354	1.25258
Br	-1.57888	0.20529	-0.11195
Br	1.09348	0.65467	-1.83078

Frequencies

12.3606	14.9212	16.8766
18.3267	19.9882	22.2387
23.2732	23.5244	24.6513
29.7433	31.9003	36.1471
36.9201	39.5400	44.6804
48.1502	50.6848	54.9527
59.9610	63.5201	67.1405
75.2294	96.6886	99.4285
101.0704	115.1603	116.8858
121.6624	123.0416	126.1303
126.2921	134.7583	139.6693
140.5642	148.9092	150.7880
158.1416	160.9387	164.2481
168.6408	174.0618	177.1366
180.9983	181.5826	181.8824
182.2940	185.5167	189.2523
199.3876	203.0184	208.0534
223.4167	228.4346	231.0885
235.9802	239.0041	241.5720
243.0733	246.0210	255.0510
259.9934	261.6849	266.1191
266.7380	272.1898	285.0397
290.0530	296.9390	299.4125
303.3308	304.6073	316.7660
323.9397	329.2470	343.0485
346.4455	347.8449	370.9776
371.9197	384.8360	385.2464
393.1209	393.7203	399.5847
403.2414	404.0256	406.6652
419.5488	426.2326	427.6924
429.1723	436.3270	436.9082
443.9885	460.3023	469.8317
478.1962	482.8996	483.7615
484.9954	486.0131	497.9825
500.6446	504.8987	527.8466
534.6707	538.3784	543.5822
549.6158	550.3851	567.8345
571.7398	575.0568	575.4724
577.7836	579.3023	581.7590
592.4058	594.8056	601.1412
606.2100	607.3668	608.7908
620.9822	623.0813	623.5328
625.6822	629.5878	634.5811
648.2008	652.4748	653.1701
655.4794	659.6690	660.2177
660.6906	664.7587	703.7763
714.9193	717.3600	721.1619
721.8775	723.7997	726.6847
733.7176	736.0529	739.2765
741.2282	741.8339	743.2080
747.8269	751.1376	758.7806
762.5937	764.2843	767.6436
768.2445	771.6583	772.0113
777.0612	779.2475	780.5842
784.1509	784.7803	785.6529

788.6665	802.3349	805.1279
813.0120	819.8994	825.3375
825.9477	834.6560	837.8853
839.7966	841.8231	854.8233
865.5073	869.2653	869.7217
877.4673	888.2960	889.0692
895.1964	897.0722	898.4912
900.6624	909.5191	911.9060
915.9002	918.7572	920.1647
923.1915	929.1007	935.3354
935.9661	936.3789	936.7593
940.7433	941.1179	941.8133
943.1107	954.5989	957.7301
959.9169	962.4715	965.6926
966.7763	968.2335	969.8213
985.5533	987.7018	996.2109
1005.7677	1007.0663	1007.3931
1009.1236	1010.1417	1011.1127
1012.7869	1014.2999	1014.9451
1016.4869	1018.9498	1030.9694
1039.8235	1043.7786	1045.0385
1066.4325	1075.4778	1078.1551
1078.9616	1098.2404	1103.9489
1107.8521	1108.4950	1117.1863
1117.9051	1120.4535	1128.3438
1138.3625	1140.2067	1153.2187
1155.1524	1155.8175	1166.2710
1166.6234	1169.3051	1176.9912
1177.5909	1177.8507	1179.2553
1179.5579	1179.7973	1186.1681
1187.8589	1190.6066	1191.3063
1191.7167	1193.4489	1222.0425
1229.2956	1231.5542	1231.8464
1237.3042	1244.4506	1244.9888
1246.1949	1249.6496	1250.4941
1254.0273	1254.1617	1254.3874
1255.9151	1259.5483	1270.2216
1275.4278	1276.5804	1277.4775
1278.4162	1278.6227	1290.6354
1291.4564	1298.4936	1300.1257
1300.7066	1301.8466	1303.8902
1314.3042	1316.3874	1318.3587
1319.8257	1322.2153	1324.2170
1326.8840	1339.4318	1340.2733
1341.5699	1344.9194	1345.4305
1346.6668	1355.4275	1365.6166
1367.8323	1373.8438	1376.6148
1376.8611	1378.0492	1380.1297
1385.5030	1400.6919	1400.8843
1406.0646	1411.1321	1413.1976
1413.7049	1414.3497	1416.8890
1420.6065	1421.6642	1451.3729
1452.1602	1468.7934	1473.2789
1473.9460	1474.4615	1474.8288
1475.3232	1475.6450	1476.0838
1476.1583	1478.8001	1484.5657
1484.7308	1484.8532	1487.6128
1489.0781	1490.5529	1491.3551
1496.8907	1498.3435	1500.7863
1501.9817	1502.4045	1503.7539
1510.1200	1520.9662	1521.1900
1521.9674	1534.9217	1535.9741
1536.2071	1605.2123	1606.1197
1628.2850	1628.8895	1633.5320
1636.3033	1636.6275	1638.5966
1649.0240	1649.9101	1650.3598
1675.5134	1675.9825	1676.8606
1678.3519	1678.5196	1679.3913
1768.6073	1770.5234	1773.4005
1819.0338	1820.0734	1822.7561
2997.6661	3015.2404	3018.1237
3018.4374	3021.5832	3026.5775
3057.7873	3058.2971	3058.4632
3062.7965	3064.3864	3064.9336
3065.2750	3067.6905	3070.7480
3080.6523	3080.8845	3081.4166
3089.3831	3097.5094	3103.6391
3104.1571	3104.7333	3109.9212
3110.4824	3128.4004	3131.9851
3133.7080	3145.2302	3149.1063
3173.8843	3174.9015	3175.3345
3181.2567	3181.2920	3181.8187
3185.1044	3188.2260	3192.4123
3197.9697	3200.8611	3200.9246
3201.2439	3204.2505	3204.7078
3205.1979	3205.2759	3220.0066
3230.4147	3230.9689	3236.1083

TS2⊂CBr_4

E(RB3LYP) = -14058.1709715

E(RB3LYP-D3) = -14058.4069860

H - Sum of electronic and thermal Enthalpies= -14056.991902

G - Sum of electronic and thermal Free Energies= -14057.173092

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.83759	1.39113	-0.79726
C	6.00150	0.04005	-1.15937
C	6.07274	-0.96108	-0.16669
C	5.96935	-0.60321	1.19050
C	5.80982	0.74728	1.56466
C	5.76065	1.73963	0.56808
C	5.77391	2.47147	-1.88169
C	5.55672	3.90858	-1.34355
C	6.41370	4.07587	-0.06982
C	5.59398	3.22015	0.92645

C	5.71470	1.14257	3.04163
C	5.67535	-0.05634	4.02109
C	5.97539	-1.66170	2.29970
C	6.29332	-2.42744	-0.54846
C	6.30408	-2.69173	-2.07268
C	6.08086	-0.39493	-2.62934
C	7.09710	-1.55587	-2.75537
C	6.70799	-1.09881	3.54088
C	2.63589	-2.89827	-3.34547
C	3.87781	-3.35931	-2.81921
C	4.91916	-2.47952	-2.65444
C	4.78290	-1.10608	-3.00913
C	3.61224	-0.63186	-3.54991
C	2.50562	-1.51345	-3.72983
C	2.24649	-2.49515	3.09264
C	2.07273	-1.52356	4.14551
C	3.17476	-0.69801	4.51654
C	4.37870	-0.83115	3.86826
C	4.55308	-1.80114	2.83887
C	3.51697	-2.61840	2.45791
C	1.80219	4.12256	0.76087
C	1.79101	4.56928	-0.61138
C	3.00157	4.52948	-1.36438
C	4.15799	4.07647	-0.77716
C	4.17324	3.66258	0.58656
C	3.02618	3.67932	1.34140
C	0.58873	4.10884	1.50829
C	-0.56597	4.52182	0.89595
C	-0.57093	4.99407	-0.43712
C	0.57313	5.02976	-1.19285
C	1.51503	-3.77206	-3.45827
C	0.32670	-3.26023	-3.91109
C	0.20253	-1.90731	-4.30515
C	1.26068	-1.03812	-4.23768
C	0.80134	-1.38704	4.77737
C	-0.23892	-2.16461	4.33722
C	-0.07243	-3.10302	3.29161
C	1.13940	-3.29273	2.67997
C	-1.39198	-3.73961	3.02578
O	-1.67807	-4.60629	2.21902
N	-2.29043	-3.14160	3.92791
C	-1.66427	-2.20775	4.77005
O	-2.21814	-1.59615	5.66646
C	-1.01249	-3.89933	-4.03268
O	-1.33858	-5.05304	-3.80723
C	-1.21352	-1.66918	-4.70649
O	-1.72153	-0.66140	-5.15933
C	-1.96430	4.55504	1.40523
O	-2.38788	4.25354	2.50547
C	-1.96626	5.38225	-0.78005
O	-2.38864	5.91384	-1.79347
N	-2.74905	5.03488	0.33399
N	-1.88225	-2.88899	-4.47095
C	-3.70049	-3.48941	4.00815
C	-3.32237	-3.08746	-4.64107
C	-4.18455	5.30218	0.44396
C	-6.72297	2.91579	-2.00135
C	-6.22850	4.10396	-2.53561
C	-5.38085	4.88854	-1.75663
C	-5.05830	4.44884	-0.46617
N	-5.53279	3.30280	0.04896
C	-6.34945	2.54053	-0.70305
C	-5.48058	-2.73501	-0.97880
C	-5.07819	-4.00924	-1.38111
C	-4.36973	-4.15997	-2.57414
C	-4.08836	-3.01247	-3.32655
N	-4.46382	-1.78772	-2.93628
C	-5.14342	-1.64437	-1.78693
C	-6.38335	-0.36350	2.95316
C	-6.61581	-1.06198	4.13428
C	-5.73218	-2.07436	4.50738
C	-4.65006	-2.34948	3.66848
N	-4.42604	-1.67927	2.52821
C	-5.26934	-0.69723	2.16533
C	-4.92195	0.04185	0.87532
C	-5.55476	-0.21132	-1.49306
C	-6.88418	1.25148	-0.08252
N	-6.00944	0.06380	-0.12959
H	6.71553	2.46507	-2.45020
H	4.98092	2.23499	-2.60251
H	5.78637	4.63213	-2.13325
H	6.43953	5.12336	0.25300
H	7.44249	3.71814	-0.19005
H	6.58301	1.76552	3.30385
H	6.31487	0.44563	-3.28401
H	7.25693	-2.76213	-0.13591
H	5.52651	-3.05988	-0.08456
H	8.05241	-1.33962	-2.26390
H	7.28747	-1.78753	-3.81002
H	4.82905	1.76791	3.20825
H	5.84407	0.30023	5.04303
H	7.68247	-0.66088	3.29672
H	6.85282	-1.88511	4.29117
H	3.97508	-4.40855	-2.54554
H	3.49731	0.41351	-3.82867
H	6.70257	-3.69305	-2.26904
H	3.03804	0.03419	5.31052
H	3.63500	-3.35523	1.66629
H	6.39694	-2.60603	1.95342
H	2.98687	4.86411	-2.40017
H	3.02329	3.35462	2.37959
H	5.86188	3.41185	1.96634
H	0.55624	5.38369	-2.22056
H	0.58313	3.75327	2.53507
H	1.14946	0.00333	-4.52756
H	1.59919	-4.81312	-3.15671
H	1.25470	-4.01520	1.87636
H	0.66150	-0.66232	5.57558

H	-3.91782	-3.85711	5.01674
H	-3.84045	-4.31428	3.30181
H	-3.46720	-4.06175	-5.11657
H	-3.67077	-2.29465	-5.30624
H	-4.44837	5.10365	1.48477
H	-4.34794	6.36303	0.22397
H	-7.39677	2.28759	-2.57759
H	-6.50200	4.41622	-3.54023
H	-4.96218	5.81461	-2.13483
H	-6.03554	-2.57715	-0.06083
H	-5.30993	-4.87672	-0.76829
H	-4.02411	-5.13333	-2.90807
H	-7.05217	0.43613	2.65789
H	-7.46524	-0.81042	4.76441
H	-5.86743	-2.62508	5.43386
H	-7.82118	0.98569	-0.58879
H	-7.12726	1.46149	0.96041
H	-6.38787	0.02015	-2.17011
H	-4.72267	0.43856	-1.81091
H	-4.06131	-0.47679	0.44874
H	-4.59224	1.06302	1.11616
C	-0.44618	-0.04652	-0.13812
Br	-1.03415	-1.90652	-0.31751
Br	-1.11381	0.68579	1.55446
Br	-1.15483	1.00572	-1.63678
Br	1.51865	0.03376	-0.15247

Frequencies

-23.7497	14.8842	16.5795
18.1675	20.1364	21.9273
22.1274	24.4744	25.5433
26.5905	30.9510	33.2676
37.2320	41.6227	44.9728
50.8782	51.8298	56.9815
58.4996	65.7988	70.8385
75.3404	96.2905	98.3353
108.1600	112.2788	115.7233
121.9059	123.6259	125.6703
127.1078	130.0328	140.3287
141.8636	147.7946	152.1309
158.6617	160.2269	160.9934
167.3178	171.5824	174.9210
181.3331	182.0470	182.4213
184.8828	186.9613	192.4052
199.1345	205.3008	210.5905
224.4405	229.6178	233.7462
236.6656	240.7175	242.5736
244.9021	250.6754	256.4107
260.0862	260.9568	262.5256
271.2117	282.2350	289.2056
293.5316	297.7454	299.5646
303.1456	307.3494	316.3568
329.8518	336.8181	344.5450
347.4400	347.8984	371.3893
371.5504	384.6211	389.3488
391.7981	393.6719	400.0756
403.0167	404.2848	410.7696
419.7586	421.4227	427.3986
428.3411	435.6152	436.2803
441.9390	461.5023	469.7727
470.3642	483.7644	484.5735
484.9483	485.8595	498.0277
500.9026	501.4559	527.6068
530.0912	535.9574	542.7467
549.2473	550.6822	567.3331
572.3307	574.1229	575.3785
578.7542	580.0575	582.0098
592.1430	593.4703	600.2061
606.2933	607.3788	608.5536
617.2653	621.8250	624.6721
625.1390	628.3852	636.5176
652.4848	653.0203	654.5290
658.4537	659.7381	661.2988
663.7381	668.3029	704.6953
714.9335	718.2162	722.1534
723.0875	724.4636	727.0372
733.4998	737.8967	740.8935
741.3448	742.1987	743.4214
749.3581	755.9176	761.6038
762.6284	767.9683	768.2826
771.9840	773.4240	777.7008
778.5902	780.7798	782.8456
783.8183	784.8228	786.1439
798.6811	801.8759	804.5102
812.9933	819.9648	824.7650
828.7533	834.7659	837.5826
840.2805	841.1290	852.5301
865.9390	869.2319	869.6407
877.2239	888.5640	888.8197
895.3706	897.4098	898.0117
900.5678	904.9478	911.0596
914.6508	917.7219	919.9779
922.7694	930.8986	934.6596
936.1691	936.6475	937.0151
940.0430	941.2811	941.8489
942.2547	948.0156	955.5511
959.5147	961.3451	965.8612
966.6109	968.9260	972.1245
984.2472	987.0469	987.6763
1001.4110	1006.7175	1007.7748
1009.7290	1010.6548	1011.0454
1013.1885	1014.6731	1014.8594
1015.8173	1018.5172	1024.4673
1039.6247	1043.5030	1044.5828
1066.4083	1075.7043	1078.3873
1078.7062	1094.9965	1101.5035
1107.8622	1108.1572	1113.6128
1118.8894	1120.5128	1124.7919

1133.4200	1138.8774	1144.1979
1147.5125	1152.2610	1155.9394
1166.3517	1166.5791	1176.2397
1177.4560	1177.5909	1178.7168
1179.3559	1180.0693	1187.2844
1190.1876	1190.9624	1191.2362
1192.7807	1195.4839	1228.7316
1230.9878	1231.4906	1234.7602
1237.4494	1245.0883	1246.9059
1249.1010	1250.0800	1250.7059
1253.9250	1254.1912	1254.5712
1259.4733	1267.8503	1272.3935
1276.9999	1278.0884	1278.1511
1278.3315	1279.7415	1290.8395
1291.4777	1299.2042	1299.8229
1300.2357	1301.6431	1303.9385
1313.8907	1314.5829	1318.6382
1319.4525	1322.0142	1324.6871
1327.6392	1339.7059	1340.1634
1341.4651	1345.3103	1345.8259
1348.2669	1356.3595	1358.0367
1365.6728	1372.6122	1374.8750
1376.8454	1377.3121	1379.2436
1387.8949	1390.2191	1400.7344
1401.2672	1409.0714	1412.0290
1413.8423	1414.1240	1415.4399
1418.7028	1425.1333	1451.1825
1451.8714	1471.6304	1472.7171
1473.7525	1474.4368	1475.1608
1475.3693	1475.8122	1476.4909
1477.7884	1483.8448	1484.4901
1484.7649	1486.5268	1487.8327
1490.8096	1493.4266	1494.6995
1495.6652	1497.9622	1501.1194
1502.0238	1503.1564	1506.9473
1512.0133	1520.9847	1521.1225
1521.9507	1535.3116	1535.6958
1536.2833	1605.2594	1605.8960
1627.6128	1628.1750	1629.8605
1635.9348	1638.3252	1640.6007
1649.6502	1649.7995	1650.0980
1675.0819	1676.1071	1676.4350
1678.3532	1678.4831	1678.7421
1767.8792	1769.8386	1771.4869
1818.4223	1819.5436	1820.9726
2992.4087	3016.2409	3016.5332
3019.0615	3029.6283	3048.1432
3055.0059	3057.9513	3058.0900
3058.4712	3062.3264	3066.0302
3066.8684	3070.1545	3073.0421
3080.6423	3081.0380	3081.4746
3092.6390	3103.7791	3104.1728
3104.7390	3116.8418	3131.2069
3131.5159	3134.0537	3136.8094
3140.6576	3149.9498	3153.9109
3174.1814	3174.5573	3175.6311
3181.7986	3183.0880	3184.1354
3189.4365	3189.8857	3193.8715
3200.4110	3200.8911	3201.5357
3205.0948	3205.3675	3205.7743
3206.4846	3207.3257	3219.6740
3232.9101	3233.2489	3237.0333

$I_2 \subset CBr_4$

E(RB3LYP) = -14058.1745147

E(RB3LYP-D3) = -14058.4149512

H - Sum of electronic and thermal Enthalpies= -14056.994299

G - Sum of electronic and thermal Free Energies= -14057.177765

Number of imaginary frequencies: 0

Cartesian Coordinates

C	-5.48155	-0.75806	-1.85006
C	-5.77029	0.49785	-1.28204
C	-5.94194	0.62780	0.11333
C	-5.84751	-0.51226	0.93353
C	-5.59572	-1.78151	0.37071
C	-5.40382	-1.89670	-1.01918
C	-5.29842	-0.88448	-3.36552
C	-4.95332	-2.31379	-3.85282
C	-5.81062	-3.31461	-3.04737
C	-5.09457	-3.24739	-1.67588
C	-5.58200	-3.03570	1.25116
C	-5.75254	-2.76009	2.76701
C	-6.00250	-0.42123	2.45591
C	-6.27759	1.98578	0.73674
C	-6.32232	3.15635	-0.27452
C	-5.89757	1.76020	-2.14625
C	-7.01619	2.65618	-1.56053
C	-6.80826	-1.64888	2.94805
C	-2.70523	4.41010	-0.95573
C	-3.97724	4.33601	-0.31653
C	-4.93060	3.46926	-0.79117
C	-4.67479	2.64779	-1.92709
C	-3.47382	2.71630	-2.58996
C	-2.45320	3.59294	-2.11811
C	-2.41509	-0.33637	4.00067
C	-2.29648	-1.75633	4.22986
C	-3.37925	-2.61183	3.87528
C	-4.51341	-2.07968	3.31384
C	-4.64660	-0.67513	3.11603
C	-3.62678	0.18218	3.45416
C	-1.23247	-3.62454	-2.11841
C	-1.15725	-3.06811	-3.44795
C	-2.35275	-2.61538	-4.07958
C	-3.55485	-2.71728	-3.42247
C	-3.63120	-3.28006	-2.11535

C	-2.50040	-3.72205	-1.47236
C	-0.03908	-4.05491	-1.46712
C	1.15697	-3.92061	-2.12441
C	1.22742	-3.39606	-3.43663
C	0.10537	-2.97692	-4.10492
C	-1.66878	5.24006	-0.43716
C	-0.44003	5.21164	-1.04445
C	-0.19451	4.41722	-2.18855
C	-1.17171	3.63111	-2.74187
C	-1.08248	-2.28902	4.75249
C	-0.03026	-1.43680	4.96406
C	-0.13058	-0.04939	4.70781
C	-1.29997	0.51453	4.26417
C	1.21899	0.55527	4.90990
O	1.56209	1.71751	4.80412
N	2.06724	-0.51777	5.25848
C	1.37101	-1.73237	5.36555
O	1.86227	-2.79350	5.71206
C	0.83987	5.86422	-0.65491
O	1.06058	6.63531	0.26457
C	1.24355	4.56107	-2.55365
O	1.84625	4.07869	-3.49317
C	2.54133	-4.24200	-1.67866
O	2.91730	-4.73312	-0.63020
C	2.65485	-3.40833	-3.85999
O	3.14301	-3.11043	-4.93701
N	3.38216	-3.87169	-2.75000
N	1.80045	5.40434	-1.56888
C	3.52963	-0.42622	5.32615
C	3.23088	5.69759	-1.44862
C	4.82696	-4.10358	-2.76519
C	7.22347	-0.58556	-2.73806
C	6.97381	-1.19790	-3.96441
C	6.17570	-2.34066	-3.99597
C	5.66489	-2.83254	-2.78954
N	5.90724	-2.24428	-1.60649
C	6.66538	-1.13113	-1.57231
C	5.09523	3.07442	1.34922
C	4.55225	4.26535	1.83065
C	3.95327	5.15500	0.93702
C	3.91342	4.80653	-0.41902
N	4.43611	3.66344	-0.88500
C	5.01753	2.81354	-0.02380
C	5.02112	-2.36989	1.84912
C	5.05982	-3.06996	3.05387
C	4.63165	-2.43641	4.22049
C	4.16889	-1.11880	4.12925
N	4.17710	-0.42576	2.98064
C	4.59907	-1.03141	1.85720
C	4.54393	-0.20767	0.58289
C	5.63418	1.58047	-0.66619
C	6.88385	-0.46903	-0.21412
N	5.82407	0.44775	0.24152
H	-6.22854	-0.57600	-3.86511
H	-4.52212	-0.18992	-3.71052
H	-5.09913	-2.37451	-4.93678
H	-5.73933	-4.32360	-3.47039
H	-6.86733	-3.03034	-2.98871
H	-6.40025	-3.69858	0.93235
H	-6.06114	1.51087	-3.19553
H	-7.26148	1.92086	1.22437
H	-5.55873	2.22681	1.52999
H	-7.94370	2.10596	-1.36585
H	-7.23580	3.48916	-2.23879
H	-4.65395	-3.59989	1.09659
H	-5.99547	-3.69476	3.28399
H	-7.72097	-1.81742	2.36546
H	-7.07986	-1.53496	4.00423
H	-4.16619	4.96471	0.55192
H	-3.26791	2.09593	-3.45963
H	-6.81123	4.02091	0.18749
H	-3.27844	-3.68321	4.03984
H	-3.70767	1.25453	3.28933
H	-6.44996	0.52595	2.75851
H	-2.29109	-2.19965	-5.08377
H	-2.54478	-4.14744	-0.47208
H	-5.35798	-4.07932	-1.02160
H	0.17055	-2.57049	-5.11109
H	-0.08326	-4.46400	-0.46140
H	-0.96759	3.01234	-3.61162
H	-1.84464	5.84912	0.44597
H	-1.36800	1.58048	4.06457
H	-0.98462	-3.35658	4.93305
H	3.86210	-0.88008	6.26442
H	3.77160	0.63849	5.32618
H	3.32928	6.75282	-1.17862
H	3.67348	5.52147	-2.43080
H	5.04987	-4.66939	-1.85783
H	5.06107	-4.71805	-3.64095
H	7.84542	0.30343	-2.67909
H	7.39188	-0.79133	-4.88173
H	5.93701	-2.83634	-4.93107
H	5.55456	2.34704	2.00984
H	4.58710	4.49423	2.89278
H	3.50265	6.08199	1.27737
H	5.29085	-2.84484	0.91077
H	5.38870	-4.10581	3.07812
H	4.60013	-2.96352	5.16836
H	7.81606	0.10797	-0.24584
H	7.00889	-1.24691	0.54338
H	6.62414	1.87241	-1.04283
H	5.03051	1.33255	-1.55541
H	3.81137	0.58529	0.74681
H	4.18117	-0.83554	-0.24601
C	0.18846	0.29011	0.06289
Br	0.84247	-1.32178	0.97363
Br	-1.76175	0.17835	-0.13603
Br	1.02290	0.42392	-1.71005

Br	0.66343	1.86579	1.12500

Frequencies

13.8941	15.0826	16.6812
18.2969	22.1640	23.2588
23.4044	24.6636	25.5633
27.8943	30.4973	35.9740
38.4162	42.4965	44.8479
50.8437	55.7293	59.2347
63.5810	66.1926	73.3239
82.0297	91.8060	100.7743
106.5912	112.6205	116.9133
122.2524	122.6354	125.6610
126.3500	134.6930	141.9069
143.7855	147.8856	152.7311
158.3050	159.5201	162.3603
172.8380	173.8621	177.5789
181.1101	181.7040	182.3546
185.0543	187.0378	197.3395
204.5057	206.8008	211.8692
225.2364	228.7701	235.7664
240.0895	243.9242	247.1447
248.7045	254.7788	259.9812
260.1901	261.7409	270.6971
273.2544	289.6858	294.7460
297.9680	300.6829	305.9072
310.0040	316.3216	321.5546
332.4962	342.5517	346.7428
347.8233	368.8376	371.0974
372.1120	384.6002	390.9749
392.8938	393.9645	403.1377
403.5057	410.2515	414.8507
419.5930	425.5418	426.9099
427.2227	435.4630	438.2587
442.1190	461.3531	467.1480
471.6341	484.1013	484.3446
485.3107	488.9333	497.5047
499.9789	500.5806	527.2690
532.0935	537.2897	547.4684
550.3778	556.4771	566.1528
570.7841	573.4276	574.6385
579.1357	582.1866	585.3250
591.2820	592.1463	601.6698
604.8549	605.6217	608.4146
616.1317	621.1624	623.4282
624.7048	628.0917	633.6265
652.9074	652.9313	654.1839
659.2390	660.3747	660.9775
665.3921	677.5121	705.1549
714.9537	717.5658	721.7721
723.0690	723.5644	727.3609
732.7505	736.7746	741.5678
741.6558	742.3134	743.6641
749.2292	761.6865	762.6146
767.9710	768.3225	771.8536
772.3656	773.8677	778.0657
778.6508	781.4859	783.8451
784.2998	785.2606	792.0054
801.6995	804.1470	811.3483
819.6200	820.3761	824.8448
832.8305	835.9602	837.5759
839.9376	842.9614	855.8914
868.5321	869.2587	870.8971
877.0910	888.2948	888.9008
895.0070	897.4025	898.0619
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916.8704	919.9788	921.9619
930.8769	935.6500	935.9061
936.4404	936.5646	936.8311
940.7565	941.3651	941.4221
942.7626	951.4889	953.6964
958.9448	960.0401	965.6497
966.7394	968.5599	969.7718
985.2903	989.7087	991.1811
1000.9185	1005.3085	1007.8705
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1013.9990	1014.1320	1014.8441
1018.1788	1021.2547	1026.2310
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1066.1569	1075.7403	1078.4925
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1102.0719	1107.8020	1107.9049
1116.1476	1119.8085	1125.8364
1132.6899	1137.1736	1138.5015
1142.4064	1151.3866	1155.5681
1165.6992	1166.5401	1175.7572
1176.1396	1176.8645	1177.6895
1179.5474	1180.2007	1188.0823
1190.1429	1190.8726	1191.1625
1192.4873	1192.7982	1228.4906
1230.6439	1231.7327	1236.6249
1237.3155	1244.8409	1248.8917
1249.5658	1250.7409	1253.8218
1254.1085	1254.5298	1255.0082
1258.8582	1265.8714	1272.2853
1276.1694	1277.7023	1277.7646
1278.2509	1281.4570	1288.0793
1291.5326	1291.9299	1299.5177
1300.0505	1300.4646	1301.0851
1313.2376	1313.7914	1317.9816
1318.8701	1319.8501	1322.6942
1327.6253	1339.6480	1340.3270
1341.4416	1344.0009	1345.5525
1345.9873	1356.1399	1358.7385
1365.6257	1366.5572	1370.3279
1374.4451	1376.0652	1376.6701
1377.5345	1384.1495	1400.2699
1400.6612	1406.7946	1408.5945

1413.4306	1414.4796	1415.5542
1419.1471	1422.7132	1450.5804
1450.5995	1471.7524	1472.2614
1473.2558	1474.1361	1474.6711
1475.1389	1475.9612	1477.3096
1477.3891	1484.0983	1484.3003
1484.6450	1487.1450	1489.8729
1491.6662	1493.3488	1494.6398
1497.7852	1499.8046	1501.0434
1501.8632	1502.7497	1509.7653
1511.4991	1520.8696	1521.0762
1521.9010	1535.1687	1535.8732
1536.3989	1603.8575	1604.8412
1626.0719	1626.8634	1628.0755
1636.6549	1637.1521	1637.7602
1648.5312	1648.7113	1650.4748
1673.2970	1675.0799	1676.8987
1677.1319	1678.3856	1679.3779
1767.8267	1769.8954	1770.3615
1817.7158	1819.3163	1820.6651
2988.0848	3009.2330	3016.9667
3018.7151	3019.0925	3047.9100
3058.0094	3058.3470	3058.4412
3059.5991	3063.7231	3063.8653
3065.0192	3078.1757	3080.9077
3081.2739	3081.5069	3090.8037
3094.7557	3104.1191	3104.3903
3104.6604	3124.5236	3128.8569
3131.5747	3133.4916	3136.4620
3145.8662	3154.3570	3158.1401
3174.6897	3174.9375	3175.6656
3182.4927	3182.8386	3183.3863
3190.4393	3193.4972	3194.9555
3200.7031	3201.0069	3201.2608
3205.1506	3206.0230	3206.1363
3206.9426	3215.9103	3220.9350
3223.5623	3226.2426	3230.9029

TS3⊂CBr_4

E(RB3LYP) = -14058.1705920

E(RB3LYP-D3) = -14058.4108084

H - Sum of electronic and thermal Enthalpies= -14056.991556

G - Sum of electronic and thermal Free Energies= -14057.172977

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.41001	0.10383	1.90151
C	5.64777	1.03602	0.87235
C	5.78620	0.60133	-0.46464
C	5.72266	-0.77455	-0.75963
C	5.51552	-1.71783	0.26908
C	5.35242	-1.27266	1.59488
C	5.24822	0.58849	3.34521
C	4.95107	-0.53495	4.36975
C	5.82957	-1.75332	4.01010
C	5.09509	-2.25616	2.74297
C	5.50821	-3.21847	-0.03877
C	5.65280	-3.56605	-1.54181
C	5.87192	-1.29545	-2.19498
C	6.04751	1.60657	-1.58936
C	6.07201	3.08248	-1.12710
C	5.76445	2.54025	1.16273
C	6.82944	3.14872	0.21788
C	6.69223	-2.60870	-2.16367
C	2.45400	4.47921	-0.81403
C	3.69009	4.14483	-1.44135
C	4.68908	3.55048	-0.71034
C	4.50958	3.25887	0.67304
C	3.34773	3.60070	1.32085
C	2.28703	4.21948	0.59564
C	2.29665	-1.88251	-3.65286
C	2.18162	-3.26838	-3.26724
C	3.26894	-3.89489	-2.59131
C	4.40008	-3.17248	-2.30099
C	4.52183	-1.80875	-2.69504
C	3.50212	-1.17625	-3.36436
C	1.25302	-2.51857	3.38793
C	1.17435	-1.47783	4.38446
C	2.36278	-0.78361	4.75796
C	3.56044	-1.11037	4.16911
C	3.63947	-2.14692	3.19439
C	2.51643	-2.83746	2.80838
C	0.06600	-3.19753	2.98334
C	-1.12898	-2.83029	3.54637
C	-1.20398	-1.82241	4.53686
C	-0.08643	-1.15335	4.96787
C	1.37485	5.03334	-1.56255
C	0.19173	5.28924	-0.91867
C	0.03467	5.05798	0.46811
C	1.05232	4.54541	1.23079
C	0.96867	-3.97347	-3.51976
C	-0.08265	-3.29302	-4.07813
C	0.02007	-1.92844	-4.43618
C	1.18495	-1.22597	-4.26016
C	-1.31921	-1.47266	-4.90980
O	-1.65739	-0.37692	-5.31576
N	-2.16280	-2.59702	-4.79906
C	-1.48095	-3.73389	-4.33761
O	-1.98098	-4.83563	-4.18787
C	-1.11446	5.76018	-1.45726
O	-1.41222	6.06414	-2.59996
C	-1.36600	5.40988	0.84192
O	-1.88838	5.40857	1.93992
C	-2.50910	-3.32340	3.27981
O	-2.87938	-4.20177	2.52325
C	-2.63179	-1.67702	4.93629

O	-3.12461	-0.96804	5.79718
N	-3.35267	-2.56118	4.11547
N	-1.99360	5.78598	-0.36364
C	-3.61307	-2.55076	-4.96762
C	-3.42598	6.03296	-0.50076
C	-4.80000	-2.75238	4.20077
C	-7.04206	0.55761	2.74039
C	-6.95008	0.38776	4.12113
C	-6.21222	-0.68487	4.61853
C	-5.60447	-1.55742	3.70809
N	-5.70528	-1.40390	2.37881
C	-6.39964	-0.35722	1.89303
C	-5.37630	2.54032	-1.97669
C	-5.42887	3.69554	-2.75739
C	-4.80842	4.86059	-2.30078
C	-4.15658	4.82082	-1.06385
N	-4.11504	3.71692	-0.30766
C	-4.70756	2.59704	-0.74887
C	-5.41918	-3.07200	-1.14962
C	-5.72633	-3.99811	-2.14526
C	-5.17600	-3.83322	-3.41693
C	-4.33441	-2.73925	-3.63895
N	-4.06951	-1.82667	-2.69425
C	-4.59921	-1.97847	-1.46886
C	-4.20645	-0.94005	-0.43321
C	-4.58280	1.41056	0.19878
C	-6.44754	-0.18066	0.37705
N	-5.17886	0.16093	-0.27735
H	6.17380	1.09220	3.66051
H	4.45501	1.34481	3.39958
H	5.11156	-0.15452	5.38435
H	5.79507	-2.51128	4.80154
H	6.87608	-1.49079	3.81821
H	6.34077	-3.69443	0.50039
H	5.97826	2.72564	2.21633
H	7.01948	1.38167	-2.05248
H	5.29726	1.49009	-2.38178
H	7.76829	2.58340	0.21354
H	7.04346	4.18644	0.49947
H	4.59090	-3.68057	0.34684
H	5.90412	-4.62686	-1.64898
H	7.61047	-2.52148	-1.57193
H	6.95610	-2.92255	-3.18054
H	3.81799	4.36576	-2.49965
H	3.20486	3.39317	2.37923
H	6.51069	3.70449	-1.91493
H	3.17517	-4.93998	-2.30115
H	3.57804	-0.13196	-3.65973
H	6.30777	-0.54131	-2.85115
H	2.29896	-0.00190	5.51289
H	2.56278	-3.62579	2.06024
H	5.37711	-3.27325	2.46800
H	-0.15470	-0.37786	5.72677
H	0.11309	-3.97568	2.22645
H	0.91604	4.35615	2.29237
H	1.48429	5.21593	-2.62862
H	1.25208	-0.17569	-4.53101
H	0.87238	-5.01821	-3.23465
H	-3.91386	-3.32552	-5.67941
H	-3.83657	-1.56791	-5.39164
H	-3.56481	6.90353	-1.14749
H	-3.79743	6.26166	0.50186
H	-5.02318	-3.62693	3.58488
H	-5.05589	-2.96998	5.24293
H	-7.60028	1.38925	2.31859
H	-7.43375	1.08681	4.79861
H	-6.08699	-0.83552	5.68585
H	-5.81752	1.60342	-2.29973
H	-5.93259	3.68485	-3.72094
H	-4.80377	5.76761	-2.89798
H	-5.77705	-3.20192	-0.13242
H	-6.35708	-4.85578	-1.92529
H	-5.35250	-4.56094	-4.20350
H	-7.16800	0.61423	0.14468
H	-6.83227	-1.09619	-0.08271
H	-5.00817	1.71961	1.16425
H	-3.51526	1.27076	0.40087
H	-3.27972	-0.49107	-0.79161
H	-4.00257	-1.44208	0.52354
C	0.11224	0.14117	-0.18671
Br	-0.38477	-1.73642	-0.47770
Br	-0.66232	0.76968	1.50796
Br	2.06205	0.29103	-0.09942
Br	-0.58047	1.22858	-1.66253

Frequencies

-30.1392	10.9367	14.4209
17.8566	19.3551	22.1848
23.7270	24.9627	27.8815
28.3155	30.1001	34.6608
37.3259	39.7601	47.5033
49.0231	51.8585	54.7166
57.2624	66.3849	66.5068
78.0385	91.0408	96.5659
99.7185	111.9851	118.2232
119.8132	123.6502	125.8636
127.2488	129.6944	141.7638
142.4610	148.6757	151.0518
153.1492	158.8901	160.1989
164.7857	173.2348	175.2030
175.8798	181.1021	181.8359
183.4971	185.6238	196.7787
201.5429	204.3957	213.1374
225.5270	229.4660	235.8605
238.6869	244.4577	248.0373
250.6301	254.0661	259.1823
260.4616	260.7025	262.9410
271.1173	291.3855	298.6059

300.1399	304.5762	305.8492	1066.1035	1075.4258	1078.1792
308.2203	313.7317	317.7017	1078.6253	1096.8466	1103.5863
332.5049	333.0260	346.5001	1105.2408	1107.3523	1108.0355
347.5031	363.4777	371.7272	1115.6326	1120.3971	1122.9342
372.5405	384.0882	387.9379	1134.6184	1140.5752	1141.0369
392.4980	395.2089	400.8434	1143.8089	1154.9260	1160.8903
403.7887	404.5611	409.3980	1165.9284	1166.2167	1176.5136
419.5268	421.7716	427.7749	1176.5851	1176.8454	1177.7608
428.8806	436.1481	437.3778	1179.8687	1180.3135	1181.5041
444.7369	463.2327	467.2635	1189.4854	1190.0043	1190.7895
473.3973	484.1520	484.9577	1191.4566	1191.6348	1229.0597
485.2604	490.4573	498.0339	1230.6738	1231.1911	1233.3223
500.2424	502.0047	527.4605	1236.8139	1239.3591	1244.9847
531.6111	534.9586	546.8685	1247.3921	1250.2332	1250.3213
549.7183	555.8817	566.5642	1254.0164	1254.3314	1254.4304
570.3692	573.0728	574.1491	1258.2836	1264.5288	1271.3566
579.3767	581.3010	583.3795	1272.4416	1277.3562	1277.5012
591.9302	592.5937	601.8152	1277.7254	1282.0995	1291.3273
604.7886	605.5629	609.6759	1291.8275	1296.7698	1299.5663
617.5085	618.0887	623.7736	1300.0054	1300.6377	1305.8737
624.8577	629.6629	633.4238	1313.5546	1314.3204	1318.2212
646.4508	653.2245	654.0653	1318.5502	1321.4035	1326.4338
654.4552	659.7138	660.5472	1333.7889	1339.6849	1340.3752
661.4289	673.2827	701.1609	1341.0827	1345.1130	1345.3835
714.1375	716.2492	720.6122	1349.2456	1350.2576	1360.0512
723.2022	724.0901	727.3075	1365.4942	1369.9620	1375.5831
732.3978	736.9752	740.7963	1376.7517	1377.4262	1378.2121
741.5921	741.8187	743.4118	1380.0157	1393.1230	1395.4528
747.1009	753.3366	762.6746	1400.4782	1410.5749	1411.6641
767.8577	768.3759	769.4193	1413.3670	1415.1349	1415.4138
769.4818	772.3374	773.6060	1418.7940	1426.6518	1449.4691
777.8641	778.4599	784.2281	1449.9424	1470.7255	1471.5237
785.2496	786.3209	791.1074	1472.2862	1473.7742	1474.1497
802.4430	804.1596	811.4525	1474.4674	1475.0727	1475.5709
814.5572	817.7316	823.9409	1476.2462	1483.9684	1484.2739
826.3270	829.9494	837.4093	1484.5084	1487.0442	1489.5092
838.9640	841.0688	846.9037	1491.3657	1494.2914	1494.8538
868.8757	869.1691	870.3812	1497.8626	1500.1624	1500.7788
876.9755	888.6279	888.7545	1501.3570	1502.4606	1505.6516
894.7500	897.5279	898.0559	1511.7082	1520.8649	1521.2025
900.7507	910.8506	913.4791	1521.9852	1534.8891	1535.4404
915.3293	919.1271	920.0564	1535.7097	1602.4384	1603.4161
928.3817	931.7014	936.1880	1626.0403	1626.3917	1627.9469
936.4852	936.6762	937.8415	1635.8000	1638.4296	1639.1884
940.8986	941.2848	942.6354	1648.2388	1648.5954	1649.4643
946.1234	950.5574	954.5375	1673.0054	1675.0231	1676.6795
959.5054	961.0745	966.2627	1676.8052	1678.0822	1678.7299
967.1199	970.2155	975.7326	1769.4599	1771.8848	1772.8331
981.7927	985.6529	994.5979	1818.8396	1821.1377	1822.5801
1006.0251	1007.0989	1008.5785	3017.5915	3019.1658	3019.2442
1009.4087	1010.0910	1010.8199	3025.8799	3029.8482	3047.9891
1012.9774	1013.4636	1014.3868	3058.1741	3058.4086	3058.6009
1014.5892	1014.7754	1018.3632	3062.0992	3064.2432	3064.4184
1039.3491	1043.0470	1043.9137	3079.3868	3080.5093	3081.0363

3081.2796	3084.1531	3086.9541
3091.0396	3104.1749	3104.4262
3104.6751	3106.4971	3129.8751
3132.7777	3135.3661	3136.1668
3142.2159	3142.3431	3145.3076
3174.3312	3174.8105	3175.4865
3181.4465	3182.7495	3183.9131
3189.0788	3189.3863	3189.6358
3199.7252	3200.3422	3200.7756
3203.3763	3204.2838	3205.8415
3206.7682	3207.9837	3211.2724
3214.4835	3222.7589	3227.4263

I3⊂CBr$_4$

E(RB3LYP) = -14058.1748589

E(RB3LYP-D3) = -14058.4160814

H - Sum of electronic and thermal Enthalpies= -14056.994796

G - Sum of electronic and thermal Free Energies= -14057.179491

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.83893	-1.01722	0.04967
C	5.69186	-0.48101	1.34410
C	5.58859	0.91487	1.52998
C	5.59857	1.76902	0.41116
C	5.70444	1.23980	-0.89232
C	5.84113	-0.15037	-1.06480
C	6.05355	-2.52367	-0.13553
C	6.18861	-2.97999	-1.61206
C	7.01842	-1.92717	-2.37688
C	5.98933	-0.77241	-2.45754
C	5.71117	2.16508	-2.11318
C	5.50810	3.66372	-1.77992
C	5.46473	3.28898	0.56282
C	5.51608	1.51276	2.93793
C	5.44933	0.46471	4.07477
C	5.63266	-1.37739	2.58873
C	6.41703	-0.68927	3.73357
C	6.33191	3.98521	-0.51384
C	1.78846	-0.77729	4.47529
C	2.93760	0.03583	4.69655
C	4.11439	-0.25349	4.05100
C	4.21424	-1.36446	3.16420
C	3.13192	-2.18178	2.93975
C	1.88789	-1.90829	3.58448
C	1.69737	4.21447	0.15292
C	1.72866	4.44419	-1.27141
C	2.96220	4.29163	-1.97080
C	4.09619	3.92547	-1.28678
C	4.06499	3.70939	0.12136
C	2.89782	3.85166	0.83034
C	2.46308	-2.03971	-3.55008
C	2.62187	-3.39926	-3.09276
C	3.84611	-3.78820	-2.47631
C	4.85147	-2.86691	-2.31705
C	4.71427	-1.53715	-2.80940
C	3.55210	-1.12858	-3.41824
C	1.19881	-1.60763	-4.05059
C	0.15644	-2.49899	-4.06171
C	0.33041	-3.84443	-3.66213
C	1.53262	-4.31176	-3.19869
C	0.54234	-0.47352	5.09773
C	-0.54533	-1.25643	4.80928
C	-0.45127	-2.36744	3.93797
C	0.73405	-2.71144	3.33861
C	0.52860	4.80107	-1.95541
C	-0.63838	4.88198	-1.23917
C	-0.67005	4.63720	0.15393
C	0.46372	4.32566	0.85751
C	-2.07906	4.76291	0.61545
O	-2.53418	4.63831	1.73851
N	-2.82682	5.08421	-0.53155
C	-2.02722	5.19676	-1.68108
O	-2.43450	5.50978	-2.78566
C	-1.96188	-1.13470	5.25198
O	-2.46821	-0.32576	6.00983
C	-1.80882	-2.97349	3.81556
O	-2.15832	-3.95822	3.18990
C	-1.29316	-2.28557	-4.33717
O	-1.86556	-1.27836	-4.70701
C	-0.99190	-4.51972	-3.72308
O	-1.26206	-5.69121	-3.51100
N	-1.91940	-3.52221	-4.06202
N	-2.65214	-2.17706	4.61320
C	-4.25867	5.31991	-0.51105
C	-4.08855	-2.36711	4.72630
C	-3.37317	-3.71216	-4.02988
C	-4.94238	-3.43722	-0.07658
C	-4.12856	-4.52723	-0.38164
C	-3.62857	-4.65045	-1.67549
C	-3.94056	-3.65332	-2.61383
N	-4.73938	-2.61541	-2.32636
C	-5.24193	-2.50862	-1.08012
C	-6.37879	0.31604	2.33265
C	-6.82971	0.03578	3.62037
C	-6.08092	-0.81880	4.43388
C	-4.90666	-1.36942	3.91363
N	-4.47006	-1.09993	2.67581
C	-5.18095	-0.26875	1.89650
C	-6.63554	2.45080	-2.56370
C	-7.01465	3.78935	-2.62159
C	-6.22436	4.73801	-1.97424
C	-5.08776	4.30327	-1.28432
N	-4.71584	3.01674	-1.23394
C	-5.47218	2.09941	-1.86311
C	-5.04018	0.64502	-1.78882

C	-4.59181	0.03727	0.53108
C	-6.17121	-1.33338	-0.79269
N	-5.55783	-0.01474	-0.57133
H	6.97248	-2.81546	0.39411
H	5.23782	-3.08608	0.33602
H	6.60984	-3.99058	-1.64525
H	7.27678	-2.28564	-3.38039
H	7.93909	-1.63798	-1.85779
H	6.67422	2.06441	-2.63512
H	5.99302	-2.38432	2.37474
H	6.40636	2.13796	3.10269
H	4.65206	2.18333	3.02208
H	7.40906	-0.34466	3.42044
H	6.53240	-1.36940	4.58581
H	4.94145	1.84940	-2.82876
H	5.77556	4.27101	-2.65147
H	7.35529	3.59510	-0.55327
H	6.37295	5.06596	-0.33396
H	2.85939	0.88217	5.37683
H	3.19302	-3.03238	2.26403
H	5.65753	0.95081	5.03412
H	2.98224	4.46862	-3.04479
H	2.85985	3.68176	1.90420
H	5.70820	3.61384	1.57514
H	3.95263	-4.81012	-2.11667
H	3.42508	-0.10866	-3.77466
H	6.25364	-0.02313	-3.20448
H	1.64406	-5.34060	-2.86583
H	1.05701	-0.57458	-4.35569
H	0.79438	-3.56118	2.66394
H	0.45788	0.37936	5.76662
H	0.42651	4.14138	1.92773
H	0.54347	4.98485	-3.02684
H	-4.45842	6.32328	-0.90248
H	-4.54528	5.30253	0.54639
H	-4.36586	-2.30410	5.78280
H	-4.28919	-3.38430	4.37302
H	-3.81713	-2.91374	-4.62644
H	-3.58784	-4.68069	-4.49282
H	-5.33623	-3.30277	0.92584
H	-3.88670	-5.26519	0.37871
H	-3.00528	-5.49074	-1.96099
H	-6.92731	0.97403	1.66552
H	-7.74667	0.48507	3.99384
H	-6.39525	-1.04412	5.44935
H	-7.22098	1.68315	-3.06198
H	-7.90115	4.09199	-3.17342
H	-6.47231	5.79517	-2.01514
H	-6.76236	-1.57418	0.09878
H	-6.87294	-1.23166	-1.62715
H	-3.73892	-0.64240	0.37883
H	-4.18903	1.05697	0.55054
H	-3.94476	0.58740	-1.84405
H	-5.42405	0.11250	-2.66187
C	-0.12518	-0.06280	-0.12597
Br	-0.75537	0.89515	-1.71570
Br	-0.83412	0.80026	1.48516
Br	1.83722	-0.03389	-0.07620
Br	-0.75858	-1.92142	-0.19540

Frequencies

9.6033	15.4495	16.5363
18.0678	18.2984	21.3302
23.8940	25.2974	27.1942
29.0866	30.9545	35.5720
36.1973	36.5167	39.4111
49.4898	52.7657	60.6361
64.1893	64.8123	76.9503
77.8088	81.8709	94.4640
101.4378	112.5705	116.0220
122.5884	125.4545	125.8077
126.7975	129.2598	141.8286
143.8908	150.0122	152.7685
159.8628	160.9893	166.0853
169.0912	171.7413	174.5258
179.7964	180.9685	182.1136
182.3747	189.3186	192.9609
200.9687	213.4765	220.4959
227.2491	232.3162	237.8226
239.6993	242.2615	245.5949
251.4188	254.6452	259.6789
260.2917	261.8999	263.2295
272.2933	286.6630	293.9396
296.0348	298.9367	301.7526
305.9641	308.5706	315.9302
321.0108	332.2901	346.5805
348.2159	359.1206	371.9002
372.3938	382.7805	386.0084
390.8272	399.2158	401.4778
403.0966	404.3227	406.9830
420.0425	426.9694	428.2092
430.6792	437.5017	440.3847
443.9341	463.9325	469.9400
472.3524	477.0947	484.1578
484.9023	485.9050	499.7060
500.9964	503.0041	527.4159
528.3579	544.1163	548.0269
549.9837	557.9294	566.2618
571.9074	574.0006	575.9346
577.9383	579.6952	586.0129
591.5300	594.2597	602.0787
605.9092	606.6269	609.5090
620.5604	622.6596	625.1483
625.9189	626.7014	627.0359
652.5424	652.7982	654.4731
658.3139	660.4090	661.1578
663.0374	668.7688	700.2448
716.8832	718.2941	722.0124

724.2358	726.4152	727.2194
733.3184	739.0954	740.0728
742.3473	743.5667	744.1080
753.0261	759.3336	760.6890
762.5893	768.4338	768.6207
772.5287	776.9068	777.9514
778.4026	780.7238	784.1107
784.9410	786.7408	786.8531
798.5432	801.2263	802.2830
813.2375	817.3005	823.3526
826.7423	829.0603	836.0540
839.8134	841.9102	854.0459
867.3545	868.5254	869.3776
876.8845	888.0972	889.0178
895.0622	897.0304	897.7335
900.7469	911.4422	913.5769
915.9799	916.6683	920.0972
921.2101	927.8964	934.6843
936.4241	936.6949	937.0740
941.1495	941.6640	941.8658
944.9383	952.3417	955.5643
957.7109	961.6190	964.3139
967.1230	967.1916	969.5221
979.8535	985.6070	1000.8733
1002.3783	1007.3764	1008.8102
1010.4861	1011.6242	1012.1042
1014.0175	1014.7118	1015.1448
1020.3248	1021.1289	1024.6697
1039.5121	1042.8993	1044.0495
1066.1186	1075.5120	1078.2871
1079.4989	1096.3336	1106.7700
1107.6382	1108.0682	1115.5216
1117.1158	1118.2007	1124.9493
1131.8483	1141.9955	1146.7797
1148.4197	1150.1650	1155.8301
1165.6969	1166.5226	1177.1823
1177.5850	1178.3405	1179.3117
1179.7562	1180.1305	1186.3467
1190.0568	1190.9340	1191.5123
1192.9643	1195.5827	1227.8754
1230.4263	1231.0610	1233.4221
1235.7131	1237.5050	1245.1185
1249.1828	1249.9810	1251.1573
1254.0866	1254.6353	1255.0084
1258.6495	1265.6767	1271.5721
1277.1044	1277.8455	1278.0872
1278.2403	1279.6567	1291.2670
1292.0313	1292.8890	1299.3796
1300.1316	1300.9837	1301.7484
1313.3753	1315.5012	1317.9957
1319.1166	1321.8424	1322.2733
1327.1812	1339.8321	1340.3841
1341.4240	1344.5148	1345.2607
1346.6652	1358.5059	1361.5074
1365.2805	1365.7034	1367.3622
1376.2261	1377.1448	1391.8064
1395.0313	1399.4551	1400.3257
1402.4872	1410.3313	1412.9949
1414.2828	1414.4709	1415.2285
1421.7083	1424.1177	1450.3155
1451.0072	1469.8589	1472.0803
1472.9549	1473.7056	1475.4201
1475.5683	1476.1841	1477.8399
1479.1058	1483.8622	1484.6874
1484.9713	1487.0123	1487.8644
1490.5755	1492.5682	1494.5539
1495.1763	1496.2069	1501.6768
1502.4642	1503.1150	1514.9633
1517.1609	1520.8354	1520.9401
1521.7876	1534.6399	1535.7565
1536.5989	1604.0714	1604.7115
1626.8349	1628.8738	1630.1502
1634.6018	1638.6172	1639.7238
1647.7678	1649.7532	1649.8255
1674.5389	1675.0151	1676.5163
1677.4982	1678.8580	1678.9377
1767.1756	1770.2091	1772.3693
1818.6436	1819.4309	1821.3202
3009.7757	3016.8248	3018.5006
3018.6773	3043.7012	3057.2066
3057.9200	3058.1797	3058.2978
3062.8348	3063.8240	3066.4512
3066.8059	3076.1108	3080.0335
3080.8070	3081.1033	3081.8697
3086.3993	3101.0917	3103.9090
3104.0786	3104.6899	3110.2039
3122.7917	3130.4183	3132.6628
3133.7681	3134.8301	3161.8505
3174.5743	3174.6677	3175.6261
3181.2816	3182.8606	3183.8818
3185.4970	3187.0534	3198.8586
3199.4558	3200.1743	3200.3944
3201.4450	3203.6259	3205.8187
3206.1501	3208.9983	3209.4032
3217.6141	3219.2559	3232.0657

TS4⊂CBr_4

E(RB3LYP) = -14058.1744384

E(RB3LYP-D3) = -14058.4142514

H - Sum of electronic and thermal Enthalpies= -14056.995440

G - Sum of electronic and thermal Free Energies= -14057.176864

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.86261	-0.99047	0.09137
C	5.63657	-0.66939	1.44431

C	5.49633	0.67761	1.84475
C	5.55183	1.70075	0.87934
C	5.75208	1.38811	-0.48177
C	5.92206	0.04524	-0.86588
C	6.09669	-2.44753	-0.32413
C	6.30802	-2.65876	-1.84688
C	7.17929	-1.50301	-2.38239
C	6.15698	-0.34143	-2.32967
C	5.82715	2.49590	-1.53637
C	5.56903	3.91833	-0.98477
C	5.37312	3.17561	1.26086
C	5.33927	1.04058	3.32435
C	5.24980	-0.17662	4.27664
C	5.53662	-1.75362	2.52574
C	6.25645	-1.24657	3.80050
C	6.29655	4.04368	0.37191
C	1.61082	-1.53984	4.32626
C	2.72888	-0.74874	4.71940
C	3.93448	-0.90427	4.08106
C	4.09539	-1.85421	3.03124
C	3.04222	-2.64221	2.63176
C	1.76996	-2.50387	3.26430
C	1.62919	4.15073	0.74430
C	1.75139	4.58175	-0.62749
C	3.02965	4.53592	-1.25766
C	4.12120	4.08078	-0.55884
C	3.99825	3.64946	0.79368
C	2.78496	3.68319	1.43615
C	2.68571	-1.37084	-3.78152
C	2.82048	-2.78972	-3.55505
C	4.01264	-3.28966	-2.95546
C	5.01085	-2.41862	-2.59466
C	4.90238	-1.02492	-2.86921
C	3.77183	-0.50746	-3.45403
C	1.44307	-0.84522	-4.24528
C	0.39789	-1.71022	-4.44581
C	0.55297	-3.10647	-4.28296
C	1.73430	-3.65938	-3.86204
C	0.33936	-1.37686	4.95015
C	-0.71488	-2.12972	4.50184
C	-0.56328	-3.07396	3.45873
C	0.64784	-3.28121	2.84823
C	0.59872	5.04635	-1.32734
C	-0.60751	5.05711	-0.67513
C	-0.72689	4.63287	0.66947
C	0.35617	4.19249	1.38465
C	-2.15105	4.78310	1.07713
O	-2.67228	4.55853	2.15506
N	-2.81673	5.29179	-0.05100
C	-1.95448	5.49157	-1.14231
O	-2.28518	5.95844	-2.21753
C	-2.14351	-2.12973	4.92151
O	-2.69451	-1.47689	5.79055
C	-1.89619	-3.68964	3.19727
O	-2.20020	-4.55839	2.39936
C	-1.04142	-1.43727	-4.72201
O	-1.59782	-0.37525	-4.92464
C	-0.76841	-3.74755	-4.50773
O	-1.04762	-4.93595	-4.52265
N	-1.68171	-2.69678	-4.68619
N	-2.78188	-3.07303	4.10070
C	-4.21663	5.65391	-0.05677
C	-4.21105	-3.32699	4.14281
C	-3.13698	-2.87199	-4.72459
C	-4.82983	-3.36747	-0.84386
C	-3.98355	-4.36760	-1.31945
C	-3.44156	-4.23629	-2.59525
C	-3.74136	-3.08275	-3.33831
N	-4.56717	-2.12714	-2.88692
C	-5.11443	-2.26902	-1.66349
C	-6.55047	-0.34039	2.19792
C	-7.05129	-0.91228	3.36553
C	-6.28918	-1.87273	4.03490
C	-5.05042	-2.23089	3.49530
N	-4.56657	-1.68203	2.37352
C	-5.29177	-0.74902	1.73539
C	-6.94995	2.69414	-1.43330
C	-7.42752	3.97095	-1.15120
C	-6.52628	4.93986	-0.71336
C	-5.17924	4.58768	-0.57288
N	-4.71420	3.36353	-0.85385
C	-5.58211	2.42794	-1.28012
C	-5.04900	1.03818	-1.59737
C	-4.64818	-0.12697	0.50794
C	-6.09527	-1.19784	-1.19673
N	-5.55238	0.04497	-0.63096
H	6.99039	-2.82367	0.19546
H	5.26218	-3.07702	0.00968
H	6.72956	-3.65442	-2.02236
H	7.49338	-1.69454	-3.41531
H	8.06954	-1.31142	-1.77289
H	6.82712	2.48762	-1.99484
H	5.92680	-2.70857	2.17147
H	6.20269	1.64951	3.63119
H	4.45360	1.67138	3.47003
H	7.25329	-0.84202	3.59177
H	6.34987	-2.05254	4.53798
H	5.11746	2.29276	-2.34804
H	5.88109	4.66076	-1.72733
H	7.32867	3.67619	0.34439
H	6.30112	5.08258	0.72222
H	2.60514	-0.02786	5.52573
H	3.14869	-3.36869	1.82888
H	5.40712	0.15377	5.30915
H	3.11898	4.87329	-2.28889
H	2.67858	3.35598	2.46818
H	5.53969	3.33723	2.32655
H	4.09773	-4.35825	-2.76605

H	3.66577	0.55893	-3.64090
H	6.46360	0.51766	-2.92720
H	1.82868	-4.73135	-3.70800
H	1.31671	0.22657	-4.37118
H	0.75301	-4.00385	2.04347
H	0.21096	-0.65210	5.75027
H	0.25265	3.87060	2.41734
H	0.68166	5.37896	-2.35906
H	-4.32094	6.55680	-0.66796
H	-4.48259	5.90620	0.97573
H	-4.51170	-3.45874	5.18662
H	-4.36772	-4.27347	3.61390
H	-3.55983	-1.96773	-5.16505
H	-3.34883	-3.72948	-5.37161
H	-5.26381	-3.43442	0.14872
H	-3.75328	-5.23430	-0.70540
H	-2.79807	-5.00165	-3.01452
H	-7.10612	0.41103	1.64522
H	-8.01784	-0.60696	3.75887
H	-6.64294	-2.32590	4.95707
H	-7.61868	1.90709	-1.76974
H	-8.48094	4.21049	-1.27407
H	-6.85728	5.95031	-0.48520
H	-6.74655	-1.64648	-0.43629
H	-6.73069	-0.92094	-2.04409
H	-3.75876	-0.72648	0.25991
H	-4.28720	0.87214	0.78379
H	-3.95228	1.07318	-1.62659
H	-5.38016	0.74591	-2.59845
C	-0.11180	-0.05847	-0.14964
Br	-0.74676	-1.87802	-0.53372
Br	-0.72346	1.15030	-1.56344
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Br	-0.83777	0.52561	1.57760

Frequencies

-15.9119	12.5225	16.1989
17.8558	19.1428	20.7406
23.5862	24.6683	26.0588
28.7248	29.0589	32.7256
34.9399	36.1787	38.9442
48.3627	52.6453	60.9676
65.1601	65.2747	76.0982
78.5644	84.1147	96.6849
102.7696	113.5631	116.9980
123.4254	124.7464	125.5641
126.8706	128.7545	141.5913
143.3753	150.5198	151.9651
160.3739	160.7917	163.1103
167.4298	170.7563	175.1145
180.0469	180.8810	182.1543
182.5262	185.5222	191.4591
199.4213	213.1612	218.1422
226.0868	233.3534	235.2787
239.5238	242.2373	245.3138
250.2047	253.6188	258.1381
260.2946	262.5943	267.0943
272.6128	282.9464	290.5036
297.0587	298.7925	301.9375
306.9998	308.3715	316.2673
321.5539	332.5167	346.6903
347.9503	349.5329	370.6994
372.6467	374.5468	386.2203
390.5427	399.4098	400.2723
402.9611	404.0546	406.0778
419.8367	427.1264	428.2320
429.9695	435.9995	438.7932
444.6688	469.1136	470.9309
472.3918	477.2703	484.0203
485.1651	485.7477	499.7190
501.7621	503.5960	526.8735
528.4776	542.9717	548.8095
549.8815	557.2363	566.6706
572.1167	573.3371	575.4983
576.7875	579.1101	586.7652
592.1494	595.1595	605.1596
606.3071	607.1714	609.4041
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626.3315	628.8919	635.2647
651.2613	653.0681	653.4026
655.1370	658.8254	661.1122
661.3373	663.7025	699.8695
716.8355	718.6835	721.8646
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733.7198	734.1028	740.2528
742.0264	743.1745	743.8819
753.1548	755.6455	760.1346
762.6225	767.6842	768.2277
771.3122	772.4813	778.4106
778.9811	780.8735	783.3212
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796.3546	797.7078	802.3361
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826.9953	828.4053	836.1321
840.0101	841.8583	852.6388
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915.8581	917.1617	919.9790
921.2553	925.6917	935.7177
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945.3631	953.2403	956.5205
957.8244	961.9294	963.8452
966.8046	967.3472	969.7472
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1009.8657	1010.7840	1011.7357	3018.7026	3048.5413	3052.4274
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1039.4642	1042.9102	1044.0824	3068.7653	3069.0483	3074.8517
1066.1844	1075.6586	1078.2592	3080.6358	3080.8944	3081.8812
1079.5915	1096.8729	1107.3082	3084.6254	3100.4684	3103.8661
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1118.1958	1120.5678	1122.7070	3113.0821	3121.1084	3132.9686
1132.8994	1143.6828	1147.7975	3133.0530	3135.9544	3161.6469
1152.6938	1154.3956	1156.5796	3174.4408	3174.8265	3175.7386
1165.7309	1166.6968	1177.5431	3181.0949	3181.7293	3183.0889
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1179.8935	1180.2991	1186.2110	3198.9650	3200.2955	3200.3097
1189.8816	1191.2427	1191.7895	3201.5507	3203.1212	3205.6039
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1228.4155	1230.6906	1232.3733	3217.1711	3219.3665	3234.6727
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1274.3211	1277.1431	1277.6504			
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1292.0665	1292.9326	1299.4121			
1300.5336	1301.0470	1302.8063			
1313.6681	1317.2762	1318.2231			
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1327.3162	1340.0629	1340.5905			
1341.2956	1344.9635	1345.4587			
1347.2570	1360.3317	1365.7193			
1366.1326	1368.8484	1373.1362			
1376.3912	1377.3238	1390.8534			
1393.8921	1400.5411	1401.3661			
1404.1905	1407.6405	1411.8259			
1414.1030	1414.3140	1415.2775			
1418.8273	1423.9761	1450.4054			
1451.0435	1468.6481	1470.1437			
1473.1997	1474.0454	1475.3852			
1475.6855	1476.6381	1477.6149			
1478.3584	1482.1837	1484.1237			
1484.7564	1485.4260	1487.0000			
1488.0269	1491.0527	1493.2306			
1494.4905	1495.0845	1501.8399			
1502.6805	1502.9524	1513.1133			
1516.3593	1520.9051	1520.9806			
1521.8308	1534.7925	1535.5659			
1536.6347	1604.0076	1605.0889			
1627.8160	1629.4822	1631.0247			
1634.5869	1638.1443	1638.9284			
1647.9197	1649.7928	1649.9781			
1674.5437	1675.1602	1676.7834			
1677.6968	1678.7944	1679.0645			
1767.4218	1770.4177	1773.2057			
1819.0520	1819.6150	1822.4102			
3012.8970	3017.4124	3017.9802			

I4⊂CBr$_4$

E(RB3LYP) = -14058.1756407

E(RB3LYP-D3) = -14058.4113628

H - Sum of electronic and thermal Enthalpies= -14056.995836

G - Sum of electronic and thermal Free Energies= -14057.181066

Number of imaginary frequencies: 0

Cartesian Coordinates

C	-5.82850	-1.45716	0.06543
C	-5.63288	-1.28492	-1.31836
C	-5.58696	0.01034	-1.87923
C	-5.76377	1.13486	-1.04994
C	-5.96747	0.97188	0.33695
C	-5.99261	-0.32248	0.88720
C	-5.89776	-2.86706	0.66282
C	-6.03164	-2.90574	2.20783
C	-7.02300	-1.80246	2.63366
C	-6.15430	-0.54437	2.39405
C	-6.20025	2.18359	1.24303
C	-6.08607	3.54549	0.52052
C	-5.72842	2.56346	-1.61106
C	-5.38601	0.20165	-3.38527
C	-5.17608	-1.11382	-4.17441
C	-5.45143	-2.48453	-2.25683
C	-6.14542	-2.17364	-3.60591
C	-6.77364	3.42170	-0.85712
C	-1.48025	-2.31058	-3.94961
C	-2.61198	-1.61016	-4.46130
C	-3.83335	-1.74124	-3.84671
C	-3.99247	-2.57404	-2.70111
C	-2.92711	-3.26905	-2.18275
C	-1.64199	-3.15541	-2.79092
C	-2.13539	4.01680	-1.13269
C	-2.34694	4.55718	0.18864
C	-3.63614	4.44732	0.78634

C	-4.64976	3.81246	0.11218
C	-4.43255	3.24722	-1.17776
C	-3.21034	3.35401	-1.79595
C	-2.54432	-0.95786	3.81538
C	-2.50789	-2.39998	3.77160
C	-3.64201	-3.11072	3.28135
C	-4.75132	-2.41898	2.86032
C	-4.80940	-0.99877	2.95810
C	-3.73511	-0.27931	3.42327
C	-1.37256	-0.23307	4.18556
C	-0.23281	-0.93454	4.48492
C	-0.21857	-2.34846	4.50168
C	-1.32305	-3.08733	4.16542
C	-0.19576	-2.18053	-4.55525
C	0.86463	-2.85059	-4.00101
C	0.70686	-3.67613	-2.86271
C	-0.51352	-3.84789	-2.26191
C	-1.26794	5.18401	0.87755
C	-0.04675	5.25448	0.25927
C	0.15606	4.74834	-1.04617
C	-0.85414	4.14125	-1.74682
C	1.57396	5.00869	-1.42474
O	2.14643	4.78056	-2.47573
N	2.16035	5.62147	-0.30533
C	1.24217	5.82242	0.74149
O	1.49155	6.37136	1.79954
C	2.30298	-2.87170	-4.38872
O	2.86285	-2.31403	-5.31631
C	2.04195	-4.23126	-2.50459
O	2.34124	-4.99624	-1.60522
C	1.15258	-0.45747	4.75797
O	1.57006	0.68123	4.84555
C	1.15751	-2.79136	4.84729
O	1.56434	-3.92345	5.05410
N	1.93697	-1.62498	4.90068
N	2.93730	-3.70620	-3.45399
C	3.53814	6.07924	-0.25494
C	4.36421	-3.96812	-3.44989
C	3.38636	-1.60678	5.12407
C	5.68716	-2.87202	1.76849
C	5.00833	-3.84499	2.49984
C	4.26012	-3.45077	3.60535
C	4.19682	-2.08473	3.92254
N	4.85751	-1.14792	3.22393
C	5.59982	-1.53292	2.16848
C	6.74129	-0.75727	-1.97010
C	7.25971	-1.54722	-2.99525
C	6.48391	-2.58544	-3.51071
C	5.21368	-2.79936	-2.96395
N	4.71562	-2.04543	-1.97759
C	5.45523	-1.03472	-1.48973
C	6.50695	3.04353	-0.48074
C	6.69303	4.20873	-1.21900
C	5.70942	5.19616	-1.17702
C	4.58144	4.97934	-0.37987
N	4.39637	3.85639	0.32903
C	5.33693	2.89904	0.27872
C	5.11229	1.65742	1.13860
C	4.77938	-0.18078	-0.42856
C	6.40068	-0.46816	1.42352
N	5.68329	0.45049	0.53209
H	-6.76487	-3.39290	0.23597
H	-5.01405	-3.44625	0.36781
H	-6.32148	-3.91351	2.52445
H	-7.28300	-1.89547	3.69480
H	-7.94641	-1.79815	2.04363
H	-7.20656	2.11238	1.68208
H	-5.81284	-3.40648	-1.79906
H	-6.26952	0.70679	-3.80264
H	-4.53610	0.87080	-3.56989
H	-7.16880	-1.80190	-3.48152
H	-6.16897	-3.06684	-4.24131
H	-5.49782	2.16892	2.08556
H	-6.50276	4.33440	1.15614
H	-7.75910	2.94487	-0.80720
H	-6.88039	4.40349	-1.33334
H	-2.48663	-0.98201	-5.34154
H	-3.03578	-3.90803	-1.30891
H	-5.30558	-0.92168	-5.24506
H	-3.79571	4.87769	1.77354
H	-3.03480	2.93532	-2.78465
H	-5.87387	2.57267	-2.69203
H	-3.59883	-4.19720	3.22901
H	-3.75689	0.80718	3.47287
H	-6.54917	0.34129	2.89250
H	-1.28984	-4.17387	4.15616
H	-1.37810	0.85349	4.17975
H	-0.62254	-4.48141	-1.38558
H	-0.06438	-1.54675	-5.42871
H	-0.68546	3.74639	-2.74510
H	-1.41466	5.58515	1.87725
H	3.64438	6.58306	0.71192
H	3.69646	6.82080	-1.04589
H	4.67173	-4.25215	-4.46125
H	4.51117	-4.82942	-2.78876
H	3.65315	-0.57237	5.34734
H	3.59816	-2.23576	5.99562
H	6.28335	-3.14243	0.90162
H	5.06372	-4.89264	2.21555
H	3.71927	-4.17176	4.20748
H	7.30562	0.06627	-1.54599
H	8.25074	-1.34947	-3.39651
H	6.84925	-3.20968	-4.32176
H	7.23845	2.24340	-0.48674
H	7.58544	4.34421	-1.82532
H	5.80602	6.10922	-1.75778
H	7.16008	-0.99130	0.82738
H	6.93547	0.14189	2.15877

H	4.00526	-0.79775	0.05342
H	4.24613	0.62490	-0.94991
H	4.03768	1.56852	1.35117
H	5.59649	1.81914	2.10878
C	0.22357	0.10841	0.03373
Br	0.91264	-1.64248	0.59891
Br	0.76674	1.46618	1.33299
Br	-1.73633	0.03443	-0.07787
Br	0.95861	0.55713	-1.73199

Frequencies

10.0146	13.6666	14.4569
17.0011	18.1981	21.0825
21.7887	25.0217	26.2730
28.1805	30.8240	35.4839
35.8618	38.3498	39.8952
47.8987	50.7522	61.3324
62.7733	64.5403	74.8887
83.0259	86.0502	98.5395
101.6502	115.5199	116.6678
123.3432	125.3619	126.7374
127.6502	130.5592	140.4264
142.8847	149.4912	151.6744
159.4157	161.3173	167.5639
172.4557	174.9260	178.5048
179.1208	181.0513	181.5431
182.6155	182.8839	193.6953
202.2424	206.6660	217.8316
225.5572	232.1292	238.0749
239.3759	240.5501	244.0083
245.8481	248.1698	257.4684
260.0622	262.0762	265.8080
272.2106	274.3672	289.9687
294.1974	296.2798	300.0650
302.7994	307.2450	316.5416
324.4380	330.8527	343.9625
346.6212	349.2267	369.0878
372.0661	373.7088	385.5813
390.1958	397.3487	399.1081
402.2935	403.2959	404.0411
419.6801	427.8248	429.1255
434.4506	436.2836	438.8829
446.6014	467.4025	470.4570
474.6446	483.6007	484.8575
485.2015	492.0282	499.6970
501.7486	504.9890	527.1986
529.2252	537.5540	548.5660
549.3736	549.9979	567.5182
572.0189	573.5587	576.4045
577.7549	579.0172	584.3400
592.5865	594.7560	605.7480
606.8533	607.6402	609.8740
619.5390	622.0460	623.0762
625.6765	631.8886	633.9157
650.4580	652.7023	653.3486
656.7493	658.9453	660.9884
662.6758	665.3313	701.7777
714.2025	716.7535	720.6599
722.4571	725.9337	726.6714
732.4987	735.4713	740.5528
741.6207	742.2366	743.9009
748.8130	754.5269	757.3395
762.6168	767.3852	767.9766
769.9162	772.2996	776.6806
778.1988	779.0526	779.4750
783.9393	786.2064	787.7496
795.8608	802.2598	806.9547
812.8605	814.2665	823.4864
826.1250	827.5496	835.9762
840.6036	843.7088	855.0458
868.6629	868.9336	869.5465
876.8455	888.0672	889.0306
895.0615	896.9249	897.4789
900.8538	909.6514	912.1387
914.7086	916.9566	920.5233
920.9777	931.4216	935.8939
936.6565	937.2869	937.9814
940.9757	941.6848	941.7787
949.4001	954.3754	958.4034
960.6580	964.1920	965.8934
967.1525	969.6833	969.9435
981.8409	986.3601	1001.3355
1004.7413	1006.0252	1009.0891
1010.4720	1011.7901	1012.4679
1012.9642	1013.9743	1015.8249
1018.0108	1022.4686	1024.0510
1039.7281	1043.0812	1044.6591
1066.2491	1075.8357	1078.5087
1078.8896	1097.3793	1107.5949
1108.1858	1109.1800	1113.3565
1117.6619	1119.7591	1128.3823
1136.5948	1148.5861	1149.7072
1151.7257	1155.9500	1166.0381
1166.8039	1167.3657	1177.2864
1177.6344	1178.8080	1179.3332
1179.3859	1180.0045	1184.6832
1187.2632	1191.0105	1191.9756
1192.5098	1194.6784	1228.7058
1228.9319	1230.8905	1232.6229
1233.4104	1237.5807	1245.2863
1249.3601	1250.3065	1250.4744
1254.2861	1254.4673	1254.6591
1259.3002	1266.7935	1270.6216
1271.8681	1274.6536	1277.8965
1277.9546	1278.2060	1291.3089
1291.4913	1292.2699	1298.9857
1300.5497	1300.7979	1301.5123
1311.3287	1314.1302	1318.2362

1319.1051	1320.0158	1322.3261
1327.0474	1339.6378	1340.2455
1341.4551	1344.4900	1345.0980
1346.2503	1350.9564	1360.1632
1365.7719	1368.5629	1371.0021
1376.7165	1377.5549	1381.5560
1395.6095	1398.7233	1400.7825
1407.3201	1410.2744	1412.2196
1413.9292	1414.4958	1415.1528
1422.1472	1425.9013	1451.0846
1451.5023	1470.4889	1471.8837
1473.2707	1474.9039	1475.5246
1475.7024	1476.8603	1476.9027
1479.5249	1484.0809	1484.6024
1484.9827	1485.5445	1486.4857
1489.3292	1493.2296	1493.3979
1494.9063	1498.2392	1501.6482
1502.4825	1502.7270	1508.9537
1512.9669	1520.9026	1520.9517
1521.7967	1535.1884	1535.9167
1536.3390	1604.5510	1606.0078
1629.4363	1629.8557	1631.1517
1635.2030	1637.4104	1639.1916
1649.2022	1649.8338	1650.0767
1674.9846	1675.6725	1677.1082
1678.1278	1678.3086	1679.5325
1767.6960	1771.3718	1772.5829
1819.1738	1820.2466	1821.8557
3012.7481	3016.9147	3017.2442
3018.6926	3035.5258	3039.8361
3058.0571	3058.1491	3058.2362
3063.1279	3063.4208	3064.0855
3065.5004	3066.5281	3071.9847
3076.9039	3080.4916	3080.7759
3081.8926	3083.6186	3099.6871
3104.0517	3104.1018	3104.3951
3110.8332	3117.0458	3129.8741
3132.2744	3137.4702	3158.2660
3174.2241	3175.1188	3175.5108
3181.5786	3182.5568	3184.0414
3186.2094	3186.4086	3193.0485
3200.5573	3200.9923	3201.4531
3203.0536	3204.0139	3204.9075
3205.3962	3207.5097	3209.5420
3225.6421	3231.1711	3238.7265

TS5⊂CBr_4

E(RB3LYP) = -14058.1657870

E(RB3LYP-D3) = -14058.4053909

H - Sum of electronic and thermal Enthalpies= -14056.987187

G - Sum of electronic and thermal Free Energies= -14057.169345

Number of imaginary frequencies: 0

Cartesian Coordinates

C	-5.38908	0.80898	-2.02667
C	-5.51251	1.70907	-0.95003
C	-5.76703	1.22955	0.35380
C	-5.94500	-0.15171	0.56739
C	-5.84546	-1.05757	-0.50969
C	-5.57372	-0.57153	-1.80272
C	-5.05903	1.33361	-3.42702
C	-4.87214	0.22756	-4.49605
C	-5.97297	-0.83210	-4.27048
C	-5.43141	-1.52335	-2.99641
C	-6.03703	-2.55990	-0.28723
C	-6.23457	-2.96044	1.19410
C	-6.22672	-0.71692	1.96769
C	-5.86235	2.19656	1.53566
C	-5.59553	3.67354	1.16446
C	-5.36406	3.22478	-1.15414
C	-6.31215	3.95839	-0.17502
C	-7.18279	-1.92723	1.84188
C	-1.78539	4.44323	0.92459
C	-3.06036	4.26556	1.53938
C	-4.14400	3.90424	0.77660
C	-4.00868	3.68378	-0.62513
C	-2.80680	3.88211	-1.25881
C	-1.66360	4.27616	-0.50339
C	-2.80818	-1.76918	3.52395
C	-2.78766	-3.11287	2.99854
C	-3.90414	-3.57955	2.24297
C	-4.96167	-2.73893	1.99337
C	-4.96652	-1.40269	2.48898
C	-3.92930	-0.93072	3.25489
C	-1.65624	-2.41726	-3.37914
C	-1.31594	-1.35458	-4.29411
C	-2.33569	-0.44763	-4.71152
C	-3.61830	-0.59265	-4.23860
C	-3.95254	-1.65356	-3.34741
C	-3.00073	-2.54844	-2.92651
C	-0.64158	-3.30507	-2.91931
C	0.64397	-3.11603	-3.35341
C	0.97833	-2.09003	-4.26830
C	0.03045	-1.22105	-4.74849
C	-0.63198	4.76961	1.69638
C	0.56976	4.91901	1.05276
C	0.68021	4.80127	-0.35275
C	-0.40219	4.48862	-1.13369
C	-1.63931	-3.93343	3.20458
C	-0.56620	-3.40635	3.87689
C	-0.59409	-2.09490	4.40576
C	-1.68710	-1.28135	4.25706
C	0.72938	-1.82140	5.03242
O	1.10996	-0.82809	5.62674
N	1.50114	-2.97276	4.81131
C	0.78395	-3.98125	4.14103

O	1.21659	-5.08387	3.85997
C	1.92669	5.19374	1.59994
O	2.27158	5.35407	2.75759
C	2.10003	5.05692	-0.72769
O	2.60475	5.12860	-1.83333
C	1.88626	-3.85655	-3.00807
O	2.02716	-4.82648	-2.28647
C	2.44189	-2.18114	-4.54123
O	3.12484	-1.53464	-5.31665
N	2.92129	-3.21709	-3.72077
N	2.78294	5.24852	0.48569
C	2.90228	-3.08951	5.18523
C	4.20476	5.50460	0.58900
C	4.28249	-3.73526	-3.76469
C	7.42827	-1.18036	-2.48729
C	7.44890	-1.64687	-3.80080
C	6.39938	-2.44939	-4.23872
C	5.37240	-2.76332	-3.33889
N	5.34521	-2.30486	-2.07930
C	6.35323	-1.52196	-1.65488
C	6.70070	2.36687	-0.84127
C	7.24581	3.64126	-0.69179
C	6.43224	4.67001	-0.22399
C	5.10007	4.37498	0.09036
N	4.58411	3.14683	-0.02324
C	5.36120	2.15076	-0.48906
C	5.44715	-0.38873	3.09196
C	5.61815	-0.52729	4.46887
C	4.78502	-1.39601	5.17234
C	3.81174	-2.10551	4.46007
N	3.65267	-1.98520	3.13666
C	4.44651	-1.13675	2.46051
C	4.15618	-1.01841	0.96602
C	4.68734	0.79597	-0.67727
C	6.32785	-1.02894	-0.20681
N	5.15816	-0.26551	0.21733
H	-5.86958	1.99452	-3.76806
H	-4.15498	1.95388	-3.38720
H	-4.88680	0.67952	-5.49378
H	-6.01473	-1.54314	-5.10398
H	-6.96844	-0.39649	-4.12814
H	-6.91871	-2.89887	-0.85143
H	-5.53358	3.50232	-2.19581
H	-6.86901	2.13558	1.97478
H	-5.16522	1.89029	2.32577
H	-7.33804	3.57407	-0.20529
H	-6.33082	5.03254	-0.39358
H	-5.18180	-3.11181	-0.69598
H	-6.59750	-3.99260	1.24856
H	-8.06684	-1.71089	1.23136
H	-7.51160	-2.25971	2.83353
H	-3.15199	4.42808	2.61193
H	-2.69917	3.73874	-2.33183
H	-5.91918	4.32051	1.98710
H	-3.89181	-4.60063	1.86543
H	-3.92587	0.08510	3.64427
H	-6.60572	0.05346	2.64068
H	-2.07561	0.35171	-5.40332
H	-3.24326	-3.35815	-2.24190
H	-5.91095	-2.48355	-2.80132
H	0.29548	-0.43219	-5.44821
H	-0.88568	-4.10018	-2.21995
H	-0.30476	4.38371	-2.21115
H	-0.70716	4.87567	2.77570
H	-1.69033	-0.26927	4.65309
H	-1.60725	-4.94220	2.80034
H	3.18928	-4.11801	4.94254
H	2.99642	-2.94983	6.26725
H	4.39714	5.69758	1.65039
H	4.44518	6.41873	0.03319
H	4.28577	-4.60061	-3.09483
H	4.49074	-4.08402	-4.78253
H	8.23527	-0.55923	-2.10758
H	8.26286	-1.38363	-4.47154
H	6.36494	-2.82002	-5.25861
H	7.29645	1.55890	-1.25200
H	8.28128	3.83518	-0.96088
H	6.81204	5.68378	-0.12406
H	6.05412	0.29146	2.50456
H	6.37963	0.04760	4.99045
H	4.87196	-1.50857	6.24940
H	7.24236	-0.44116	-0.04042
H	6.40758	-1.89962	0.45421
H	4.79288	0.49876	-1.73384
H	3.62356	0.95523	-0.49979
H	3.19103	-0.51264	0.86822
H	4.00724	-2.03014	0.56228
C	-0.15416	-0.00770	0.23782
Br	0.29891	-1.89899	0.46724
Br	0.51665	1.00749	1.77706
Br	0.68653	0.67044	-1.40593
Br	-2.09681	0.20076	0.09829

Frequencies

-18.6768	11.4206	14.2963
16.9121	18.6494	20.6631
22.3268	25.4283	26.7672
28.0818	32.2728	33.8699
37.4395	38.1955	43.8419
47.7504	50.5802	52.9260
59.6839	65.0633	65.5048
75.1014	84.0110	99.9289
104.6467	111.4820	115.4758
120.6389	122.9393	125.5399
127.0631	127.5841	141.0767
142.8677	150.7724	152.3711
159.4734	159.9298	164.3629
170.7361	173.2707	178.5231

180.2534	180.9735	181.6365	960.9637	964.8053	966.3346
183.5163	184.4987	190.7218	967.4417	970.4016	974.6625
198.9329	203.2714	213.2549	987.7500	989.3095	998.3290
228.1248	232.5037	235.8097	999.9391	1003.3044	1004.3947
238.1922	241.4999	244.0922	1009.6495	1011.0871	1012.5190
246.4148	247.5910	254.7174	1013.0586	1013.5774	1015.1610
257.5939	260.7851	262.3078	1018.3866	1018.7949	1028.0548
265.8209	272.7809	287.9628	1039.4231	1043.7650	1044.6184
293.5411	298.6704	298.8646	1066.2665	1075.3752	1077.9990
303.3975	305.4718	310.8243	1078.1181	1106.5432	1107.1310
317.5753	329.1382	344.8281	1109.2048	1112.4872	1117.0159
346.2663	347.6904	358.3834	1117.4025	1120.7609	1128.7204
371.2773	372.2729	372.9948	1142.8512	1147.5789	1150.6296
386.5791	396.6058	399.2871	1153.4071	1154.8279	1166.2052
401.5022	404.5210	405.7167	1166.4040	1175.1358	1177.9150
419.6660	428.4448	428.8674	1178.1760	1178.6230	1179.7937
433.1651	436.2071	438.5427	1180.0368	1180.3319	1183.7920
460.3499	470.0799	471.3582	1190.0816	1191.1131	1191.4415
475.1695	484.0105	484.7846	1192.5569	1193.6258	1222.9613
485.2961	493.8288	500.8401	1229.1422	1230.5383	1231.7268
501.7454	502.8313	524.0791	1232.3613	1236.6081	1238.3701
529.3646	531.7104	546.9164	1245.5271	1249.8869	1250.2492
549.3678	549.5236	567.8735	1253.7539	1253.9746	1254.3430
572.4842	574.4585	578.0964	1258.8755	1263.9151	1266.0307
578.2276	579.5510	581.4953	1269.4325	1272.7059	1277.6512
593.7850	594.8384	603.6025	1277.7366	1278.1765	1290.7000
606.8241	606.9518	612.2212	1290.9765	1295.7018	1298.6889
617.4993	621.2764	625.1820	1299.7642	1300.4796	1306.9294
626.3540	627.0265	632.0787	1314.1193	1314.8620	1317.8842
645.8328	653.1249	654.5565	1318.8323	1320.8299	1325.8033
656.2274	659.5592	660.1755	1333.1313	1339.1954	1339.9397
661.0688	663.9865	695.5085	1340.9129	1345.4659	1345.8763
712.1676	715.9721	718.4677	1349.1631	1350.1255	1355.0056
720.8816	724.7084	726.2560	1365.0322	1370.5858	1376.7482
733.4823	734.2473	740.3173	1377.4762	1386.7361	1389.5352
740.9754	742.9306	744.2493	1393.5792	1398.6636	1400.4711
747.4704	750.4061	754.2375	1404.3982	1413.3481	1413.9247
762.9018	766.1327	767.3134	1414.4755	1415.6296	1418.9756
768.5111	769.9474	772.4888	1425.7670	1428.7565	1449.8807
773.7851	779.4124	780.3280	1450.2143	1469.9174	1471.8860
785.8246	786.7053	787.3937	1472.9037	1474.5725	1474.7547
797.1686	803.9832	805.0219	1475.0343	1475.2142	1477.3037
809.5412	817.8772	823.4994	1479.0590	1482.1271	1484.3894
826.1671	828.3270	835.3875	1484.5753	1484.7366	1488.8737
839.4732	842.6754	846.3947	1489.6846	1492.6628	1498.2701
866.8010	869.2511	869.6498	1498.4225	1498.8239	1500.3362
877.2194	888.6168	889.0970	1500.9122	1501.9930	1506.2668
894.9903	897.6085	898.0717	1519.1912	1520.9169	1521.1461
900.7564	905.2904	909.4229	1521.9705	1535.2732	1535.3592
911.7863	915.3991	918.9630	1535.6694	1603.1046	1603.8384
919.7776	923.3341	936.1035	1628.3527	1629.2632	1632.7452
936.6746	937.2825	941.1781	1636.3900	1637.6291	1638.6986
941.4519	942.2250	944.7545	1648.5870	1649.3340	1649.6063
950.0504	957.5648	959.4577	1674.7458	1676.1324	1676.2965

1678.1098	1678.3968	1678.6441
1769.9989	1772.8472	1773.4249
1820.1392	1821.2811	1822.7897
2990.0860	3017.2667	3017.7931
3018.6729	3019.0339	3032.7469
3058.2602	3058.3898	3058.5587
3059.5471	3064.3380	3066.1726
3067.1131	3068.2759	3072.2628
3080.0938	3080.4428	3080.9363
3082.2949	3104.0083	3104.1249
3104.2798	3104.5366	3106.7105
3117.9622	3121.2053	3126.3201
3130.6878	3130.8545	3151.3553
3173.9376	3174.7220	3174.9879
3182.0587	3182.5757	3183.5157
3184.7864	3186.0343	3186.1773
3199.3109	3199.6024	3199.8312
3200.7678	3200.7815	3202.6874
3204.2822	3204.9308	3205.5776
3215.0513	3224.7446	3227.4558

I5⊂CBr$_4$

E(RB3LYP) = -14058.1660973

E(RB3LYP-D3) = -14058.4078077

H - Sum of electronic and thermal Enthalpies= -14056.986535

G - Sum of electronic and thermal Free Energies= -14057.171963

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.27902	1.37721	1.84901
C	5.48471	1.87678	0.54789
C	5.77419	0.99380	-0.51606
C	5.92613	-0.38365	-0.25885
C	5.75679	-0.88638	1.04855
C	5.43290	-0.00290	2.09579
C	4.88699	2.33162	2.98039
C	4.60924	1.63564	4.33703
C	5.69144	0.55119	4.53429
C	5.20091	-0.51256	3.52318
C	5.92869	-2.37907	1.34004
C	6.19557	-3.24302	0.08465
C	6.26297	-1.37771	-1.38124
C	5.93178	1.52007	-1.94412
C	5.69389	3.04154	-2.08311
C	5.39004	3.38102	0.24535
C	6.38662	3.73141	-0.88551
C	7.19177	-2.47904	-0.81545
C	1.90223	3.93035	-2.23018
C	3.18429	3.52942	-2.71223
C	4.24031	3.41872	-1.84034
C	4.06715	3.68153	-0.44997
C	2.86282	4.11804	0.04303
C	1.74906	4.26259	-0.83446
C	2.90461	-2.88163	-2.67594
C	2.83473	-3.97565	-1.73790
C	3.90820	-4.17128	-0.81902
C	4.96784	-3.29714	-0.80802
C	5.01945	-2.19835	-1.71419
C	4.02872	-2.00527	-2.64497
C	1.39190	-1.21219	3.97397
C	1.03058	0.09285	4.47244
C	2.04861	1.08240	4.62153
C	3.34917	0.78539	4.28834
C	3.70264	-0.51040	3.81105
C	2.75302	-1.48932	3.65674
C	0.38305	-2.19980	3.78468
C	-0.91691	-1.87638	4.07181
C	-1.27428	-0.60531	4.58007
C	-0.33280	0.37148	4.79178
C	0.76935	3.98482	-3.09477
C	-0.44248	4.35559	-2.56959
C	-0.57884	4.73380	-1.21342
C	0.48254	4.69893	-0.34716
C	1.67754	-4.80909	-1.71043
C	0.64102	-4.52348	-2.56215
C	0.71772	-3.46123	-3.49272
C	1.82305	-2.65489	-3.57652
C	-0.57932	-3.39210	-4.22196
O	-0.91632	-2.64665	-5.12505
N	-1.38805	-4.39140	-3.65820
C	-0.71481	-5.13511	-2.67069
O	-1.18155	-6.07819	-2.05901
C	-1.79257	4.40425	-3.19750
O	-2.11970	4.13572	-4.33981
C	-2.00527	5.08841	-0.97282
O	-2.53028	5.52423	0.03618
C	-2.15335	-2.69119	3.94030
O	-2.27711	-3.84616	3.57643
C	-2.74973	-0.60249	4.80514
O	-3.45537	0.26416	5.29101
N	-3.20834	-1.85450	4.35832
N	-2.66927	4.83580	-2.18480
C	-2.78752	-4.59102	-4.01014
C	-4.10644	4.95387	-2.36748
C	-4.56995	-2.34129	4.52979
C	-7.68098	-0.39369	2.38616
C	-7.81759	-0.54168	3.76473
C	-6.78101	-1.13969	4.47722
C	-5.65258	-1.58310	3.77665
N	-5.51914	-1.44018	2.44970
C	-6.51108	-0.85006	1.76096
C	-6.30331	2.69833	0.49553
C	-6.81290	3.93234	0.09428
C	-6.10696	4.67843	-0.84738
C	-4.91741	4.14911	-1.35972
N	-4.44713	2.94790	-1.00426

C	-5.11715	2.22848	-0.08651
C	-5.22108	-1.24387	-2.99831
C	-5.30370	-1.75227	-4.29402
C	-4.51166	-2.84413	-4.64710
C	-3.66677	-3.39274	-3.67641
N	-3.59706	-2.91848	-2.42627
C	-4.35218	-1.85892	-2.08902
C	-4.17234	-1.35902	-0.65746
C	-4.48541	0.90927	0.33637
C	-6.37126	-0.70298	0.24145
N	-5.08262	-0.27781	-0.28437
H	5.69518	3.06078	3.13919
H	4.00477	2.91239	2.68387
H	4.58258	2.38797	5.13279
H	5.66860	0.14968	5.55424
H	6.70468	0.90865	4.31843
H	6.77213	-2.51596	2.03315
H	5.54601	3.97523	1.14746
H	6.94899	1.30491	-2.30282
H	5.25086	0.98242	-2.61614
H	7.39789	3.35336	-0.69708
H	6.43627	4.81735	-1.02730
H	5.04180	-2.76490	1.85735
H	6.54390	-4.23548	0.39086
H	8.04783	-2.07343	-0.26438
H	7.56383	-3.11860	-1.62450
H	3.30226	3.31906	-3.77382
H	2.73008	4.34879	1.09782
H	6.05711	3.37899	-3.05998
H	3.85982	-5.01037	-0.12698
H	4.06097	-1.17427	-3.34630
H	6.68721	-0.87079	-2.24910
H	1.77326	2.06479	5.00137
H	3.01111	-2.47992	3.28898
H	5.66421	-1.48770	3.67953
H	-0.61432	1.34692	5.18103
H	0.64415	-3.18235	3.40079
H	0.36190	4.96871	0.69885
H	0.86564	3.70641	-4.14119
H	1.86258	-1.83023	-4.28331
H	1.60798	-5.62643	-0.99686
H	-3.11330	-5.46988	-3.44488
H	-2.85815	-4.81708	-5.07914
H	-4.30426	4.60601	-3.38741
H	-4.39761	6.00894	-2.30880
H	-4.55011	-3.38091	4.18656
H	-4.81118	-2.33822	5.59889
H	-8.46658	0.07203	1.79638
H	-8.70838	-0.18605	4.27652
H	-6.83574	-1.25257	5.55585
H	-6.79661	2.12040	1.27107
H	-7.72847	4.32185	0.53266
H	-6.44993	5.66337	-1.15264
H	-5.79288	-0.37754	-2.68478
H	-5.96251	-1.29108	-5.02591
H	-4.52670	-3.24656	-5.65593
H	-7.15365	-0.00727	-0.09388
H	-6.61354	-1.66789	-0.22172
H	-4.50110	0.84404	1.43752
H	-3.44153	0.95662	0.02830
H	-3.14167	-1.00361	-0.56862
H	-4.24516	-2.21876	0.02338
C	0.20696	-0.04924	-0.32394
Br	-0.24366	-1.91022	0.09392
Br	-0.50252	0.39757	-2.09628
Br	2.15065	0.18564	-0.29716
Br	-0.59705	1.13684	1.02304

Frequencies

10.4082	12.0842	13.7289
18.5529	19.5513	21.8567
22.3861	24.6063	27.6379
28.9809	31.4465	33.8661
38.0006	40.5987	45.4976
47.9892	51.2147	53.6383
56.3424	65.3051	67.4144
75.2652	85.6744	99.0483
104.6061	114.3993	116.6093
120.2110	122.3138	125.0476
127.9159	130.1124	141.7797
144.1393	150.9201	152.9342
159.2000	160.4587	164.2348
169.9020	175.8475	178.7843
180.8617	181.5839	184.1136
184.2836	185.0023	190.2138
199.0031	204.7226	213.4518
227.4103	230.4631	236.8706
239.9666	244.7684	245.2807
245.6850	248.7484	257.1959
259.5925	260.9180	264.7424
265.3275	273.1838	287.1270
291.3878	298.8185	299.4936
305.1916	306.7873	308.3653
317.8653	329.1179	345.7558
346.5073	349.4394	355.9590
371.1957	371.8025	377.4098
386.6199	396.9752	399.1634
401.6431	405.2875	406.1879
419.8835	428.5931	428.8071
433.0569	436.3165	438.2373
457.8420	469.5806	471.1582
475.2086	483.9603	484.6806
485.4813	494.3661	500.4198
501.3104	501.8824	525.8705
529.7762	531.7779	547.7687
549.7656	550.2721	567.3720
572.3853	574.2118	578.0322
578.1235	580.4847	582.3239

593.8986	594.5790	600.7695
606.5449	607.1378	612.6036
617.9109	619.5902	625.0766
625.8837	629.4790	632.6267
644.4183	653.1718	654.6548
656.8192	660.1026	660.7348
662.9167	667.8099	688.6949
710.3089	715.4241	717.6037
720.7493	724.2179	726.0008
732.8529	738.3565	740.2900
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746.6768	749.7156	759.2089
762.8751	765.6619	768.6755
768.7809	770.2287	773.0427
779.0065	779.3856	782.5342
785.9468	786.4950	787.0550
802.8605	804.9947	807.2465
809.5689	816.6171	819.2977
826.3234	828.0665	831.2533
839.9041	842.6259	847.6212
869.3018	869.5057	875.3032
877.4514	888.7931	889.2292
894.9607	897.5870	898.3639
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914.7757	918.6188	919.3977
920.1857	929.0619	935.8905
936.8838	937.2973	941.3989
941.4754	942.3578	947.1497
950.5718	958.9432	960.3646
960.8766	965.3013	966.6444
967.9470	970.7045	976.5285
987.9321	991.2742	995.7051
1002.6266	1004.9280	1008.6522
1009.6767	1011.9406	1012.7392
1013.2907	1013.8070	1015.1023
1016.1368	1019.7884	1021.4471
1039.3260	1043.8154	1044.6454
1066.1879	1075.1602	1077.7875
1078.0507	1105.8128	1106.8856
1108.0557	1113.6294	1114.8513
1117.3546	1123.1673	1129.1457
1143.9610	1146.1907	1147.9209
1153.5184	1153.9773	1165.8858
1166.1460	1175.7712	1177.5517
1177.9773	1178.6771	1179.1012
1179.8993	1180.5033	1183.6336
1190.1047	1190.9690	1191.2465
1192.7040	1193.4576	1224.2384
1229.6243	1230.7181	1231.4833
1233.1307	1236.3209	1237.7415
1245.5244	1249.8391	1250.1412
1253.5062	1253.8177	1254.1219
1258.8492	1262.9001	1266.2395
1267.1328	1276.8303	1277.4864
1277.6269	1277.7158	1290.7479
1291.0194	1294.3095	1298.4379
1299.0397	1300.3591	1305.6222
1308.7873	1314.7229	1317.5558
1318.4295	1320.3918	1325.4629
1330.5187	1338.1968	1339.5716
1339.9355	1341.2730	1345.1123
1345.9678	1351.2623	1351.4789
1364.5014	1364.8014	1376.7734
1377.4014	1386.1850	1389.3276
1392.8684	1394.7006	1400.2818
1400.8926	1413.4103	1413.8163
1414.2723	1416.7140	1419.1645
1426.5296	1431.3329	1449.3493
1449.9632	1469.5783	1472.3349
1472.5706	1473.9621	1474.5721
1474.7521	1475.1560	1477.7682
1479.4960	1483.5366	1484.3029
1484.5689	1485.1543	1487.4641
1493.5486	1494.9165	1497.7333
1498.7631	1500.8698	1501.2336
1501.6356	1503.3848	1506.9857
1516.5434	1520.9413	1521.2670
1522.0870	1534.9136	1535.3517
1535.7359	1602.4436	1603.2954
1627.8815	1629.4171	1631.4351
1635.7697	1638.4588	1639.2157
1647.6642	1649.2713	1649.5697
1673.8771	1675.9488	1676.2055
1677.3532	1678.3236	1678.5744
1769.8395	1772.4281	1773.4276
1820.2356	1820.6333	1822.6515
2986.2057	3017.2096	3018.9325
3019.8614	3023.8888	3037.5303
3058.2855	3058.3742	3058.7658
3062.7059	3063.8328	3063.8937
3067.5693	3068.3761	3068.8232
3074.8637	3079.9439	3080.4061
3081.0943	3104.1193	3104.2720
3104.6984	3106.8261	3107.4607
3114.0715	3122.7910	3124.4607
3130.0193	3130.5695	3158.4629
3173.8532	3174.8592	3175.0428
3182.0252	3182.2823	3184.0474
3184.1531	3185.5212	3186.9515
3198.5026	3198.8286	3199.8422
3200.9128	3201.6342	3202.3491
3204.2644	3205.3323	3206.6855
3212.2559	3213.6574	3229.2113

TS6⊂CBr_4

E(RB3LYP) = -14058.1642760

E(RB3LYP-D3) = -14058.4081219

H - Sum of electronic and thermal Enthalpies= -14056.985872

G - Sum of electronic and thermal Free Energies= -14057.167414

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.24466	1.38772	1.87990
C	5.53148	1.75393	0.55050
C	5.80651	0.76246	-0.41713
C	5.89753	-0.58881	-0.02451
C	5.65068	-0.95852	1.31499
C	5.31044	0.03056	2.25776
C	4.85428	2.46248	2.89732
C	4.45269	1.90856	4.28646
C	5.45474	0.79053	4.65043
C	4.96530	-0.33437	3.70722
C	5.75601	-2.42094	1.75430
C	6.06642	-3.40736	0.60344
C	6.25936	-1.69510	-1.02903
C	6.00017	1.14420	-1.88615
C	5.82151	2.65431	-2.16995
C	5.52936	3.22791	0.11279
C	6.54510	3.41971	-1.03785
C	7.12821	-2.75574	-0.31029
C	2.07207	3.70623	-2.41399
C	3.33274	3.19826	-2.85225
C	4.38556	3.12283	-1.97206
C	4.22769	3.53417	-0.61605
C	3.05092	4.08370	-0.17340
C	1.94198	4.19043	-1.06122
C	2.92966	-3.23855	-2.34691
C	2.77691	-4.22798	-1.30802
C	3.80081	-4.36371	-0.32411
C	4.88537	-3.52089	-0.34467
C	5.01510	-2.51880	-1.34952
C	4.08084	-2.39769	-2.34808
C	1.10184	-0.79268	4.00563
C	0.78868	0.57677	4.33508
C	1.85149	1.52356	4.44191
C	3.14995	1.12601	4.22719
C	3.45439	-0.22731	3.89879
C	2.46015	-1.16801	3.79050
C	0.05174	-1.75022	3.89877
C	-1.24000	-1.33839	4.09979
C	-1.55136	0.00362	4.42289
C	-0.57060	0.95600	4.55052
C	0.93400	3.71355	-3.27403
C	-0.25946	4.18172	-2.78442
C	-0.36895	4.70753	-1.47595
C	0.69893	4.72809	-0.61782
C	1.58265	-5.00523	-1.24327
C	0.58771	-4.75857	-2.15484
C	0.74728	-3.80247	-3.18453
C	1.89345	-3.06123	-3.30935
C	-0.52882	-3.72942	-3.94844
O	-0.80122	-3.05994	-4.92974
N	-1.41173	-4.60934	-3.30293
C	-0.80250	-5.29341	-2.23330
O	-1.33914	-6.13765	-1.54031
C	-1.61590	4.20345	-3.40141
O	-1.96469	3.82678	-4.50601
C	-1.78191	5.12542	-1.26035
O	-2.28210	5.67840	-0.29697
C	-2.50627	-2.11942	4.08660
O	-2.67308	-3.31288	3.91344
C	-3.02689	0.09592	4.62287
O	-3.70070	1.04992	4.96857
N	-3.52978	-1.19563	4.37580
N	-2.46825	4.76294	-2.43045
C	-2.82528	-4.72721	-3.64364
C	-3.90450	4.90441	-2.60793
C	-4.87969	-1.60474	4.70594
C	-7.97071	-1.23604	1.80271
C	-8.29032	-1.66602	3.08748
C	-7.26749	-1.77473	4.02582
C	-5.95978	-1.45747	3.63662
N	-5.64642	-1.05322	2.39854
C	-6.63590	-0.93741	1.49425
C	-6.14059	2.99304	0.46897
C	-6.59540	4.22016	-0.01334
C	-5.87367	4.85456	-1.02217
C	-4.72518	4.22576	-1.51788
N	-4.30666	3.03325	-1.07993
C	-4.99230	2.42161	-0.09708
C	-4.91362	-1.07210	-2.99131
C	-4.95303	-1.63400	-4.26622
C	-4.27874	-2.83209	-4.50146
C	-3.59084	-3.42632	-3.43886
N	-3.56781	-2.90027	-2.20647
C	-4.20961	-1.74136	-1.98194
C	-4.08723	-1.18393	-0.56492
C	-4.43871	1.09862	0.40908
C	-6.33567	-0.45123	0.06626
N	-4.98817	-0.06990	-0.28977
H	5.69930	3.15185	3.04279
H	4.03131	3.06704	2.49757
H	4.42043	2.72994	5.01053
H	5.34591	0.48650	5.69815
H	6.49858	1.07244	4.47147
H	6.55345	-2.51303	2.50667
H	5.71701	3.89025	0.96001
H	7.01150	0.86087	-2.21230
H	5.30542	0.56900	-2.51154
H	7.53576	3.01107	-0.80819
H	6.64946	4.48385	-1.27967
H	4.82902	-2.73242	2.25144
H	6.37180	-4.37285	1.02133

H	7.96487	-2.31683	0.24496
H	7.52458	-3.47886	-1.03280
H	3.43504	2.87428	-3.88649
H	2.93473	4.43009	0.85118
H	6.20060	2.88246	-3.17210
H	3.69191	-5.12682	0.44472
H	4.17378	-1.64281	-3.12583
H	6.74130	-1.28313	-1.91703
H	1.61196	2.55290	4.70325
H	2.68184	-2.20373	3.54257
H	5.36122	-1.31388	3.97853
H	-0.81687	1.98272	4.81029
H	0.27823	-2.78565	3.65863
H	0.59821	5.11170	0.39427
H	1.00958	3.31975	-4.28442
H	1.99438	-2.31331	-4.09138
H	1.44937	-5.73935	-0.45245
H	-3.22397	-5.51084	-2.99260
H	-2.91518	-5.05379	-4.68471
H	-4.12601	4.46389	-3.58620
H	-4.16402	5.96843	-2.64985
H	-4.81934	-2.66013	4.99439
H	-5.18740	-1.02873	5.58608
H	-8.74050	-1.13037	1.04164
H	-9.31607	-1.90772	3.35480
H	-7.47400	-2.09787	5.04328
H	-6.64803	2.49496	1.29073
H	-7.48044	4.68825	0.41042
H	-6.17266	5.83049	-1.39503
H	-5.39467	-0.12669	-2.76554
H	-5.48505	-1.13453	-5.07233
H	-4.25973	-3.28188	-5.48981
H	-7.00837	0.39531	-0.13459
H	-6.65650	-1.24215	-0.62553
H	-4.59354	1.03240	1.49601
H	-3.36419	1.11527	0.22768
H	-3.05676	-0.83805	-0.44009
H	-4.20774	-2.01708	0.14393
C	0.30082	-0.08137	-0.45492
Br	-0.20585	-1.87294	0.15919
Br	-0.50342	1.26756	0.72600
Br	2.24757	0.11252	-0.39709
Br	-0.35338	0.17382	-2.28529

Frequencies

-26.9856	13.6299	14.5181
16.6065	17.2919	20.2838
22.0568	24.8985	26.7683
30.3549	32.2375	35.9958
39.0623	40.4129	46.7782
49.1368	50.7850	54.8229
58.0769	67.1206	68.9629
78.0225	85.8210	98.9877
104.6776	116.8261	117.1593
119.8771	123.2639	125.3184
128.6018	131.1877	143.0906
145.7259	150.5594	153.0238
153.9753	159.9853	162.2130
170.5319	173.7645	178.8782
180.8515	181.7112	183.0359
184.9515	188.1442	191.5203
198.5041	206.6722	211.6715
227.0792	231.2902	234.9585
238.9866	243.1900	244.6382
245.4959	249.6641	252.8232
261.2483	263.6687	264.9851
266.2734	274.0261	287.9673
290.8884	298.2152	299.7929
302.9517	307.0239	309.9017
317.0060	321.6372	329.3128
346.7426	347.4067	359.5333
370.5850	372.1022	377.6256
386.9987	396.6628	399.3643
401.9725	405.9021	406.8708
420.0353	428.5162	429.0047
431.5989	434.0068	436.8506
452.2808	467.9330	472.5749
478.2151	484.0176	484.7689
486.2475	488.6831	500.1210
501.8215	504.3404	529.9693
533.6330	536.9990	547.9398
549.9815	551.3361	567.1472
572.3587	573.8480	576.7105
577.9452	580.4767	583.3545
594.3402	595.1977	602.7751
606.0325	607.4361	615.7727
619.0133	621.9739	624.7883
625.5423	633.0439	635.0153
645.9647	653.0497	654.0833
655.6431	660.2516	660.6272
662.4879	663.7502	669.1150
714.2548	715.4137	718.2089
720.4556	723.2384	724.6888
732.8821	738.0831	738.5387
740.7557	742.5330	743.2829
745.4692	750.3829	756.0330
759.9274	762.9493	768.3661
768.8208	770.8781	772.7087
778.2008	779.0936	780.5998
782.6468	785.9530	786.8115
787.4511	803.8784	806.1829
809.9582	811.1090	818.0594
826.4589	827.5111	828.6894
841.2837	842.5641	847.3262
869.1749	869.5398	877.5776
882.0281	888.9273	889.4213
894.8649	897.8213	898.0179
900.6179	903.4092	911.0385

916.3795	918.3383	919.0625
919.6334	933.4058	935.9486
936.4160	937.7952	941.1472
941.4435	942.6016	949.0739
950.6644	953.8380	959.3878
960.4944	963.5710	966.2169
966.8505	968.6351	971.0501
988.2535	991.3498	999.3062
1002.3232	1002.9337	1008.8009
1009.6386	1010.5005	1012.1607
1013.3161	1014.6884	1014.8347
1015.1815	1021.0711	1032.0431
1039.3797	1044.0730	1044.2666
1066.1926	1074.6861	1077.1504
1078.3304	1104.6644	1106.5860
1107.5780	1114.3594	1117.5454
1117.9459	1122.4356	1124.8868
1144.3338	1147.4095	1151.1993
1153.7796	1161.3801	1166.0273
1166.0821	1176.4167	1177.2277
1178.1038	1178.9087	1179.8539
1180.2331	1180.6141	1184.1458
1189.4026	1190.9322	1191.3184
1192.5119	1193.5542	1214.7125
1229.6099	1230.7532	1230.8300
1234.2324	1235.3072	1236.4231
1245.1491	1249.2420	1250.0243
1253.4539	1253.8249	1253.8955
1258.4782	1259.4434	1262.0394
1268.2647	1275.7734	1277.2124
1277.6065	1277.8322	1290.0426
1290.8950	1294.6157	1298.0660
1298.8547	1300.2833	1303.4421
1308.2906	1314.7963	1317.4871
1318.1412	1319.8850	1325.1916
1330.8005	1338.0479	1339.4908
1339.7099	1341.1239	1344.8735
1346.1391	1353.4999	1363.2048
1364.2912	1376.8205	1377.2197
1379.3089	1384.4677	1388.9875
1392.6669	1399.9709	1401.4177
1404.4189	1413.2403	1413.7576
1414.0480	1416.2559	1418.4606
1422.2855	1432.2606	1449.1422
1449.2750	1467.1727	1469.9162
1471.9458	1473.1445	1474.3185
1474.6923	1474.8774	1475.9730
1478.4208	1479.2668	1483.6011
1484.4471	1484.6015	1486.0278
1488.5498	1493.2473	1494.3892
1498.6280	1501.5363	1501.7723
1502.2294	1502.8402	1503.0469
1520.8677	1520.9937	1521.3922
1522.1999	1534.2796	1535.4365
1535.6998	1601.9651	1602.4066
1627.2302	1630.2069	1632.3026
1634.7049	1637.5579	1638.6770
1647.1989	1649.0455	1649.2883
1672.9695	1675.6597	1675.9968
1676.2888	1678.4125	1678.4930
1769.9490	1772.4843	1773.9482
1820.3889	1821.0306	1823.2160
3017.3188	3017.3492	3017.8635
3020.5093	3021.4819	3028.4089
3055.2197	3058.1980	3058.5573
3058.8891	3062.8293	3063.1216
3063.4903	3065.8742	3073.2450
3077.5087	3080.1525	3080.4245
3080.8158	3103.9960	3104.5227
3104.7524	3104.9400	3107.0428
3108.0901	3121.4367	3127.8833
3128.2583	3131.8547	3156.1769
3173.8209	3174.4604	3175.3576
3179.3742	3183.0057	3183.0757
3183.6291	3184.9661	3187.9399
3188.4379	3198.0842	3198.7697
3199.6849	3200.7489	3202.1586
3203.9531	3204.4237	3204.4786
3208.2849	3208.8372	3228.2420

I6⊂CBr$_4$

E(RB3LYP) = -14058.1709754

E(RB3LYP-D3) = -14058.4135407

H - Sum of electronic and thermal Enthalpies= -14056.991038

G - Sum of electronic and thermal Free Energies= -14057.176416

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.73356	0.75263	1.16093
C	5.64066	1.70037	0.12295
C	5.61577	1.28183	-1.22372
C	5.69416	-0.09105	-1.52748
C	5.78580	-1.04675	-0.49378
C	5.85506	-0.61805	0.84702
C	5.67176	1.21473	2.61729
C	5.70429	0.05590	3.63955
C	6.78781	-0.93949	3.16265
C	6.03550	-1.62388	1.99763
C	5.77738	-2.54229	-0.81468
C	5.56687	-2.86135	-2.31415
C	5.63745	-0.58626	-2.98034
C	5.48535	2.30203	-2.35590
C	5.29571	3.75804	-1.87167
C	5.54163	3.20383	0.42236
C	6.26893	3.99069	-0.69396
C	6.46044	-1.88825	-3.11658

C	1.60574	4.44878	-0.82895
C	2.73177	4.32558	-1.69677
C	3.95150	3.95107	-1.18752
C	4.10564	3.66685	0.20089
C	3.05597	3.81313	1.07343
C	1.77889	4.21506	0.58435
C	1.90848	-1.22140	-3.91902
C	1.83364	-2.57251	-3.41857
C	3.00826	-3.17790	-2.87601
C	4.18093	-2.46349	-2.80683
C	4.23507	-1.11277	-3.26082
C	3.13730	-0.50742	-3.81917
C	2.50869	-2.80113	3.14443
C	2.22620	-1.67669	4.00298
C	3.24955	-0.70702	4.23363
C	4.45324	-0.81162	3.57835
C	4.68561	-1.87259	2.65401
C	3.76132	-2.86906	2.47094
C	1.51088	-3.79234	2.92481
C	0.26744	-3.59722	3.46453
C	-0.03942	-2.45802	4.24289
C	0.91893	-1.52565	4.55466
C	0.31452	4.78202	-1.33376
C	-0.73357	4.87063	-0.45316
C	-0.55372	4.68534	0.93747
C	0.66971	4.36721	1.46679
C	0.58918	-3.26965	-3.46415
C	-0.50910	-2.62859	-3.98116
C	-0.42353	-1.31460	-4.49854
C	0.75159	-0.61033	-4.48356
C	-1.77600	-0.91438	-4.97484
O	-2.13150	0.12141	-5.50879
N	-2.61506	-2.00575	-4.70010
C	-1.92736	-3.07544	-4.09812
O	-2.43004	-4.13550	-3.76883
C	-2.17813	5.13544	-0.69783
O	-2.75314	5.34850	-1.75060
C	-1.87136	4.88228	1.60543
O	-2.13896	4.88735	2.79338
C	-0.97763	-4.38631	3.28521
O	-1.11838	-5.47733	2.75630
C	-1.50783	-2.46831	4.50733
O	-2.18122	-1.67221	5.13324
N	-2.00536	-3.62046	3.85516
N	-2.79230	5.10450	0.56812
C	-4.04349	-1.99998	-4.95762
C	-4.20368	5.37616	0.76866
C	-3.42826	-3.96985	3.77462
C	-5.05340	-3.41508	-0.12639
C	-4.30832	-4.56833	0.11297
C	-3.78660	-4.77725	1.38757
C	-4.00826	-3.80293	2.37282
N	-4.73942	-2.70016	2.14711
C	-5.26258	-2.50828	0.92027
C	-6.43970	2.35222	2.75749
C	-6.81665	3.68251	2.92605
C	-6.06946	4.67397	2.29428
C	-4.97954	4.29086	1.50335
N	-4.61620	3.01295	1.33704
C	-5.32752	2.05342	1.95804
C	-6.28119	0.50447	-2.33040
C	-6.74236	0.33168	-3.63394
C	-6.00773	-0.46352	-4.51558
C	-4.83825	-1.06999	-4.04642
N	-4.39534	-0.91031	-2.79356
C	-5.09129	-0.12987	-1.94892
C	-4.48356	0.07260	-0.57282
C	-4.89450	0.60911	1.77274
C	-6.12634	-1.26875	0.70263
N	-5.44440	0.02235	0.53231
H	6.52160	1.87813	2.83481
H	4.76664	1.81523	2.77289
H	5.88340	0.45934	4.64216
H	7.02803	-1.67227	3.94181
H	7.71314	-0.44544	2.84539
H	6.73163	-2.99474	-0.50631
H	5.91918	3.43663	1.41933
H	6.38823	2.26781	-2.98375
H	4.64802	2.02786	-3.00885
H	7.28012	3.61678	-0.89082
H	6.33012	5.05400	-0.43403
H	4.99822	-3.03857	-0.22370
H	5.78814	-3.91887	-2.49517
H	7.47329	-1.79944	-2.70739
H	6.52994	-2.18647	-4.16922
H	2.60177	4.53750	-2.75669
H	3.17057	3.62209	2.13825
H	5.44363	4.44488	-2.71218
H	2.95253	-4.20843	-2.52945
H	3.17703	0.51544	-4.18702
H	5.95528	0.19031	-3.67803
H	3.04928	0.11113	4.92326
H	3.94900	-3.70448	1.80019
H	6.52544	-2.53583	1.65049
H	0.68035	-0.65722	5.16326
H	1.72115	-4.65391	2.29642
H	0.79507	4.21023	2.53494
H	0.16661	4.93986	-2.39922
H	0.80225	0.40419	-4.87046
H	0.51537	-4.28179	-3.07430
H	-4.37851	-3.03389	-4.81895
H	-4.21273	-1.72235	-6.00317
H	-4.61963	5.51896	-0.23515
H	-4.31375	6.32206	1.31227
H	-3.53891	-5.00615	4.11117
H	-3.95022	-3.30408	4.46405
H	-5.46752	-3.21638	-1.11014
H	-4.13555	-5.28945	-0.68173

H	-3.19964	-5.65860	1.61899
H	-6.98667	1.55128	3.24695
H	-7.66570	3.94425	3.55264
H	-6.31358	5.72524	2.42237
H	-6.81405	1.11881	-1.61107
H	-7.65488	0.82089	-3.96585
H	-6.32909	-0.60311	-5.54447
H	-6.81078	-1.16784	1.55141
H	-6.74249	-1.43602	-0.18890
H	-5.24174	0.01965	2.62435
H	-3.79811	0.55670	1.78453
H	-4.02731	1.06932	-0.54756
H	-3.66613	-0.65667	-0.45966
C	-0.05971	-0.05439	0.20771
Br	-0.67062	0.72297	1.90253
Br	-0.75834	-1.88211	0.04247
Br	1.90135	-0.09222	0.16576
Br	-0.72508	1.03340	-1.28077

Frequencies

6.5389	13.3084	14.9334
16.5047	17.6810	22.2473
22.4449	26.5083	26.7253
30.9814	31.9985	35.5611
36.1647	36.8605	41.5668
49.0088	51.6279	59.6227
61.8206	65.1952	76.2165
80.4893	82.7421	95.8317
101.8724	112.1421	114.2345
122.2144	123.8821	125.5797
126.7356	127.2880	141.2629
144.5350	151.5978	153.2056
160.1093	161.5052	168.3873
170.6865	172.8719	176.3376
181.0021	181.8722	182.5939
183.1313	188.9600	191.8416
201.1625	214.1788	221.4332
229.4955	233.3526	235.0179
235.8740	241.3922	243.7949
246.2967	248.6657	251.3836
260.4869	262.9705	263.6842
273.6300	279.2398	288.8640
293.1171	299.3028	301.5735
305.9543	308.1176	314.2836
319.0654	327.3987	345.3941
346.4632	360.2934	369.8561
370.9858	382.7320	385.5044
391.6894	397.0061	401.7694
404.8090	406.3046	407.8191
420.4057	427.6965	428.6565
429.1624	436.1892	441.0793
444.4962	465.8614	471.1108
473.2308	476.8988	484.0382
484.0918	484.9154	498.7415
502.0583	504.6438	527.5128
532.7025	545.9279	547.6629
548.6462	556.9867	566.6040
572.5484	572.8328	577.0585
579.1565	579.8177	584.4186
594.2039	595.6609	602.4250
606.1720	606.4858	609.4829
620.4811	621.3999	624.6783
625.8042	626.6905	628.1305
651.0085	653.2896	655.0464
657.1476	659.4670	660.2164
663.9472	666.0605	701.7952
715.8474	716.4187	719.5147
721.5450	724.3877	726.7780
734.9030	737.9938	738.8970
740.5001	744.1758	745.6676
752.8185	756.4278	758.7969
763.0879	767.8838	768.7379
771.6278	773.3114	777.1366
779.4307	780.0135	782.7950
784.1703	786.3673	787.7444
795.2579	800.9300	803.5754
811.1848	816.4315	823.1853
826.1802	827.1794	838.3802
842.7473	846.8011	858.0010
867.7681	869.8189	869.9368
877.7136	888.7643	889.4397
894.8428	897.4782	898.3741
900.2280	910.3180	911.7244
914.8054	916.4985	919.1188
919.7388	928.5759	934.3096
936.0912	936.7836	937.1377
941.0713	941.6130	942.1959
944.6276	955.0050	958.9682
961.6549	964.3885	965.6671
967.1546	967.6987	971.1708
982.8767	990.2295	1000.8373
1001.7446	1007.2377	1008.1554
1010.8926	1011.3369	1012.5637
1013.4097	1014.1312	1015.1617
1018.6759	1023.3508	1025.6127
1039.6376	1044.9371	1045.3688
1066.3083	1074.7099	1077.1909
1077.8689	1095.8467	1106.5223
1107.0801	1109.9635	1116.2411
1117.3217	1118.9601	1125.7453
1131.6407	1142.2201	1148.9355
1149.7237	1150.5623	1153.3228
1166.0433	1166.3537	1177.0960
1178.3002	1178.9306	1179.7129
1179.9538	1180.3295	1186.3693
1190.4024	1191.2240	1191.7995
1193.5843	1194.7834	1228.3913
1229.2510	1231.9336	1232.2628

1233.5459 1236.1492 1245.5068
1248.3998 1249.2273 1250.3661
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1260.0363 1266.1153 1270.7016
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1299.5167 1300.0081 1300.1653
1314.9520 1315.9790 1317.9023
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1325.2435 1338.3316 1339.2776
1340.8227 1343.7962 1345.7680
1346.0326 1351.6362 1358.7237
1363.8955 1367.4720 1369.2961
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1396.5070 1400.2586 1400.6887
1407.9362 1410.7994 1413.4578
1414.4212 1415.2445 1416.4282
1422.8127 1425.1002 1449.9136
1450.2574 1470.5653 1472.4616
1472.9214 1473.7065 1475.1986
1475.8971 1476.5470 1478.8758
1480.5900 1483.7439 1484.3492
1484.9867 1488.1133 1489.5513
1491.5760 1493.8133 1495.1048
1495.6700 1500.6864 1500.7209
1501.2413 1501.7349 1515.9066
1518.5123 1521.1943 1521.5553
1522.3261 1534.5221 1535.6645
1536.7285 1602.9803 1603.9935
1627.8006 1628.5868 1631.2503
1634.5232 1638.3989 1639.3500
1648.0593 1649.3143 1649.7069
1674.6392 1675.5088 1676.1242
1677.6711 1678.7823 1679.4808
1767.4408 1770.2946 1772.5854
1818.9465 1819.6081 1821.8626
3010.0721 3017.4744 3018.2063
3020.0278 3049.7672 3056.4739
3057.8027 3058.4978 3058.5787
3059.1760 3066.0331 3070.7526
3072.1859 3073.4519 3079.7408
3079.9053 3080.1189 3080.2121
3080.2652 3100.4342 3101.6655
3104.1946 3104.4256 3105.2099
3113.9295 3119.3248 3126.4927
3126.7812 3130.5723 3158.3288
3174.3802 3174.6984 3175.6830
3182.4944 3183.9718 3184.0471
3184.6372 3185.5734 3197.3740
3198.0853 3200.0018 3200.3866
3201.3197 3201.9623 3202.1441
3203.1109 3203.1735 3209.0510
3215.9691 3218.0391 3238.5845

TS7⊂CBr_4

E(RB3LYP) = -14058.1708349

E(RB3LYP-D3) = -14058.4116138

H - Sum of electronic and thermal Enthalpies= -14056.991994

G - Sum of electronic and thermal Free Energies= -14057.174993

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.77737	0.88560	1.01582
C	5.65877	1.69674	-0.12936
C	5.60478	1.11487	-1.41290
C	5.68936	-0.28458	-1.54612
C	5.80476	-1.10491	-0.40402
C	5.89188	-0.51378	0.87241
C	5.75353	1.52755	2.40352
C	5.79138	0.50569	3.56180
C	6.85543	-0.55620	3.19808
C	6.07831	-1.36980	2.13737
C	5.80668	-2.62870	-0.53835
C	5.59031	-3.13299	-1.98521
C	5.61998	-0.95588	-2.92574
C	5.43769	1.98730	-2.65822
C	5.25242	3.49221	-2.35306
C	5.56034	3.22503	-0.01581
C	6.25465	3.86983	-1.23906
C	6.46151	-2.25340	-2.91074
C	1.59200	4.32195	-1.30407
C	2.69395	4.08838	-2.18034
C	3.92588	3.76920	-1.66259
C	4.11668	3.65387	-0.25456
C	3.08902	3.90104	0.62134
C	1.79999	4.24785	0.12184
C	1.89420	-1.75686	-3.74233
C	1.84614	-3.03970	-3.08388
C	3.03434	-3.55619	-2.48242
C	4.19471	-2.81932	-2.50930
C	4.22317	-1.53256	-3.12306
C	3.11121	-1.01611	-3.73961
C	2.54603	-2.33522	3.45443
C	2.29198	-1.10885	4.17070
C	3.33369	-0.13674	4.27064
C	4.52838	-0.34347	3.62339
C	4.73306	-1.51368	2.83434
C	3.78937	-2.50752	2.78220
C	1.53078	-3.32956	3.37156
C	0.29868	-3.04976	3.89990
C	0.01938	-1.81793	4.53419
C	0.99486	-0.86895	4.71463
C	0.29264	4.61915	-1.81064
C	-0.73023	4.82517	-0.92002
C	-0.51787	4.78478	0.47795

C	0.71473	4.50744	1.00891
C	0.61423	-3.75855	-3.03675
C	-0.49809	-3.20247	-3.61796
C	-0.43926	-1.95792	-4.28824
C	0.72317	-1.23687	-4.36600
C	-1.80120	-1.64133	-4.79949
O	-2.17803	-0.68363	-5.45156
N	-2.61872	-2.70655	-4.39010
C	-1.90831	-3.68489	-3.67053
O	-2.38982	-4.70692	-3.21419
C	-2.17110	5.11692	-1.15765
O	-2.76599	5.24694	-2.21299
C	-1.81150	5.08947	1.15216
O	-2.04916	5.22494	2.33855
C	-0.95745	-3.84007	3.84726
O	-1.11880	-4.98929	3.46923
C	-1.44312	-1.77617	4.82579
O	-2.09502	-0.90005	5.36094
N	-1.96578	-2.99465	4.33334
N	-2.74991	5.24431	0.11811
C	-4.04786	-2.75902	-4.63632
C	-4.13163	5.61962	0.32920
C	-3.39102	-3.34192	4.34943
C	-5.13958	-3.44310	0.46451
C	-4.41913	-4.55900	0.88638
C	-3.85606	-4.55081	2.16017
C	-4.01211	-3.40676	2.95726
N	-4.71837	-2.33751	2.55719
C	-5.28242	-2.35436	1.33394
C	-6.70846	2.65016	1.96220
C	-7.16179	3.96436	1.87913
C	-6.30960	4.93247	1.35285
C	-5.03670	4.54197	0.91914
N	-4.59893	3.27934	0.99420
C	-5.41671	2.34366	1.51308
C	-6.31824	0.04076	-2.35820
C	-6.79130	-0.33048	-3.61551
C	-6.04691	-1.22631	-4.38476
C	-4.85558	-1.72987	-3.85205
N	-4.40208	-1.38088	-2.64249
C	-5.10781	-0.50303	-1.90895
C	-4.48421	-0.08661	-0.58807
C	-4.90486	0.91465	1.60570
C	-6.12907	-1.15234	0.92302
N	-5.43493	0.07448	0.51231
H	6.61722	2.19899	2.51812
H	4.86069	2.15740	2.50199
H	5.99042	1.02843	4.50371
H	7.09841	-1.18947	4.05932
H	7.78187	-0.11823	2.80965
H	6.76693	-3.03129	-0.18322
H	5.96235	3.58005	0.93445
H	6.32345	1.87913	-3.30178
H	4.58493	1.63143	-3.24895
H	7.26227	3.47626	-1.41486
H	6.31726	4.95713	-1.11354
H	5.03586	-3.05506	0.11504
H	5.82676	-4.20140	-2.03680
H	7.47672	-2.10074	-2.52707
H	6.52545	-2.67785	-3.91949
H	2.53674	4.17627	-3.25403
H	3.23086	3.83534	1.69790
H	5.37595	4.06950	-3.27584
H	2.99895	-4.53864	-2.01473
H	3.13121	-0.04447	-4.22820
H	5.91817	-0.26724	-3.71804
H	3.15502	0.76367	4.85584
H	3.95439	-3.42117	2.21562
H	6.55126	-2.32523	1.90200
H	0.77754	0.07150	5.21453
H	1.71996	-4.26619	2.85356
H	0.86613	4.46871	2.08453
H	0.12009	4.66578	-2.88304
H	0.75367	-0.27482	-4.87099
H	0.56077	-4.71848	-2.52921
H	-4.36359	-3.77101	-4.35933
H	-4.22762	-2.62597	-5.70831
H	-4.51473	5.92380	-0.65107
H	-4.15498	6.49617	0.98745
H	-3.49753	-4.30703	4.85646
H	-3.88981	-2.56648	4.93346
H	-5.58843	-3.41297	-0.52387
H	-4.29792	-5.41907	0.23293
H	-3.28448	-5.39447	2.52909
H	-7.33785	1.86780	2.37710
H	-8.15502	4.23319	2.23031
H	-6.61796	5.97312	1.28631
H	-6.85687	0.74068	-1.72672
H	-7.72072	0.08291	-3.99954
H	-6.37728	-1.52124	-5.37737
H	-6.78860	-0.89258	1.75751
H	-6.77284	-1.46347	0.09104
H	-5.21083	0.48309	2.56268
H	-3.80874	0.92940	1.60499
H	-4.00288	0.88749	-0.73886
H	-3.68063	-0.80407	-0.35930
C	-0.05630	-0.01954	0.17642
Br	-0.71075	-1.86988	0.23071
Br	-0.73908	0.86549	-1.43499
Br	1.90508	-0.01686	0.14264
Br	-0.69387	0.94078	1.76296

Frequencies

-13.9733	6.2678	12.6229
15.0349	16.8995	18.5772
21.4379	23.5364	25.3074
28.7725	30.4147	34.8103
35.4743	36.3419	40.3387

48.6043	51.2592	58.4371	867.7861	869.5643	869.8182
61.9612	65.6650	73.7015	877.4386	888.4709	889.2023
79.5940	83.0960	96.3949	894.7335	896.9442	898.0103
102.7412	111.8019	112.8590	900.0307	910.2028	911.8965
121.5060	123.5078	125.4361	914.8542	916.1774	919.2220
126.3368	126.9209	141.4047	919.7971	922.5756	934.0318
144.2091	151.4209	152.7785	935.8798	936.7493	937.2822
158.4338	160.5107	165.7364	941.1338	941.2939	941.7271
168.5371	171.9235	176.7227	943.0684	955.4012	958.5388
180.2091	180.8922	181.7078	961.6273	964.1756	965.3782
182.3386	187.7257	190.9038	967.1130	967.6050	970.9623
199.9827	212.2706	220.8899	980.1487	990.1993	998.4595
230.2955	232.7756	233.7229	1001.2195	1006.3906	1008.0049
235.8387	241.3091	243.6096	1009.8753	1010.9482	1011.5675
246.9370	247.8118	252.0979	1012.8532	1013.8711	1015.0518
260.4116	262.6732	264.2555	1017.7456	1023.6089	1030.7911
271.6304	275.2621	284.7937	1039.7272	1044.7999	1045.4926
295.8208	298.0655	301.3831	1066.3616	1074.8542	1077.2513
305.8665	307.3744	314.0871	1077.8632	1096.6420	1106.7133
319.1663	327.5884	344.9330	1107.3439	1110.4313	1117.1280
345.9645	352.9950	369.3124	1117.9426	1121.3076	1122.9961
371.2854	377.7017	385.7077	1132.4228	1142.9786	1149.4562
391.5409	396.4984	400.6115	1151.2499	1153.0523	1154.2193
402.3859	406.1684	407.3406	1166.0038	1166.2870	1177.1762
420.1110	426.7988	428.3462	1178.3815	1178.9114	1179.8423
428.9913	435.7691	440.5753	1180.1029	1180.2181	1186.1691
445.3290	469.6930	470.7777	1190.3276	1191.2414	1191.8544
474.9835	476.5748	483.2243	1193.3568	1194.7130	1227.0336
484.5638	485.3740	498.7701	1228.2905	1231.8760	1232.1031
502.3621	504.6900	527.5198	1232.9792	1236.4001	1245.6319
532.5503	545.5026	548.0842	1247.5522	1249.2879	1250.3678
548.9408	556.0290	567.0792	1253.5068	1253.8573	1254.1910
572.5359	573.0448	576.9669	1260.1696	1265.3516	1270.8757
578.3499	579.4128	584.2581	1273.7943	1275.7521	1277.3762
594.2130	595.8385	604.6765	1277.8939	1277.9563	1289.8149
606.3117	606.8892	609.3782	1290.7344	1296.7978	1298.1480
621.4911	622.1033	624.1924	1299.6405	1300.0592	1300.3900
626.4236	627.6867	631.3869	1315.4184	1316.8069	1318.3101
649.8893	653.2968	654.1860	1318.5965	1319.4935	1325.2886
656.0454	659.2449	660.0456	1325.3462	1338.6175	1339.3377
660.3570	663.9935	701.4080	1340.8364	1344.8305	1345.9936
715.7884	716.5964	718.9711	1346.2642	1357.7906	1363.3518
721.7009	724.4623	726.6939	1364.2874	1369.3646	1370.9660
732.8395	735.4860	738.9591	1377.3826	1377.7848	1394.2220
740.5130	743.7458	745.6641	1396.2670	1400.5268	1404.8815
752.4347	754.2527	758.1626	1407.0867	1409.4212	1412.3759
763.0903	767.8951	768.3796	1414.1656	1414.7445	1416.4289
770.2894	771.8089	775.8930	1419.2044	1424.1146	1450.1828
779.1591	779.6631	781.4667	1450.5582	1470.5537	1471.0747
784.1217	786.7935	787.8615	1473.0630	1473.8140	1475.0697
795.1257	797.9837	802.5156	1476.1035	1476.6112	1478.8400
810.2817	816.7825	822.8265	1479.7842	1483.7907	1484.4692
826.3460	827.0810	837.8785	1484.7603	1486.1229	1487.6340
843.0442	844.8739	857.6169	1489.8558	1493.4412	1494.4212

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1536.7141	1603.3168	1604.4048
1628.2393	1629.0677	1631.6192
1635.0368	1638.0468	1638.8378
1648.1933	1649.4831	1649.5863
1674.7709	1675.7155	1676.2577
1677.7491	1678.8042	1679.5699
1767.8371	1770.7448	1773.2316
1819.2500	1819.9830	1822.6482
3008.1524	3017.8581	3018.3825
3019.3877	3051.2650	3058.5280
3058.6100	3059.0888	3060.7989
3063.6911	3067.7898	3069.9539
3070.6273	3071.8296	3075.0969
3077.2684	3080.0889	3080.1365
3080.2634	3099.0748	3104.2353
3104.4136	3105.0408	3106.6841
3112.9029	3120.8134	3122.7337
3125.9671	3127.0068	3156.9788
3174.4533	3174.5768	3175.4216
3181.3549	3182.3329	3183.5373
3184.2447	3185.3796	3194.7295
3196.1455	3200.0749	3200.2262
3201.1421	3201.8330	3202.3081
3202.7442	3203.1686	3207.9269
3213.6081	3217.7917	3239.8511

I7⊂CBr_4

E(RB3LYP) = -14058.1739989

E(RB3LYP-D3) = -14058.4101579

H - Sum of electronic and thermal Enthalpies= -14056.994298

G - Sum of electronic and thermal Free Energies= -14057.179972

Number of imaginary frequencies: 0

Cartesian Coordinates

C	6.04761	0.46953	0.74642
C	5.95885	1.07016	-0.52341
C	5.72384	0.28584	-1.67135
C	5.64402	-1.11511	-1.54790
C	5.76543	-1.72915	-0.28298
C	5.97729	-0.93468	0.86086
C	6.19107	1.34920	1.98913
C	6.10283	0.56454	3.31651
C	6.98356	-0.69645	3.16156
C	6.07123	-1.56106	2.26218
C	5.66042	-3.24897	-0.14058
C	5.33784	-3.98826	-1.46066
C	5.40487	-2.01112	-2.77103
C	5.54725	0.94630	-3.04115
C	5.59102	2.49423	-3.00897
C	6.07668	2.59070	-0.68946
C	6.73384	2.90588	-2.05403
C	6.17877	-3.33836	-2.58244
C	2.18777	4.02683	-1.87990
C	3.16876	3.50571	-2.77669
C	4.38457	3.08434	-2.29400
C	4.68527	3.17276	-0.90317
C	3.77612	3.68639	-0.01293
C	2.50021	4.11869	-0.47442
C	1.58818	-2.71761	-3.17189
C	1.53909	-3.88050	-2.31908
C	2.74424	-4.35157	-1.71741
C	3.92711	-3.68960	-1.94201
C	3.96663	-2.52132	-2.75802
C	2.83103	-2.04657	-3.36666
C	2.44091	-1.69037	3.66478
C	2.40011	-0.33339	4.15403
C	3.58624	0.45976	4.09452
C	4.72456	-0.05080	3.51760
C	4.72843	-1.36053	2.95322
C	3.63056	-2.17728	3.05151
C	1.28213	-2.51188	3.76207
C	0.12863	-1.95985	4.25251
C	0.06284	-0.60938	4.66422
C	1.17372	0.19715	4.65473
C	0.90211	4.43698	-2.34196
C	-0.01725	4.87944	-1.42452
C	0.29032	4.95859	-0.04616
C	1.52208	4.60697	0.43856
C	0.29369	-4.53984	-2.09824
C	-0.83113	-4.04623	-2.70926
C	-0.77735	-2.92085	-3.56512
C	0.39725	-2.25651	-3.80566
C	-2.15113	-2.66711	-4.08249
O	-2.53539	-1.82637	-4.87570
N	-2.96725	-3.64298	-3.48703
C	-2.24564	-4.51007	-2.64728
O	-2.72274	-5.44662	-2.03088
C	-1.43232	5.31343	-1.60184
O	-2.08130	5.43112	-2.62674
C	-0.92221	5.43060	0.67659
O	-1.06703	5.65741	1.86375
C	-1.21976	-2.56155	4.41726
O	-1.55341	-3.72725	4.28149
C	-1.35292	-0.31118	5.02538
O	-1.83871	0.72465	5.43747
N	-2.06837	-1.51056	4.79688
N	-1.91176	5.59120	-0.31085
C	-4.39180	-3.75717	-3.72365
C	-3.26683	6.04375	-0.02640
C	-3.49777	-1.66258	5.08764
C	-5.91758	-2.83644	1.78622
C	-5.30008	-3.83719	2.53412

C	-4.50685	-3.46807	3.61648
C	-4.34099	-2.10398	3.89674
N	-4.94134	-1.13925	3.18114
C	-5.72530	-1.49656	2.14670
C	-6.28441	3.10352	-0.60793
C	-6.36987	4.28559	-1.33791
C	-5.37623	5.25160	-1.17683
C	-4.33709	4.99269	-0.27889
N	-4.24627	3.84951	0.41846
C	-5.19892	2.91716	0.26064
C	-6.76879	-0.67791	-1.98453
C	-7.29043	-1.40221	-3.05691
C	-6.51119	-2.39509	-3.64596
C	-5.23504	-2.63826	-3.12108
N	-4.73772	-1.95567	-2.08651
C	-5.48016	-0.97991	-1.53116
C	-4.79488	-0.18859	-0.42844
C	-5.08472	1.66664	1.12967
C	-6.46492	-0.39872	1.38571
N	-5.69233	0.48663	0.50760
H	7.15908	1.87185	1.96682
H	5.42137	2.12988	1.97895
H	6.39969	1.21418	4.14712
H	7.14549	-1.19158	4.12622
H	7.95777	-0.48413	2.70667
H	6.61239	-3.64378	0.24459
H	6.60860	3.04188	0.14981
H	6.34315	0.60341	-3.71857
H	4.60135	0.61953	-3.49116
H	7.65947	2.34376	-2.22206
H	6.95184	3.97729	-2.13459
H	4.89980	-3.50176	0.60811
H	5.52157	-5.06060	-1.33262
H	7.22681	-3.18435	-2.30152
H	6.14337	-3.93640	-3.50062
H	2.93175	3.45123	-3.83783
H	3.99997	3.76535	1.04852
H	5.70509	2.87586	-4.02942
H	2.70549	-5.24564	-1.09740
H	2.85330	-1.16523	-4.00400
H	5.66640	-1.49707	-3.69729
H	3.56354	1.46669	4.50777
H	3.63581	-3.18954	2.65342
H	6.38646	-2.60473	2.21429
H	1.12042	1.23008	4.98923
H	1.31038	-3.54391	3.42224
H	1.74562	4.66919	1.50039
H	0.65437	4.37380	-3.39858
H	0.42641	-1.38756	-4.45769
H	0.24308	-5.41136	-1.45026
H	-4.69218	-4.71943	-3.29391
H	-4.56745	-3.79821	-4.80436
H	-3.47268	6.93305	-0.63088
H	-3.26886	6.32695	1.03051
H	-3.60515	-2.38725	5.90332
H	-3.83855	-0.68395	5.43113
H	-6.54706	-3.08519	0.93636
H	-5.43426	-4.88502	2.27834
H	-3.99934	-4.21089	4.22055
H	-7.03082	2.32306	-0.69976
H	-7.19411	4.45203	-2.02728
H	-5.39386	6.17682	-1.74505
H	-7.33406	0.11431	-1.50608
H	-8.28631	-1.18594	-3.43607
H	-6.87781	-2.96657	-4.49492
H	-6.98719	0.23493	2.11022
H	-7.23574	-0.89067	0.77799
H	-5.60266	1.86280	2.07585
H	-4.02790	1.52108	1.39324
H	-4.19021	0.58553	-0.91820
H	-4.07949	-0.85877	0.07320
C	-0.25971	0.22487	-0.00257
Br	-0.91973	-1.58443	0.37567
Br	-0.87215	1.45113	1.39504
Br	1.70336	0.20248	-0.05964
Br	-0.95789	0.82052	-1.74060

Frequencies

9.8490	11.0062	13.8019
15.6830	20.0361	20.7707
22.0295	24.8161	26.5999
27.4189	31.6701	35.1793
36.5712	39.7877	41.1675
48.0240	51.0130	52.9079
61.9891	65.4993	69.9580
83.6510	89.4752	99.2182
101.2073	111.2243	117.9368
120.7742	125.6142	126.4247
127.1240	131.1925	140.2926
141.1837	149.8042	151.5269
159.9547	162.0547	169.0455
170.3572	176.5023	178.0609
180.9921	181.0714	181.7824
182.1896	182.8983	189.5232
202.0531	207.2636	220.1689
227.2071	229.6280	234.2283
236.9127	240.2860	242.4697
244.9119	246.9431	257.4553
260.0346	262.5314	263.0405
265.9991	273.0098	286.0171
293.1951	296.9368	300.1501
303.7896	306.1915	317.6799
326.1900	327.2450	344.7400
345.7584	349.1702	369.0485
371.4708	376.4391	385.4428
392.8976	394.3672	398.5175
400.5848	404.2139	406.3761
420.1504	428.4572	429.1704

433.6036 435.8262 438.8545
448.7353 462.9579 470.7114
475.5761 482.3383 484.5007
484.7753 493.2689 498.7076
502.3545 506.3822 527.2926
531.5180 539.7219 547.1738
548.2808 549.9177 567.8256
572.0429 574.7705 576.9710
577.9877 579.4612 581.6528
594.3060 594.7332 605.3575
606.7324 607.7885 609.4917
620.0525 621.6792 623.4142
626.1037 629.8077 632.5731
649.9115 652.5133 653.2098
656.9519 658.3268 660.0604
662.7120 667.0103 702.4965
714.2987 716.0028 718.2914
721.2769 724.4656 726.9735
730.4824 737.2662 739.4320
740.8941 741.8843 744.0029
748.0802 753.3241 755.9103
762.9324 766.9782 767.8013
769.7534 771.2105 771.8127
773.1417 779.4221 780.7063
784.1890 784.8117 787.4770
791.4269 803.0742 805.6969
813.6050 817.9250 821.4685
825.7825 831.5242 836.7299
839.9190 843.5747 858.4366
867.8698 869.3273 869.9798
877.1781 888.2039 888.8604
894.8496 897.0096 897.7822
900.2330 909.2224 911.7129
914.2967 917.4594 919.9412
920.6560 930.3544 934.0649
935.5216 936.7230 936.8468
941.0375 941.5113 941.9561
946.4414 956.1628 960.4935
961.9121 964.2876 966.2929
966.8292 969.2341 970.1707
986.1894 989.7726 1002.0022
1004.2782 1006.4416 1009.6326
1009.9517 1010.5833 1011.6381
1012.9383 1014.7229 1015.1148
1015.5327 1017.2564 1027.3548
1039.7215 1044.1738 1046.2077
1066.5470 1075.0759 1077.3846
1078.4033 1099.7619 1105.5001
1107.5025 1108.0029 1111.9009
1117.1640 1120.0214 1129.2406
1137.0471 1145.6902 1150.9795
1153.2562 1154.7276 1166.0180
1166.5189 1169.2976 1177.0198
1178.0450 1178.3273 1179.4045
1179.6388 1180.4439 1183.9911
1186.9365 1190.4806 1191.9641
1192.3808 1194.1234 1225.3015
1230.9049 1231.7370 1231.9997
1236.2046 1236.9789 1245.2517
1247.7986 1249.2382 1250.3812
1253.5283 1253.9691 1254.2717
1260.1938 1265.3948 1269.7198
1272.6346 1274.5057 1277.5434
1277.6677 1278.7986 1289.4577
1291.1688 1292.0656 1297.6850
1298.5098 1299.6928 1301.1232
1310.0818 1315.3142 1318.2674
1319.0584 1320.5331 1321.7521
1325.7721 1338.9461 1339.1875
1340.8255 1341.4140 1345.7127
1345.9704 1351.3842 1359.1595
1364.6995 1368.8433 1372.8435
1376.9942 1377.9248 1383.0752
1391.4271 1397.6235 1400.5619
1411.4765 1413.0889 1413.4695
1414.3411 1415.2913 1417.9861
1421.6767 1424.7238 1450.9943
1451.5110 1470.4470 1471.5982
1473.1417 1474.4852 1475.0565
1476.0653 1476.4494 1476.8757
1479.6260 1483.1212 1484.0471
1484.9053 1485.1916 1486.7734
1491.0835 1493.1130 1494.1713
1496.6231 1499.7531 1500.6028
1501.7883 1502.2667 1505.4774
1512.4168 1521.2226 1521.5916
1522.4344 1534.8411 1535.8932
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1628.7876 1629.3212 1632.2226
1636.4398 1637.0608 1639.2177
1648.9733 1649.4793 1650.1480
1675.1671 1675.5383 1677.2745
1677.9255 1679.0323 1679.8719
1768.5372 1772.0038 1772.2998
1819.8305 1820.4681 1822.1255
3011.5079 3017.0838 3017.7154
3019.0657 3036.7633 3041.1209
3058.4378 3058.5504 3058.7691
3065.1574 3065.1699 3065.6556
3065.8351 3069.6011 3074.8640
3076.4475 3080.1420 3080.4221
3080.7844 3082.6217 3097.7689
3104.1809 3104.4630 3104.7418
3108.4366 3125.8410 3126.2280
3126.9889 3127.3765 3151.2356
3174.2770 3174.8274 3175.0352
3182.6807 3183.0014 3184.1887
3184.3910 3188.3961 3192.3986

3200.1537	3200.4245	3200.8143
3201.9453	3203.2968	3203.4419
3204.5163	3208.2443	3210.8637
3226.8261	3235.0424	3240.5284

TS8⊂CBr_4

E(RB3LYP) = -14058.1711301

E(RB3LYP-D3) = -14058.4068412

H - Sum of electronic and thermal Enthalpies= -14056.992466

G - Sum of electronic and thermal Free Energies= -14057.175498

Number of imaginary frequencies: 0

Cartesian Coordinates

C	-5.80582	-1.14257	0.73111
C	-5.81490	-1.08065	-0.67516
C	-5.72649	0.16252	-1.33628
C	-5.70628	1.35063	-0.57918
C	-5.69592	1.29875	0.83131
C	-5.74272	0.05025	1.48187
C	-5.86179	-2.50358	1.42784
C	-5.70268	-2.43105	2.96373
C	-6.56103	-1.25121	3.47191
C	-5.68951	-0.05821	3.01289
C	-5.64359	2.58579	1.65809
C	-5.56736	3.88089	0.81384
C	-5.69452	2.72843	-1.25642
C	-5.64927	0.22743	-2.86356
C	-5.60037	-1.15800	-3.55259
C	-5.87919	-2.35697	-1.52520
C	-6.63382	-2.06122	-2.84248
C	-6.51816	3.71514	-0.39301
C	-2.03638	-2.73979	-3.44669
C	-3.11254	-1.94002	-3.93740
C	-4.30622	-1.90289	-3.25693
C	-4.48438	-2.65733	-2.06047
C	-3.48172	-3.45526	-1.56947
C	-2.23036	-3.51751	-2.24700
C	-2.01942	3.97541	-1.63387
C	-1.92637	4.62838	-0.35055
C	-3.06730	4.64009	0.50620
C	-4.22567	4.01474	0.11296
C	-4.30640	3.35011	-1.14530
C	-3.23877	3.33923	-2.00782
C	-1.96365	-0.57700	4.04667
C	-1.95262	-2.01529	3.92778
C	-3.16148	-2.69254	3.58884
C	-4.30612	-1.97175	3.34824
C	-4.30220	-0.54810	3.41943
C	-3.16708	0.13749	3.77577
C	-0.76929	0.10927	4.41349
C	0.37670	-0.61880	4.60098
C	0.39852	-2.02414	4.44312
C	-0.73615	-2.73077	4.13419
C	-0.77353	-2.77445	-4.10974
C	0.23262	-3.53773	-3.57303
C	0.03600	-4.30409	-2.40016
C	-1.16501	-4.31719	-1.74149
C	-0.69636	5.23253	0.04542
C	0.37790	5.15782	-0.80447
C	0.28061	4.52771	-2.06728
C	-0.88584	3.95089	-2.49709
C	1.61478	4.59933	-2.72353
O	1.95732	4.19704	-3.82190
N	2.45489	5.25399	-1.80983
C	1.78154	5.63106	-0.63246
O	2.28112	6.23062	0.30181
C	1.64457	-3.72944	-4.01285
O	2.22309	-3.26452	-4.97914
C	1.31285	-4.99818	-2.07722
O	1.55838	-5.77111	-1.16912
C	1.74811	-0.17377	4.97190
O	2.13586	0.93903	5.28370
C	1.79625	-2.48982	4.66253
O	2.24129	-3.62231	4.64354
N	2.55077	-1.32595	4.92552
N	2.22098	-4.60128	-3.07421
C	3.88053	5.44205	-2.02705
C	3.60756	-5.02366	-3.10826
C	3.95754	-1.36953	5.31944
C	6.61019	1.20161	3.21379
C	6.28526	1.52654	4.53016
C	5.39780	0.70497	5.21849
C	4.86676	-0.41326	4.56249
N	5.17266	-0.72348	3.29400
C	6.02980	0.06979	2.62497
C	6.38618	-2.11725	-1.70526
C	6.79670	-3.00529	-2.70038
C	5.89018	-3.94348	-3.18795
C	4.60055	-3.96502	-2.64215
N	4.20576	-3.11806	-1.68711
C	5.07387	-2.19919	-1.22666
C	6.04203	1.77137	-1.98124
C	6.31471	2.68386	-3.00085
C	5.61270	3.88782	-3.04205
C	4.66058	4.13396	-2.04650
N	4.40237	3.26407	-1.06399
C	5.07420	2.10087	-1.02726
C	4.70150	1.19047	0.14016
C	4.51997	-1.27872	-0.14208
C	6.38558	-0.30749	1.18899
N	5.34680	-0.11673	0.17314
H	-6.82626	-2.98546	1.20766
H	-5.08899	-3.16489	1.01851
H	-5.96886	-3.39728	3.40598
H	-6.64600	-1.26500	4.56491
H	-7.56820	-1.23470	3.04019

H	-6.54327	2.64680	2.28788
H	-6.31500	-3.18624	-0.96572
H	-6.52644	0.76363	-3.25465
H	-4.77282	0.81508	-3.16437
H	-7.59840	-1.56662	-2.68090
H	-6.80217	-2.98881	-3.40202
H	-4.78996	2.55403	2.34696
H	-5.80058	4.74329	1.44780
H	-7.50256	3.32076	-0.11662
H	-6.65420	4.66554	-0.92232
H	-2.96588	-1.37084	-4.85372
H	-3.61356	-4.04294	-0.66374
H	-5.78020	-1.03621	-4.62629
H	-2.99864	5.15318	1.46393
H	-3.29392	2.84516	-2.97541
H	-6.05244	2.66612	-2.28541
H	-3.15412	-3.77950	3.52827
H	-3.15700	1.22291	3.84769
H	-5.97061	0.88087	3.49155
H	-0.71210	-3.81256	4.02880
H	-0.77086	1.19059	4.52210
H	-1.30269	-4.90579	-0.83811
H	-0.61300	-2.18917	-5.01169
H	-0.94508	3.45999	-3.46493
H	-0.61274	5.72014	1.01354
H	4.22819	6.07560	-1.20448
H	4.02978	5.97942	-2.96901
H	3.85286	-5.33506	-4.12842
H	3.67400	-5.89967	-2.45327
H	4.02698	-1.16005	6.39355
H	4.27879	-2.39979	5.14554
H	7.30404	1.81455	2.64448
H	6.71136	2.40537	5.00713
H	5.10295	0.92890	6.23864
H	7.06125	-1.36548	-1.31278
H	7.80782	-2.95816	-3.09770
H	6.16819	-4.63639	-3.97757
H	6.54608	0.81414	-1.92239
H	7.05370	2.45206	-3.76406
H	5.77949	4.60903	-3.83711
H	6.67622	-1.36292	1.17225
H	7.27614	0.27254	0.90399
H	4.32117	-1.88704	0.75377
H	3.54174	-0.93681	-0.49063
H	3.61064	1.08124	0.12966
H	4.91475	1.74887	1.06160
C	0.00091	0.09496	-0.14918
Br	0.59618	-1.61308	0.60426
Br	0.60700	1.56562	1.00278
Br	-1.95554	0.11500	-0.26510
Br	0.77524	0.32160	-1.94066

Frequencies

-29.7629	11.3004	14.9816
16.3290	18.4610	20.0436
21.7569	23.0911	25.6879
26.0180	30.2616	32.2363
36.1295	38.5465	44.0312
45.3012	48.1996	50.5334
51.7942	63.1520	65.4755
68.0496	89.5315	98.8039
102.1370	113.5594	116.7363
119.5191	121.6100	125.7534
126.3296	134.3436	140.7745
141.3967	150.2333	151.6258
155.0672	159.3663	160.8802
163.5807	174.2605	178.4821
180.3577	181.0908	181.4474
181.6314	182.9100	183.9865
194.4997	203.1937	210.6312
224.0453	225.7966	230.2605
236.7892	238.6062	242.6673
246.2325	248.0884	255.1129
260.3818	261.6419	262.2575
270.5226	272.7086	286.2296
290.6439	299.7719	301.2536
306.7221	309.1505	318.2216
328.5664	331.1915	343.5530
346.3154	348.3604	358.0341
370.8461	372.2452	385.4660
388.1587	395.5469	399.9735
401.5850	404.8817	406.8663
419.6939	427.6492	428.6199
432.8234	436.4016	437.0577
459.3024	466.5855	470.7542
481.9460	484.0890	484.4799
486.3567	493.1788	499.9084
501.8919	505.5737	528.7033
530.4729	533.7969	538.5521
548.5261	550.6839	568.2296
571.5404	574.3713	576.8186
578.8010	578.9934	580.6637
593.9372	595.4127	603.8730
606.7034	607.3109	609.9220
617.9634	621.1356	623.4672
624.6423	629.4968	631.5960
644.2190	650.4524	652.7396
654.8661	658.0071	660.4583
661.1221	662.5042	700.2771
714.0607	714.8649	717.2907
720.7092	723.7149	725.0746
729.5440	734.6869	739.3790
740.3336	742.2774	743.2403
746.6422	748.6868	752.3662
762.8936	766.2887	768.0102
768.1392	769.3591	771.9629
772.4774	779.3487	779.8809
785.3640	786.7495	786.9806

795.9250	803.1792	805.2756
807.0378	814.0973	822.5769
825.7710	827.3795	835.7281
840.5878	842.6420	850.7696
862.6740	869.2223	869.5722
877.2178	888.7285	888.9833
895.0106	897.2406	897.9443
900.4653	904.6605	909.7163
911.4475	915.3786	919.4134
919.9675	930.8189	936.5986
937.0542	937.5423	940.5832
941.3347	941.6218	942.7804
952.0137	953.9103	960.1056
961.3456	963.8461	966.8784
967.0312	970.5836	973.6655
986.3948	988.6423	994.0941
1003.3306	1003.8965	1005.7732
1007.0719	1010.3713	1012.8138
1013.4772	1014.0005	1015.1906
1015.6824	1019.0091	1024.9691
1039.7263	1044.0517	1045.3254
1066.3945	1075.2389	1077.6126
1078.6526	1104.8106	1106.9814
1107.2165	1109.9689	1113.7520
1116.5324	1120.1904	1129.5312
1140.8394	1146.8625	1150.2580
1154.4237	1165.0127	1166.1348
1166.6428	1176.2525	1177.6721
1178.0613	1178.5210	1179.1248
1180.0710	1180.5345	1182.9728
1187.2909	1190.2773	1191.6134
1192.3390	1193.0307	1228.9400
1230.2053	1231.0739	1232.6593
1233.5067	1237.1210	1240.8426
1245.5720	1249.8428	1250.4620
1253.7055	1254.1087	1254.2601
1259.5643	1263.5984	1267.4496
1270.2192	1274.2671	1277.8184
1278.0570	1278.1435	1290.3609
1291.3004	1298.6415	1298.9009
1300.2564	1300.9603	1312.9805
1315.2604	1315.5029	1318.1459
1319.0303	1320.6924	1325.7637
1338.9892	1339.2247	1340.8449
1341.1466	1343.4193	1345.3037
1346.2773	1349.5668	1361.2805
1365.0546	1377.1463	1377.4889
1378.3559	1380.0289	1385.2473
1394.0692	1395.6821	1400.7590
1404.5456	1410.2545	1413.8897
1414.1081	1415.0511	1418.3010
1423.3724	1425.6316	1450.4169
1450.9152	1469.1887	1470.2521
1473.4102	1474.4522	1474.7258
1474.9548	1475.5578	1476.1117
1476.4171	1478.7063	1482.8152
1484.3453	1484.8784	1485.4662
1489.5665	1490.9589	1494.5053
1497.4374	1499.6836	1501.3542
1501.9963	1502.6332	1504.8130
1512.3162	1521.2298	1521.4543
1522.2780	1535.2155	1535.5120
1535.8626	1603.8945	1604.4588
1628.3657	1628.8873	1631.3835
1637.3846	1637.5466	1640.7675
1649.2080	1649.3282	1649.7714
1674.6925	1676.4989	1676.5986
1677.9257	1679.1466	1679.2078
1769.9851	1772.5008	1773.6996
1819.8446	1821.0663	1822.8471
3010.4466	3016.5853	3017.3902
3019.1891	3019.4585	3039.5652
3058.2697	3058.6206	3058.7201
3061.7423	3063.8372	3066.0507
3071.8996	3073.9085	3075.4294
3079.8904	3080.3583	3080.5933
3080.7022	3097.7351	3104.1072
3104.2896	3104.8208	3115.2865
3117.7249	3121.2812	3126.1766
3127.2793	3130.9924	3132.4499
3174.5083	3174.6865	3175.1314
3183.0753	3183.4124	3183.5966
3185.1171	3187.6594	3188.7238
3200.0252	3200.6436	3200.8819
3202.5861	3202.6869	3203.5973
3203.9859	3204.7166	3206.6827
3219.8974	3230.0948	3242.4422

I8⊂CBr$_4$

E(RB3LYP) = -14058.1724605

E(RB3LYP-D3) = -14058.4073417

H - Sum of electronic and thermal Enthalpies= -14056.992764

G - Sum of electronic and thermal Free Energies= -14057.178098

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.94302	-1.46136	-0.09032
C	5.93755	-0.82278	1.16398
C	5.88565	0.58361	1.24968
C	5.90896	1.35108	0.06907
C	5.88769	0.72059	-1.19330
C	5.90824	-0.68589	-1.26833
C	5.98008	-2.98929	-0.16006
C	5.82352	-3.55662	-1.58908
C	6.70104	-2.70746	-2.53551
C	5.85087	-1.41757	-2.61752

C	5.84102	1.55160	-2.47781
C	5.77830	3.07958	-2.24054
C	5.93621	2.88521	0.11872
C	5.78398	1.27766	2.60992
C	5.63614	0.30385	3.80410
C	5.91913	-1.63412	2.46610
C	6.64304	-0.84719	3.58270
C	6.75052	3.41395	-1.08649
C	1.99280	-1.04926	4.15605
C	3.09460	-0.15864	4.33619
C	4.31330	-0.44953	3.77005
C	4.49174	-1.63612	2.99989
C	3.46204	-2.52451	2.81753
C	2.18561	-2.25612	3.38912
C	2.28351	4.23745	0.00604
C	2.16119	4.28365	-1.43082
C	3.28318	3.92039	-2.23476
C	4.44899	3.50586	-1.63729
C	4.55328	3.42938	-0.21746
C	3.50756	3.80099	0.58973
C	2.11153	-2.25408	-3.35401
C	2.07583	-3.50938	-2.64268
C	3.27510	-4.00664	-2.05185
C	4.43402	-3.27394	-2.13451
C	4.45416	-2.00879	-2.79113
C	3.32914	-1.51402	-3.40384
C	0.92761	-1.76417	-3.97883
C	-0.23151	-2.48409	-3.84726
C	-0.27692	-3.69109	-3.11203
C	0.84602	-4.22229	-2.53052
C	0.70909	-0.76898	4.71320
C	-0.31554	-1.65445	4.48941
C	-0.11976	-2.83735	3.73859
C	1.09801	-3.15598	3.19902
C	0.92076	4.66961	-2.01978
C	-0.13389	4.97084	-1.19568
C	-0.00449	4.94212	0.21256
C	1.17261	4.59613	0.82210
C	-1.32411	5.28814	0.80555
O	-1.63430	5.40813	1.97899
N	-2.19571	5.46770	-0.27849
C	-1.54531	5.32559	-1.52164
O	-2.06599	5.48240	-2.60996
C	-1.74199	-1.62162	4.92558
O	-2.32139	-0.80036	5.61380
C	-1.41230	-3.57164	3.67927
O	-1.66420	-4.64172	3.15487
C	-1.59534	-2.21749	-4.38197
O	-1.96082	-1.33865	-5.14370
C	-1.68175	-4.18363	-3.12280
O	-2.14415	-5.19758	-2.63413
N	-2.41893	-3.22636	-3.85436
N	-2.32842	-2.78477	4.39744
C	-3.61772	5.75742	-0.12420
C	-3.70604	-3.17318	4.61967
C	-3.81903	-3.43546	-4.22284
C	-6.56140	-0.25119	-3.59227
C	-6.09728	-0.47221	-4.88682
C	-5.16979	-1.48871	-5.09624
C	-4.74165	-2.24683	-3.99979
N	-5.17549	-2.02419	-2.74852
C	-6.06963	-1.03940	-2.54105
C	-6.62798	-1.19713	2.23453
C	-7.01736	-1.74947	3.45590
C	-6.06013	-2.37027	4.25205
C	-4.74099	-2.43117	3.78126
N	-4.36507	-1.91018	2.61064
C	-5.28647	-1.28997	1.84878
C	-5.80910	2.45454	1.43461
C	-5.67719	3.58946	2.23375
C	-4.96115	4.68375	1.74857
C	-4.39852	4.59454	0.47107
N	-4.51397	3.50112	-0.29466
C	-5.20695	2.44929	0.17042
C	-5.34537	1.29282	-0.81074
C	-4.76175	-0.68032	0.55221
C	-6.58683	-0.81620	-1.12160
N	-5.78096	0.02906	-0.22419
H	6.93703	-3.34782	0.24846
H	5.19706	-3.41356	0.47904
H	6.07209	-4.62351	-1.59017
H	6.78439	-3.17469	-3.52386
H	7.70887	-2.52958	-2.14356
H	6.73670	1.34131	-3.08060
H	6.32944	-2.63461	2.32056
H	6.68345	1.88681	2.78407
H	4.93837	1.97626	2.60369
H	7.63720	-0.49641	3.28308
H	6.74369	-1.46662	4.48164
H	4.98272	1.24541	-3.08929
H	6.00304	3.60299	-3.17626
H	7.72622	2.92577	-1.18962
H	6.90434	4.49588	-0.99881
H	2.94763	0.74172	4.93029
H	3.59174	-3.43599	2.23844
H	5.78583	0.85143	4.74099
H	3.19364	3.98263	-3.31794
H	3.58417	3.76403	1.67417
H	6.31702	3.24277	1.07706
H	3.24895	-4.96887	-1.54325
H	3.33807	-0.55786	-3.92270
H	6.14740	-0.76581	-3.44058
H	0.80307	-5.15847	-1.97954
H	0.94726	-0.82890	-4.53200
H	1.23479	-4.06717	2.62240
H	0.55046	0.13707	5.29263
H	1.25532	4.56419	1.90536
H	0.81274	4.69542	-3.10119

H	-3.98991	5.98188	-1.12733
H	-3.72607	6.64548	0.50657
H	-3.93638	-3.03684	5.68145
H	-3.75868	-4.24403	4.39207
H	-3.85990	-3.72734	-5.27936
H	-4.15771	-4.27938	-3.61693
H	-7.30407	0.51720	-3.39509
H	-6.45523	0.13189	-5.71648
H	-4.77340	-1.69100	-6.08579
H	-7.33822	-0.68753	1.59329
H	-8.05187	-1.68541	3.78483
H	-6.32163	-2.79536	5.21766
H	-6.35848	1.58415	1.77344
H	-6.12056	3.61777	3.22602
H	-4.81680	5.57493	2.35145
H	-6.70582	-1.79187	-0.64114
H	-7.58630	-0.36504	-1.19892
H	-4.26617	-1.46948	-0.03279
H	-3.97354	0.02896	0.82695
H	-4.39908	1.21040	-1.36974
H	-6.09802	1.59807	-1.54828
C	-0.33430	0.21629	-0.04944
Br	-0.91797	-1.64631	0.09846
Br	-1.01974	1.23911	1.48127
Br	1.62850	0.29116	-0.06038
Br	-1.03282	0.99169	-1.71229

Frequencies

11.4878	13.7215	14.3605
17.3877	18.8097	21.5261
23.3623	23.9903	26.5172
29.7295	31.5733	34.9305
39.8311	42.6804	44.3675
47.5156	49.1183	52.7088
58.6605	62.1722	66.9178
74.5532	97.3348	98.4218
104.1113	112.8721	116.8058
120.5479	121.9873	125.7174
126.1901	136.0899	139.8653
140.8283	149.8776	151.0159
158.8972	161.2417	166.1840
170.7350	175.8064	180.7777
181.2385	181.6639	182.1046
183.6871	184.2911	186.2114
198.7620	200.9619	211.2002
222.8517	225.0487	229.5863
237.2450	238.5521	241.1058
245.1541	245.7468	257.1016
260.0652	261.4652	262.3941
268.3973	271.4057	284.1978
287.3056	298.0450	298.7290
304.6805	305.4142	317.6804
321.1980	327.4786	341.7369
346.1531	347.9715	370.1015
371.0790	379.6152	385.5125
392.2702	395.2301	399.6079
403.2830	406.0085	407.4308
419.8934	425.2334	427.5358
428.6234	436.7264	437.4955
447.0089	461.0954	469.7479
477.6706	483.5917	484.0271
484.7472	487.0370	498.2317
501.9389	504.3762	530.0132
533.0522	538.9847	542.0613
548.5788	550.8064	567.7938
572.2462	575.0908	576.1854
578.1543	579.1432	581.4075
593.4694	595.5103	601.0816
606.6854	607.9622	608.7651
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627.7021	629.5445	633.6928
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655.4503	658.9881	660.4786
660.9464	665.0095	703.1714
714.6580	715.3492	718.2964
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730.9896	735.6020	739.8753
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747.2957	750.6065	757.0129
762.9024	767.3767	768.0806
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776.0866	779.6786	780.4839
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813.5807	819.1856	822.2807
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840.5334	843.1116	856.4508
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877.0379	888.3007	888.9207
894.9561	897.2740	897.7050
900.0973	910.1821	912.1628
916.7311	918.8407	919.7927
921.7475	929.6093	936.2612
936.7142	937.6484	939.4809
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946.5701	952.8920	959.8003
961.1551	963.8082	966.1482
966.6508	969.8801	970.8927
988.0372	989.3694	997.1187
1006.2774	1006.6809	1009.2121
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1016.1828	1019.5583	1027.8680
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1066.5091	1075.2232	1077.5678
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1107.5628	1109.4949	1115.0153
1118.5078	1121.0530	1129.0834

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1154.6288	1154.9763	1166.2428
1166.8888	1170.0208	1177.4665
1177.7698	1178.0868	1179.5063
1180.0751	1180.3564	1185.5703
1187.6395	1190.5927	1191.6432
1192.1305	1193.8182	1225.4773
1230.3108	1231.6195	1232.0231
1236.8267	1242.3747	1242.7656
1245.4010	1249.2240	1250.2807
1253.8269	1254.1699	1254.2956
1259.7378	1260.2382	1269.6691
1275.3431	1275.7519	1277.8982
1278.3171	1278.5319	1289.9161
1290.9390	1297.5568	1298.2218
1300.3274	1301.3177	1303.8737
1313.6290	1315.3101	1318.3696
1319.0947	1320.8801	1321.9908
1325.9471	1338.8040	1339.6886
1340.7798	1341.9031	1345.4430
1346.3160	1351.7811	1364.2367
1365.1606	1374.5510	1377.0145
1377.5514	1379.0169	1381.8544
1387.7484	1400.5876	1400.7268
1404.6013	1408.6397	1413.8432
1414.3550	1414.9812	1419.5505
1422.3932	1426.0810	1451.0548
1451.8134	1469.5010	1472.9617
1473.5049	1474.6058	1475.0195
1475.4036	1475.7490	1476.3519
1477.1022	1479.8454	1484.5395
1484.8989	1484.9883	1487.6796
1489.7130	1491.4471	1494.0719
1497.4858	1500.6991	1501.9997
1502.4053	1504.0341	1505.7467
1510.0352	1521.2198	1521.4058
1522.1809	1535.0948	1535.7831
1536.0907	1604.8510	1605.5329
1628.5353	1629.1578	1632.6971
1636.3120	1637.5300	1639.8086
1649.0047	1649.7532	1650.2490
1675.1097	1676.3057	1676.9937
1678.1994	1679.3315	1679.6181
1769.0941	1771.3404	1773.4388
1819.7045	1820.3950	1822.6190
3000.4073	3015.7660	3017.5828
3019.3804	3023.0311	3027.8185
3058.1516	3058.3958	3058.5058
3058.8574	3063.2806	3067.8664
3068.8515	3069.8725	3075.3345
3080.3991	3080.5130	3080.6960
3081.0175	3094.2518	3103.9175
3104.1498	3105.0055	3111.0861
3112.0644	3123.3205	3127.5650
3130.3828	3136.0695	3137.1410
3174.5199	3174.8364	3174.9236
3182.7330	3183.5620	3183.7679
3185.0258	3188.7186	3191.9554
3200.5779	3200.7496	3201.2039
3201.3282	3202.6768	3203.3912
3204.1143	3204.6003	3215.7899
3222.4301	3229.4233	3240.2792

TS9⊂CBr_4

E(RB3LYP) = -14058.1697900

E(RB3LYP-D3) = -14058.4040945

H - Sum of electronic and thermal Enthalpies= -14056.991227

G - Sum of electronic and thermal Free Energies= -14057.174142

Number of imaginary frequencies: 0

Cartesian Coordinates

C	5.76272	0.65099	1.31451
C	5.77329	1.40743	0.12719
C	5.75992	0.76579	-1.12952
C	5.79304	-0.64109	-1.19124
C	5.79115	-1.40804	-0.00641
C	5.77569	-0.75787	1.24249
C	5.74364	1.36376	2.66887
C	5.62069	0.41286	3.88325
C	6.54940	-0.79592	3.63313
C	5.73491	-1.55067	2.55558
C	5.81943	-2.93733	-0.06577
C	5.76847	-3.51719	-1.49928
C	5.81451	-1.38258	-2.53527
C	5.71700	1.58522	-2.42184
C	5.62363	3.11440	-2.20036
C	5.77076	2.94138	0.16104
C	6.58098	3.47784	-1.04329
C	6.68582	-2.65415	-2.39399
C	1.98282	4.26839	-1.42569
C	3.11714	3.91959	-2.21837
C	4.28278	3.52098	-1.60961
C	4.37548	3.44784	-0.18910
C	3.31066	3.78792	0.60758
C	2.08586	4.20776	0.01224
C	2.15156	-2.30505	-3.50658
C	2.10955	-3.57745	-2.82726
C	3.27806	-4.04486	-2.15612
C	4.41409	-3.27273	-2.14190
C	4.44479	-2.00434	-2.79103
C	3.34916	-1.53297	-3.47094
C	2.00109	-1.91627	3.62632
C	1.92488	-0.69932	4.39827
C	3.08992	0.11263	4.53199
C	4.25983	-0.26174	3.91678
C	4.32860	-1.45582	3.14161

C	3.23261	-2.27136	3.00239
C	0.84372	-2.73706	3.48682
C	-0.32564	-2.33253	4.07674
C	-0.40336	-1.13428	4.82533
C	0.68985	-0.32574	5.00531
C	0.75320	4.67015	-2.02692
C	-0.30895	4.97644	-1.21443
C	-0.20327	4.92246	0.19549
C	0.96186	4.55578	0.81644
C	0.90036	-4.33348	-2.81926
C	-0.20284	-3.81646	-3.44886
C	-0.15574	-2.57649	-4.12838
C	0.98896	-1.82450	-4.17663
C	-1.50991	-2.30258	-4.68321
O	-1.89168	-1.36402	-5.36055
N	-2.31279	-3.38020	-4.27818
C	-1.59322	-4.34417	-3.54696
O	-2.05219	-5.38571	-3.11505
C	-1.69934	5.39287	-1.55451
O	-2.20755	5.56972	-2.64764
C	-1.51878	5.31037	0.77513
O	-1.84418	5.41702	1.94375
C	-1.66860	-2.97609	4.09505
O	-2.02258	-4.04203	3.62193
C	-1.79977	-0.98983	5.32265
O	-2.27696	-0.12702	6.03618
N	-2.49937	-2.10516	4.81865
N	-2.35245	5.57681	-0.32446
C	-3.73351	-3.48135	-4.57309
C	-3.74445	5.95100	-0.20023
C	-3.87292	-2.41658	5.17886
C	-6.84404	-2.29578	2.14449
C	-6.74687	-3.44446	2.92583
C	-5.73867	-3.51684	3.88586
C	-4.87031	-2.42909	4.03018
N	-4.93957	-1.33786	3.25315
C	-5.90494	-1.26708	2.32077
C	-6.49205	2.69695	-0.36588
C	-6.98099	3.99668	-0.51534
C	-6.08885	5.06410	-0.48249
C	-4.72792	4.78691	-0.28936
N	-4.25781	3.54728	-0.14322
C	-5.11815	2.51199	-0.18667
C	-6.10906	-0.53371	-2.62661
C	-6.27666	-0.71516	-3.99816
C	-5.49594	-1.66432	-4.65685
C	-4.57404	-2.40146	-3.90673
N	-4.40507	-2.22463	-2.58984
C	-5.15623	-1.30993	-1.95460
C	-4.94500	-1.22097	-0.44650
C	-4.47549	1.13842	-0.06263
C	-6.00295	0.01426	1.50833
N	-5.40773	0.03254	0.14560
H	6.67093	1.94427	2.78614
H	4.92252	2.09034	2.69709
H	5.84513	0.96355	4.80323
H	6.65179	-1.40952	4.53596
H	7.54866	-0.50768	3.28752
H	6.74081	-3.29954	0.41396
H	6.13623	3.31869	1.11736
H	6.62528	1.38679	-3.00968
H	4.87364	1.25701	-3.04240
H	7.56743	3.00947	-1.13640
H	6.71164	4.56341	-0.96330
H	4.98786	-3.35128	0.51797
H	6.04163	-4.57776	-1.47455
H	7.66378	-2.45256	-1.94238
H	6.83902	-3.12435	-3.37249
H	3.03885	3.98476	-3.30225
H	3.37473	3.74422	1.69263
H	5.84536	3.63229	-3.13986
H	3.24698	-5.01470	-1.66251
H	3.36450	-0.57037	-3.97747
H	6.14573	-0.73022	-3.34462
H	3.03000	1.02145	5.12831
H	3.27558	-3.18701	2.41663
H	6.07175	-2.57847	2.41400
H	0.62041	0.58957	5.58781
H	0.89201	-3.65711	2.91033
H	1.03025	4.51384	1.90037
H	0.66318	4.71751	-3.10932
H	1.00998	-0.86757	-4.69137
H	0.85478	-5.28840	-2.30159
H	-4.04176	-4.46924	-4.21584
H	-3.87536	-3.44313	-5.65821
H	-3.97006	6.68235	-0.98278
H	-3.85390	6.44249	0.77306
H	-3.88966	-3.38987	5.68125
H	-4.16871	-1.64858	5.90134
H	-7.63328	-2.19033	1.40458
H	-7.44687	-4.26566	2.79508
H	-5.62757	-4.39477	4.51542
H	-7.15360	1.83841	-0.39110
H	-8.04432	4.17152	-0.66061
H	-6.43266	6.08842	-0.60302
H	-6.68739	0.19784	-2.07476
H	-6.99800	-0.11674	-4.54932
H	-5.58093	-1.81595	-5.72902
H	-5.52667	0.79992	2.10354
H	-7.07040	0.27227	1.43344
H	-3.70987	1.19330	0.72859
H	-3.93042	0.95385	-0.99633
H	-3.88163	-1.42555	-0.24328
H	-5.49628	-2.05353	-0.00022
C	-0.02346	0.01074	-0.10418
Br	-0.69828	-1.83074	-0.05220
Br	-0.69345	0.89979	-1.72182
Br	1.93777	-0.00421	-0.12979

Br	-0.64851	0.97814	1.48327

Frequencies

-43.2922	13.0285	14.9290
16.1045	17.7335	20.1207
20.5809	22.8489	26.7295
27.3624	30.4182	33.0074
35.0067	39.7596	41.0377
46.4154	47.9075	51.1014
54.0106	60.7813	65.1241
72.3155	93.6358	98.4025
103.6339	109.5725	115.8498
119.9964	121.9019	125.4977
126.4224	131.4450	139.9348
140.7958	149.5413	151.5477
159.1344	160.0462	168.0078
172.8575	174.4326	177.4781
179.9642	180.8123	181.7210
182.2505	182.4796	185.8558
194.7186	203.1166	211.3834
226.9178	228.9717	231.5552
235.8504	239.0272	242.7345
244.8283	247.6504	257.4583
260.2634	261.5661	267.1339
270.2838	272.7222	281.7976
289.9759	297.7873	298.8052
301.9038	305.0224	310.4101
317.5907	322.6361	329.5046
346.1321	346.8563	361.5726
370.5339	372.2156	374.5944
386.5100	396.2924	399.7060
400.8313	404.0597	405.1526
419.3185	419.4171	428.2674
428.7677	437.5147	438.3321
449.3587	460.4641	470.2784
477.1932	481.8322	484.0948
484.4566	485.0251	500.9915
502.6133	503.9434	528.8974
533.0938	542.8682	548.8659
549.5915	554.3825	568.7466
572.2678	573.6779	576.6869
578.0854	578.7473	580.0850
594.3934	595.6246	605.1322
607.0631	607.6918	612.1988
621.5274	624.0029	624.2562
627.4580	633.2941	633.7974
648.0865	652.3319	653.3024
654.0767	658.3268	660.0459
660.7442	663.5012	696.0575
713.9533	715.3090	718.5863
720.4446	724.1271	728.0308
734.3143	736.7966	740.3294
741.0242	743.5015	743.7003
748.4380	751.6659	755.5273
762.8309	767.6346	768.0070
769.3461	770.4533	772.4113
775.2061	779.5074	780.4735
785.8706	786.1215	786.9092
790.0279	804.8890	806.1589
811.3120	813.9165	823.9960
826.0377	827.9296	838.9031
841.1935	842.8270	843.7695
858.1473	869.0783	869.4460
876.7531	888.4172	888.6113
894.9868	897.3250	897.6448
900.2991	910.0566	912.0368
913.4671	918.3531	919.7892
920.4732	928.8667	936.6218
937.1473	937.2616	941.3966
941.5417	942.0199	943.0276
950.4212	954.6066	957.9573
961.3446	962.9539	966.5715
966.7464	970.0018	970.9185
988.2655	998.2443	1001.1765
1004.2866	1005.8989	1008.0775
1010.0334	1011.1288	1012.4684
1014.0361	1014.4221	1015.2899
1019.2278	1023.4968	1028.8214
1039.7274	1044.2561	1044.4710
1066.3330	1075.4443	1077.9475
1078.5513	1106.0106	1107.4963
1107.9211	1112.0906	1113.9507
1117.7708	1118.8530	1126.1646
1145.1641	1147.3174	1151.7497
1152.7610	1155.0677	1166.1680
1166.4984	1177.7396	1178.4448
1178.5690	1179.4433	1179.7593
1180.0580	1180.3262	1185.6361
1187.2792	1190.0376	1191.6384
1192.3093	1193.1665	1224.7046
1230.0795	1231.1974	1232.1018
1234.8821	1237.2684	1238.8440
1245.6920	1249.9878	1250.3442
1253.8850	1254.1409	1254.2831
1259.5662	1262.3989	1269.3460
1272.5775	1277.7600	1277.9527
1278.1665	1278.6191	1290.8709
1291.3256	1296.6563	1298.9233
1299.8504	1301.1977	1305.2747
1314.5274	1314.9760	1318.6760
1318.7396	1320.9348	1325.0028
1326.2301	1332.8216	1339.3373
1339.9924	1341.1434	1345.4366
1346.0873	1352.2587	1365.0688
1365.7101	1366.9897	1377.1004
1377.3482	1384.4827	1386.9323
1392.6369	1397.4305	1400.4949
1411.2057	1414.1142	1414.1593

1414.7318	1418.8976	1422.2528
1424.6715	1428.7346	1450.7956
1451.0617	1468.7998	1471.6127
1472.2574	1475.0212	1475.1812
1475.7154	1475.8574	1477.2355
1477.9619	1478.4549	1484.2912
1484.8159	1485.0848	1486.7525
1490.0694	1490.3158	1494.9659
1496.2852	1499.2535	1500.8521
1501.4506	1501.9909	1508.0252
1521.0622	1521.2155	1522.0248
1526.8326	1535.1912	1535.3724
1535.8980	1604.4871	1604.7708
1628.8048	1629.6191	1633.2513
1636.6329	1637.0121	1639.3554
1649.1731	1649.5489	1650.0880
1675.3493	1676.5368	1676.8267
1678.2142	1678.9876	1679.2602
1770.6249	1773.1386	1773.7910
1820.5827	1821.1894	1822.9681
2997.4728	3002.0953	3007.0955
3017.0928	3017.9774	3019.0679
3058.2021	3058.3976	3058.4817
3064.8426	3065.3812	3068.2086
3069.6208	3071.9256	3073.2209
3077.0183	3080.4003	3080.4971
3080.8654	3093.3735	3104.0157
3104.2074	3104.5033	3107.3553
3116.0824	3117.6484	3120.3213
3127.5080	3128.7917	3131.4767
3174.4891	3174.8105	3174.9602
3182.2918	3182.9103	3182.9555
3183.4744	3187.4916	3188.6470
3199.8151	3200.1988	3200.5801
3200.8498	3200.8927	3203.1798
3204.3787	3204.5827	3208.0860
3213.1135	3229.3980	3238.5344

B(–)⊂CBr_4

E(RB3LYP) = -14058.1824538

E(RB3LYP-D3) = -14058.4209980

H - Sum of electronic and thermal Enthalpies= -14057.002899

G - Sum of electronic and thermal Free Energies= -14057.187780

Number of imaginary frequencies: 0

Cartesian Coordinates

C	-5.62431	1.22684	-0.70950
C	-5.63045	1.22708	0.69915
C	-5.62378	0.00988	1.41378
C	-5.63353	-1.21014	0.70964
C	-5.62709	-1.22050	-0.70176
C	-5.63314	-0.00069	-1.40621
C	-5.62363	2.55536	-1.47009
C	-5.56025	2.40782	-3.00978
C	-6.48648	1.23909	-3.41309
C	-5.63293	0.03711	-2.94046
C	-5.62932	-2.54338	-1.47206
C	-5.56617	-3.80298	-0.57450
C	-5.63478	-2.55778	1.44421
C	-5.62237	0.00398	2.94452
C	-5.55609	1.41092	3.58670
C	-5.62757	2.53681	1.49918
C	-6.48100	2.34634	2.77676
C	-6.49069	-3.56685	0.64047
C	-1.90545	2.76202	3.67832
C	-3.06553	2.06156	4.12342
C	-4.20414	2.06360	3.35460
C	-4.24660	2.75942	2.11169
C	-3.15412	3.45566	1.65584
C	-1.95344	3.47524	2.42490
C	-1.96356	-3.83685	1.79402
C	-1.91710	-4.56550	0.54944
C	-3.07740	-4.59865	-0.27950
C	-4.21459	-3.93155	0.10684
C	-4.25557	-3.20346	1.33119
C	-3.16309	-3.15924	2.16216
C	-1.95966	0.36752	-4.21899
C	-1.91133	1.80960	-4.22942
C	-3.07091	2.54597	-3.84524
C	-4.20933	1.87975	-3.46102
C	-4.25237	0.45549	-3.44143
C	-3.16038	-0.28807	-3.81658
C	-0.80410	-0.37925	-4.59389
C	0.33606	0.29914	-4.93937
C	0.38466	1.71339	-4.94730
C	-0.70795	2.47229	-4.61304
C	-0.70187	2.76111	4.44377
C	0.39107	3.43004	3.95439
C	0.34249	4.13231	2.72679
C	-0.79770	4.17367	1.96663
C	-0.71460	-5.22952	0.16528
C	0.37897	-5.14134	0.98856
C	0.33205	-4.42916	2.21050
C	-0.80729	-3.79062	2.62736
C	1.67387	-4.52231	2.85105
O	2.05780	-4.06298	3.91212
N	2.45837	-5.29460	1.97891
C	1.75264	-5.69747	0.83119
O	2.20978	-6.37908	-0.06858
C	1.76538	3.57206	4.51304
O	2.22396	3.13335	5.55246
C	1.68383	4.73411	2.48574
O	2.06651	5.42350	1.55700
C	1.67723	-0.21120	-5.33970
O	2.05985	-1.36044	-5.47051
C	1.75868	2.12550	-5.35128

O	2.21713	3.24478	-5.49338
N	2.46296	0.92895	-5.57455
N	2.46974	4.36505	3.58967
C	3.86354	-5.56758	2.19432
C	3.87505	4.68818	3.71637
C	3.86792	0.87667	-5.91904
C	6.44985	0.17521	-2.59758
C	6.94900	-0.02557	-3.88516
C	6.11108	0.18483	-4.97867
C	4.79394	0.59623	-4.73810
N	4.31053	0.77958	-3.50680
C	5.11709	0.57500	-2.45002
C	6.45406	2.15629	1.45158
C	6.95519	3.37104	1.92125
C	6.11829	4.21496	2.64894
C	4.80010	3.80372	2.88396
N	4.31480	2.64649	2.42718
C	5.12034	1.83155	1.72279
C	6.44677	-2.34015	1.14495
C	6.94521	-3.35560	1.96205
C	6.10673	-4.40771	2.32554
C	4.78977	-4.40425	1.84853
N	4.30692	-3.42868	1.07482
C	5.11401	-2.41120	0.72472
C	4.49363	-1.37925	-0.19794
C	4.49667	0.51767	1.29181
C	4.49585	0.85906	-1.09562
N	4.97436	-0.00146	-0.00069
H	-6.53945	3.11224	-1.22274
H	-4.78618	3.17915	-1.13328
H	-5.82033	3.36313	-3.47851
H	-6.62864	1.20495	-4.49964
H	-7.46912	1.27965	-2.92953
H	-6.54608	-2.60637	-2.07669
H	-5.96283	3.37663	0.88904
H	-6.53879	-0.48726	3.30353
H	-4.78565	-0.60112	3.31552
H	-7.46451	1.90908	2.57043
H	-6.62129	3.30453	3.29073
H	-4.79289	-2.56477	-2.18185
H	-5.82796	-4.68628	-1.16713
H	-7.47316	-3.16708	0.36479
H	-6.63338	-4.49063	1.21339
H	-3.02821	1.53774	5.07703
H	-3.17671	3.99377	0.71068
H	-5.81582	1.33954	4.64850
H	-3.04109	-5.16220	-1.21023
H	-3.18451	-2.60972	3.10079
H	-5.96990	-2.44808	2.47652
H	-3.03315	3.63371	-3.86900
H	-3.18326	-1.37566	-3.80919
H	-5.96918	-0.91116	-3.36206
H	-0.66069	3.55840	-4.62393
H	-0.82929	-1.46574	-4.58673
H	-0.82269	4.71198	1.02283
H	-0.65469	2.22596	5.38895
H	-0.83105	-3.24235	3.56543
H	-0.66861	-5.78052	-0.77081
H	4.11271	-6.43173	1.56844
H	4.00454	-5.85002	3.24262
H	4.12516	4.58196	4.77783
H	4.01595	5.73619	3.43284
H	4.00787	0.10795	-6.68590
H	4.11806	1.84942	-6.35689
H	7.06480	0.01550	-1.71787
H	7.97680	-0.34758	-4.03379
H	6.46416	0.02608	-5.99455
H	7.06819	1.47272	0.87437
H	7.98379	3.65853	1.71758
H	6.47304	5.17351	3.01937
H	7.06227	-1.49855	0.84415
H	7.97293	-3.32404	2.31552
H	6.45934	-5.20873	2.97047
H	3.40202	0.80186	-1.21222
H	4.72529	1.89838	-0.82856
H	3.40320	0.64973	1.30043
H	4.72440	-0.23367	2.05847
H	3.39979	-1.45013	-0.08942
H	4.72201	-1.66774	-1.23178
C	-0.20863	-0.00526	0.00232
Br	0.44498	-1.55586	-1.00947
Br	0.44553	1.64451	-0.83762
Br	0.45256	-0.10466	1.84847
Br	-2.16237	-0.00569	0.00823

Frequencies

13.2810	13.6319	15.7420
17.2667	17.6100	20.6675
25.1432	25.5187	27.2759
29.8781	32.1369	32.3382
34.7300	35.0079	43.9609
48.1833	48.9439	52.8170
62.9065	63.7215	63.8837
89.4434	95.7589	95.8690
107.1644	119.4490	119.5975
123.9663	125.5154	125.6040
128.9273	129.0629	141.0943
141.5604	149.8595	153.3708
159.6136	159.8038	168.3615
173.1133	173.1992	178.8748
178.9994	180.3471	181.2174
181.2426	183.7323	191.9527
192.0507	209.0267	225.2509
225.5915	232.8588	234.7831
241.1248	241.2197	248.9689
249.0420	250.1052	259.8035
260.3540	261.2786	264.9273
270.0686	270.2273	273.1289

300.8009	301.1582	306.2970	1066.1687	1075.1645	1077.9114
312.4892	312.5867	319.9080	1077.9595	1107.3361	1107.4167
321.5686	321.8118	329.8801	1109.3059	1109.4056	1112.6222
341.3443	346.5853	347.0998	1117.3900	1117.5636	1117.5881
373.3218	373.4054	382.4422	1148.0546	1148.0963	1150.5079
388.4011	398.3753	400.4990	1152.6193	1152.6610	1155.1697
400.6336	405.1949	405.5904	1166.1102	1166.1661	1177.8813
419.0411	428.7127	428.9758	1179.3416	1179.4170	1179.6914
436.3098	436.4159	439.4845	1180.1871	1180.2617	1185.4523
459.8763	459.9752	468.8283	1185.5125	1186.7848	1191.4944
479.3134	479.3450	484.7863	1192.2429	1192.3256	1224.7818
485.2583	486.3823	502.6696	1224.8810	1228.3763	1231.6694
503.4840	503.6386	528.3004	1231.8770	1231.9358	1237.5995
532.0635	549.5901	549.6603	1245.6267	1250.2416	1250.3468
556.4762	556.5798	569.3974	1254.0818	1254.3729	1254.3965
571.7002	571.7411	576.3248	1258.3487	1269.6878	1270.8281
578.3814	578.4471	579.3631	1270.9713	1277.5109	1277.5748
595.5243	595.5948	605.8940	1277.6282	1287.9166	1288.2783
606.1764	606.2060	620.4608	1291.3025	1291.4186	1293.5478
620.5600	624.2756	629.7562	1299.4558	1299.9580	1300.4729
636.3880	646.5656	646.5950	1314.8449	1318.3109	1318.3492
651.6631	653.9964	654.0312	1320.8155	1322.9591	1325.0130
654.3274	655.5551	655.6113	1325.2629	1326.1986	1339.6954
660.3429	660.4029	660.9414	1339.8470	1340.7124	1345.4131
716.7954	716.9013	718.4689	1345.5661	1361.7932	1363.0854
721.4969	721.5245	729.4705	1363.1942	1365.5823	1377.1348
736.2194	738.2344	738.2638	1377.2688	1386.7799	1391.4126
740.2662	744.0572	744.1293	1391.4489	1400.2960	1409.7436
751.5217	753.2938	753.3731	1409.8394	1412.0717	1413.7174
762.8887	767.8201	768.0352	1413.7371	1414.6326	1417.8874
768.9310	772.5420	775.7774	1417.9131	1423.2239	1449.7990
775.7951	780.2613	780.3077	1449.9352	1469.3171	1469.3244
788.4003	788.6717	788.7437	1470.4232	1474.3030	1474.5360
797.5762	800.2119	800.2858	1474.5877	1477.4524	1477.4718
809.1306	809.1945	816.2202	1478.9637	1482.5562	1482.5725
826.5390	826.5797	827.8252	1483.7470	1484.6528	1484.7871
841.3156	841.4118	842.5624	1484.8940	1492.8334	1492.8446
869.1855	869.4337	877.3813	1496.6412	1500.6999	1501.4025
883.4955	888.7300	889.2306	1501.8914	1512.0622	1512.1295
894.8920	897.6837	898.3884	1513.4585	1520.8132	1520.9411
900.9785	911.0671	913.9139	1521.7707	1534.9078	1534.9260
913.9728	914.9678	919.6057	1535.2491	1603.0362	1603.1988
919.7675	935.9644	936.0388	1631.7059	1631.7380	1633.3838
936.8834	937.4343	937.9268	1637.1202	1637.1296	1638.2746
941.6560	941.8740	942.2514	1648.8543	1648.8953	1648.9858
957.2856	957.3573	957.7949	1675.4318	1675.5656	1675.5870
963.3265	963.3794	967.3424	1677.8686	1677.9785	1678.0327
967.5451	970.5639	975.9622	1771.2307	1773.7241	1773.7353
987.1146	1005.2704	1005.7389	1821.3773	1821.3889	1823.1479
1005.8439	1010.3736	1010.4049	3010.3881	3011.2178	3015.6353
1011.6559	1014.1588	1014.2230	3018.6474	3018.7426	3018.8583
1015.7882	1015.8550	1027.5271	3058.3325	3058.3403	3058.4500
1027.7832	1027.8239	1035.8614	3065.1554	3065.2667	3065.5451
1039.4742	1043.6901	1043.8174	3068.4850	3069.4590	3069.6063

3072.5360	3072.5618	3072.6106
3080.6515	3080.6802	3080.8322
3104.1424	3104.1547	3104.4480
3116.5884	3116.5966	3116.6963
3130.4144	3130.4567	3130.5303
3174.7241	3174.7563	3174.8262
3182.8242	3183.1110	3183.7688
3184.5745	3184.6132	3184.6703
3200.2484	3200.2678	3200.2935
3200.3077	3200.3208	3200.5189
3204.0717	3204.1432	3204.2629
3220.3306	3220.3945	3221.6497

Force field data

B(+) empty

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"C2" "ca" 0 1 131072 2 6 -0.059573
"C3" "ca" 0 1 131072 3 6 -0.037067
"C4" "ca" 0 1 131072 4 6 -0.059573
"C5" "ca" 0 1 131072 5 6 -0.037067
"C6" "ca" 0 1 131072 6 6 -0.059573
"C7" "c3" 0 1 131072 7 6 0.003613
"C8" "c3" 0 1 131072 8 6 -0.013600
"C9" "c3" 0 1 131072 9 6 -0.062368
"C10" "c3" 0 1 131072 10 6 0.012061
"C11" "c3" 0 1 131072 11 6 0.003613
"C12" "c3" 0 1 131072 12 6 -0.013600
"C13" "c3" 0 1 131072 13 6 0.012061
"C14" "c3" 0 1 131072 14 6 0.003613
"C15" "c3" 0 1 131072 15 6 -0.013600
"C16" "c3" 0 1 131072 16 6 0.012061
"C17" "c3" 0 1 131072 17 6 -0.062368
"C18" "c3" 0 1 131072 18 6 -0.062368
"C19" "ca" 0 1 131072 19 6 0.074886
"C20" "ca" 0 1 131072 20 6 -0.235654
"C21" "ca" 0 1 131072 21 6 0.029487
"C22" "ca" 0 1 131072 22 6 0.018730
"C23" "ca" 0 1 131072 23 6 -0.225410
"C24" "ca" 0 1 131072 24 6 0.068161
"C25" "ca" 0 1 131072 25 6 0.068161
"C26" "ca" 0 1 131072 26 6 0.074886
"C27" "ca" 0 1 131072 27 6 -0.235654
"C28" "ca" 0 1 131072 28 6 0.029487
"C29" "ca" 0 1 131072 29 6 0.018730
"C30" "ca" 0 1 131072 30 6 -0.225410
"C31" "ca" 0 1 131072 31 6 0.068161
"C32" "ca" 0 1 131072 32 6 0.074886
"C33" "ca" 0 1 131072 33 6 -0.235654
"C34" "ca" 0 1 131072 34 6 0.029487
"C35" "ca" 0 1 131072 35 6 0.018730
"C36" "ca" 0 1 131072 36 6 -0.225410
"C37" "ca" 0 1 131072 37 6 -0.141903
"C38" "ca" 0 1 131072 38 6 -0.028040
"C39" "ca" 0 1 131072 39 6 -0.081079
"C40" "ca" 0 1 131072 40 6 -0.152883
"C41" "ca" 0 1 131072 41 6 -0.152883
"C42" "ca" 0 1 131072 42 6 -0.081079
"C43" "ca" 0 1 131072 43 6 -0.028040
"C44" "ca" 0 1 131072 44 6 -0.141903
"C45" "ca" 0 1 131072 45 6 -0.152883
"C46" "ca" 0 1 131072 46 6 -0.081079
"C47" "ca" 0 1 131072 47 6 -0.028040
"C48" "ca" 0 1 131072 48 6 -0.141903
"C49" "c" 0 1 131072 49 6 0.373942
"O1" "o" 0 1 131072 50 8 -0.497602
"N1" "n" 0 1 131072 51 7 -0.020135
"C50" "c" 0 1 131072 52 6 0.460664
"O2" "o" 0 1 131072 53 8 -0.523258
"C51" "c" 0 1 131072 54 6 0.460664
"O3" "o" 0 1 131072 55 8 -0.523258
"C52" "c" 0 1 131072 56 6 0.373942
"O4" "o" 0 1 131072 57 8 -0.497602
"C53" "c" 0 1 131072 58 6 0.373942
"O5" "o" 0 1 131072 59 8 -0.497602
"C54" "c" 0 1 131072 60 6 0.460664
"O6" "o" 0 1 131072 61 8 -0.523258
"N2" "n" 0 1 131072 62 7 -0.020135
"N3" "n" 0 1 131072 63 7 -0.020135
"C55" "c3" 0 1 131072 64 6 -0.221365
"C56" "c3" 0 1 131072 65 6 -0.221365
"C57" "c3" 0 1 131072 66 6 -0.221365
"C58" "ca" 0 1 131072 67 6 -0.234917
"C59" "ca" 0 1 131072 68 6 -0.063399
"C60" "ca" 0 1 131072 69 6 -0.330303
"C61" "ca" 0 1 131072 70 6 0.437326
"N4" "nb" 0 1 131072 71 7 -0.373183
"C62" "ca" 0 1 131072 72 6 0.181141
"C63" "ca" 0 1 131072 73 6 -0.234917
"C64" "ca" 0 1 131072 74 6 -0.063399
"C65" "ca" 0 1 131072 75 6 -0.330303
"C66" "ca" 0 1 131072 76 6 0.437326
"N5" "nb" 0 1 131072 77 7 -0.373183
"C67" "ca" 0 1 131072 78 6 0.181141
"C68" "ca" 0 1 131072 79 6 -0.234917
"C69" "ca" 0 1 131072 80 6 -0.063399
"C70" "ca" 0 1 131072 81 6 -0.330303
"C71" "ca" 0 1 131072 82 6 0.437326
"N6" "nb" 0 1 131072 83 7 -0.373183
"C72" "ca" 0 1 131072 84 6 0.181141
"C73" "c3" 0 1 131072 85 6 -0.010570
"C74" "c3" 0 1 131072 86 6 -0.010570
"C75" "c3" 0 1 131072 87 6 -0.010570
"N7" "n3" 0 1 131072 88 7 0.007395
"H1" "hc" 0 1 131072 89 1 0.047365
"H2" "hc" 0 1 131072 90 1 0.047365
"H3" "hc" 0 1 131072 91 1 0.044432
"H4" "hc" 0 1 131072 92 1 0.036184

"H5" "hc" 0 1 131072 93 1 0.036184
"H6" "hc" 0 1 131072 94 1 0.047365
"H7" "hc" 0 1 131072 95 1 0.053935
"H8" "hc" 0 1 131072 96 1 0.047365
"H9" "hc" 0 1 131072 97 1 0.047365
"H10" "hc" 0 1 131072 98 1 0.036184
"H11" "hc" 0 1 131072 99 1 0.036184
"H12" "hc" 0 1 131072 100 1 0.047365
"H13" "hc" 0 1 131072 101 1 0.044432
"H14" "hc" 0 1 131072 102 1 0.036184
"H15" "hc" 0 1 131072 103 1 0.036184
"H16" "ha" 0 1 131072 104 1 0.153800
"H17" "ha" 0 1 131072 105 1 0.140063
"H18" "hc" 0 1 131072 106 1 0.044432
"H19" "ha" 0 1 131072 107 1 0.153800
"H20" "ha" 0 1 131072 108 1 0.140063
"H21" "hc" 0 1 131072 109 1 0.053935
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"H24" "hc" 0 1 131072 112 1 0.053935
"H25" "ha" 0 1 131072 113 1 0.173343
"H26" "ha" 0 1 131072 114 1 0.171302
"H27" "ha" 0 1 131072 115 1 0.171302
"H28" "ha" 0 1 131072 116 1 0.173343
"H29" "ha" 0 1 131072 117 1 0.171302
"H30" "ha" 0 1 131072 118 1 0.173343
"H31" "h1" 0 1 131072 119 1 0.116892
"H32" "h1" 0 1 131072 120 1 0.116892
"H33" "h1" 0 1 131072 121 1 0.116892
"H34" "h1" 0 1 131072 122 1 0.116892
"H35" "h1" 0 1 131072 123 1 0.116892
"H36" "h1" 0 1 131072 124 1 0.116892
"H37" "ha" 0 1 131072 125 1 0.120210
"H38" "ha" 0 1 131072 126 1 0.155223
"H39" "ha" 0 1 131072 127 1 0.157338
"H40" "ha" 0 1 131072 128 1 0.120210
"H41" "ha" 0 1 131072 129 1 0.155223
"H42" "ha" 0 1 131072 130 1 0.157338
"H43" "ha" 0 1 131072 131 1 0.120210
"H44" "ha" 0 1 131072 132 1 0.155223
"H45" "ha" 0 1 131072 133 1 0.157338
"H46" "h1" 0 1 131072 134 1 0.039652
"H47" "h1" 0 1 131072 135 1 0.039652
"H48" "h1" 0 1 131072 136 1 0.039652
"H49" "h1" 0 1 131072 137 1 0.039652
"H50" "h1" 0 1 131072 138 1 0.039652
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"C2" "ca" 0 1 131072 2 6 -0.069938
"C3" "ca" 0 1 131072 3 6 -0.033525
"C4" "ca" 0 1 131072 4 6 -0.069938
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"C6" "ca" 0 1 131072 6 6 -0.069938
"C7" "c3" 0 1 131072 7 6 0.021891
"C8" "c3" 0 1 131072 8 6 -0.010952
"C9" "c3" 0 1 131072 9 6 -0.060775
"C10" "c3" 0 1 131072 10 6 0.020082
"C11" "c3" 0 1 131072 11 6 0.021891
"C12" "c3" 0 1 131072 12 6 -0.010952
"C13" "c3" 0 1 131072 13 6 0.020082
"C14" "c3" 0 1 131072 14 6 0.021891
"C15" "c3" 0 1 131072 15 6 -0.010952
"C16" "c3" 0 1 131072 16 6 0.020082
"C17" "c3" 0 1 131072 17 6 -0.060775
"C18" "c3" 0 1 131072 18 6 -0.060775
"C19" "ca" 0 1 131072 19 6 0.069865
"C20" "ca" 0 1 131072 20 6 -0.248776
"C21" "ca" 0 1 131072 21 6 0.029610
"C22" "ca" 0 1 131072 22 6 0.026918
"C23" "ca" 0 1 131072 23 6 -0.243164
"C24" "ca" 0 1 131072 24 6 0.081713
"C25" "ca" 0 1 131072 25 6 0.081713
"C26" "ca" 0 1 131072 26 6 0.069865
"C27" "ca" 0 1 131072 27 6 -0.248776
"C28" "ca" 0 1 131072 28 6 0.029610
"C29" "ca" 0 1 131072 29 6 0.026918
"C30" "ca" 0 1 131072 30 6 -0.243164
"C31" "ca" 0 1 131072 31 6 0.081713
"C32" "ca" 0 1 131072 32 6 0.069865
"C33" "ca" 0 1 131072 33 6 -0.248776
"C34" "ca" 0 1 131072 34 6 0.029610
"C35" "ca" 0 1 131072 35 6 0.026918
"C36" "ca" 0 1 131072 36 6 -0.243164
"C37" "ca" 0 1 131072 37 6 -0.132455
"C38" "ca" 0 1 131072 38 6 -0.071127
"C39" "ca" 0 1 131072 39 6 -0.053021
"C40" "ca" 0 1 131072 40 6 -0.138465
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"C44" "ca" 0 1 131072 44 6 -0.132455
"C45" "ca" 0 1 131072 45 6 -0.138465
"C46" "ca" 0 1 131072 46 6 -0.053021
"C47" "ca" 0 1 131072 47 6 -0.071127
"C48" "ca" 0 1 131072 48 6 -0.132455
"C49" "c" 0 1 131072 49 6 0.394758
"O1" "o" 0 1 131072 50 8 -0.496854
"N1" "n" 0 1 131072 51 7 -0.041688
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"C52" "c" 0 1 131072 56 6 0.394758
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"C53" "c" 0 1 131072 58 6 0.394758
"O5" "o" 0 1 131072 59 8 -0.496854

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"N2" "n" 0 1 131072 62 7 -0.041688
"N3" "n" 0 1 131072 63 7 -0.041688
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"C56" "c3" 0 1 131072 65 6 -0.085101
"C57" "c3" 0 1 131072 66 6 -0.085101
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"C59" "ca" 0 1 131072 68 6 -0.108557
"C60" "ca" 0 1 131072 69 6 -0.291161
"C61" "ca" 0 1 131072 70 6 0.351128
"N4" "nb" 0 1 131072 71 7 -0.357949
"C62" "ca" 0 1 131072 72 6 0.190256
"C63" "ca" 0 1 131072 73 6 -0.203392
"C64" "ca" 0 1 131072 74 6 -0.108557
"C65" "ca" 0 1 131072 75 6 -0.291161
"C66" "ca" 0 1 131072 76 6 0.351128
"N5" "nb" 0 1 131072 77 7 -0.357949
"C67" "ca" 0 1 131072 78 6 0.190256
"C68" "ca" 0 1 131072 79 6 -0.203392
"C69" "ca" 0 1 131072 80 6 -0.108557
"C70" "ca" 0 1 131072 81 6 -0.291161
"C71" "ca" 0 1 131072 82 6 0.351128
"N6" "nb" 0 1 131072 83 7 -0.357949
"C72" "ca" 0 1 131072 84 6 0.190256
"C73" "c3" 0 1 131072 85 6 0.008200
"C74" "c3" 0 1 131072 86 6 0.008200
"C75" "c3" 0 1 131072 87 6 0.008200
"N7" "n3" 0 1 131072 88 7 -0.044155
"H1" "hc" 0 1 131072 89 1 0.041607
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"H5" "hc" 0 1 131072 93 1 0.034062
"H6" "hc" 0 1 131072 94 1 0.041607
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"H8" "hc" 0 1 131072 96 1 0.041607
"H9" "hc" 0 1 131072 97 1 0.041607
"H10" "hc" 0 1 131072 98 1 0.034062
"H11" "hc" 0 1 131072 99 1 0.034062
"H12" "hc" 0 1 131072 100 1 0.041607
"H13" "hc" 0 1 131072 101 1 0.042469
"H14" "hc" 0 1 131072 102 1 0.034062
"H15" "hc" 0 1 131072 103 1 0.034062
"H16" "ha" 0 1 131072 104 1 0.157196
"H17" "ha" 0 1 131072 105 1 0.146930
"H18" "hc" 0 1 131072 106 1 0.042469
"H19" "ha" 0 1 131072 107 1 0.157196
"H20" "ha" 0 1 131072 108 1 0.146930
"H21" "hc" 0 1 131072 109 1 0.049411
"H22" "ha" 0 1 131072 110 1 0.157196
"H23" "ha" 0 1 131072 111 1 0.146930
"H24" "hc" 0 1 131072 112 1 0.049411
"H25" "ha" 0 1 131072 113 1 0.166641
"H26" "ha" 0 1 131072 114 1 0.169812
"H27" "ha" 0 1 131072 115 1 0.169812
"H28" "ha" 0 1 131072 116 1 0.166641
"H29" "ha" 0 1 131072 117 1 0.169812
"H30" "ha" 0 1 131072 118 1 0.166641
"H31" "h1" 0 1 131072 119 1 0.084633
"H32" "h1" 0 1 131072 120 1 0.084633
"H33" "h1" 0 1 131072 121 1 0.084633
"H34" "h1" 0 1 131072 122 1 0.084633
"H35" "h1" 0 1 131072 123 1 0.084633
"H36" "h1" 0 1 131072 124 1 0.084633
"H37" "ha" 0 1 131072 125 1 0.114083
"H38" "ha" 0 1 131072 126 1 0.166719
"H39" "ha" 0 1 131072 127 1 0.151500
"H40" "ha" 0 1 131072 128 1 0.114083
"H41" "ha" 0 1 131072 129 1 0.166719
"H42" "ha" 0 1 131072 130 1 0.151500
"H43" "ha" 0 1 131072 131 1 0.114083
"H44" "ha" 0 1 131072 132 1 0.166719
"H45" "ha" 0 1 131072 133 1 0.151500
"H46" "h1" 0 1 131072 134 1 0.035593
"H47" "h1" 0 1 131072 135 1 0.035593
"H48" "h1" 0 1 131072 136 1 0.035593
"H49" "h1" 0 1 131072 137 1 0.035593
"H50" "h1" 0 1 131072 138 1 0.035593
"H51" "h1" 0 1 131072 139 1 0.035593

B(+)⊂CCl_4
"C1" "ca" 0 1 131072 1 6 -0.027972
"C2" "ca" 0 1 131072 2 6 -0.073038
"C3" "ca" 0 1 131072 3 6 -0.027972
"C4" "ca" 0 1 131072 4 6 -0.073038
"C5" "ca" 0 1 131072 5 6 -0.027972
"C6" "ca" 0 1 131072 6 6 -0.073038
"C7" "c3" 0 1 131072 7 6 0.015253
"C8" "c3" 0 1 131072 8 6 -0.003396
"C9" "c3" 0 1 131072 9 6 -0.057944
"C10" "c3" 0 1 131072 10 6 0.016311
"C11" "c3" 0 1 131072 11 6 0.015253
"C12" "c3" 0 1 131072 12 6 -0.003396
"C13" "c3" 0 1 131072 13 6 0.016311
"C14" "c3" 0 1 131072 14 6 0.015253
"C15" "c3" 0 1 131072 15 6 -0.003396
"C16" "c3" 0 1 131072 16 6 0.016311
"C17" "c3" 0 1 131072 17 6 -0.057944
"C18" "c3" 0 1 131072 18 6 -0.057944
"C19" "ca" 0 1 131072 19 6 0.065465
"C20" "ca" 0 1 131072 20 6 -0.244219
"C21" "ca" 0 1 131072 21 6 0.033716
"C22" "ca" 0 1 131072 22 6 0.015018
"C23" "ca" 0 1 131072 23 6 -0.223394
"C24" "ca" 0 1 131072 24 6 0.064111
"C25" "ca" 0 1 131072 25 6 0.064111
"C26" "ca" 0 1 131072 26 6 0.065465

"C27" "ca" 0 1 131072 27 6 -0.244219
"C28" "ca" 0 1 131072 28 6 0.033716
"C29" "ca" 0 1 131072 29 6 0.015018
"C30" "ca" 0 1 131072 30 6 -0.223394
"C31" "ca" 0 1 131072 31 6 0.064111
"C32" "ca" 0 1 131072 32 6 0.065465
"C33" "ca" 0 1 131072 33 6 -0.244219
"C34" "ca" 0 1 131072 34 6 0.033716
"C35" "ca" 0 1 131072 35 6 0.015018
"C36" "ca" 0 1 131072 36 6 -0.223394
"C37" "ca" 0 1 131072 37 6 -0.127459
"C38" "ca" 0 1 131072 38 6 -0.047458
"C39" "ca" 0 1 131072 39 6 -0.092059
"C40" "ca" 0 1 131072 40 6 -0.132133
"C41" "ca" 0 1 131072 41 6 -0.132133
"C42" "ca" 0 1 131072 42 6 -0.092059
"C43" "ca" 0 1 131072 43 6 -0.047458
"C44" "ca" 0 1 131072 44 6 -0.127459
"C45" "ca" 0 1 131072 45 6 -0.132133
"C46" "ca" 0 1 131072 46 6 -0.092059
"C47" "ca" 0 1 131072 47 6 -0.047458
"C48" "ca" 0 1 131072 48 6 -0.127459
"C49" "c" 0 1 131072 49 6 0.364782
"O1" "o" 0 1 131072 50 8 -0.491552
"N1" "n" 0 1 131072 51 7 -0.025881
"C50" "c" 0 1 131072 52 6 0.488962
"O2" "o" 0 1 131072 53 8 -0.532197
"C51" "c" 0 1 131072 54 6 0.488962
"O3" "o" 0 1 131072 55 8 -0.532197
"C52" "c" 0 1 131072 56 6 0.364782
"O4" "o" 0 1 131072 57 8 -0.491552
"C53" "c" 0 1 131072 58 6 0.364782
"O5" "o" 0 1 131072 59 8 -0.491552
"C54" "c" 0 1 131072 60 6 0.488962
"O6" "o" 0 1 131072 61 8 -0.532197
"N2" "n" 0 1 131072 62 7 -0.025881
"N3" "n" 0 1 131072 63 7 -0.025881
"C55" "c3" 0 1 131072 64 6 -0.162100
"C56" "c3" 0 1 131072 65 6 -0.162100
"C57" "c3" 0 1 131072 66 6 -0.162100
"C58" "ca" 0 1 131072 67 6 -0.236128
"C59" "ca" 0 1 131072 68 6 -0.057606
"C60" "ca" 0 1 131072 69 6 -0.340798
"C61" "ca" 0 1 131072 70 6 0.415252
"N4" "nb" 0 1 131072 71 7 -0.396620
"C62" "ca" 0 1 131072 72 6 0.205203
"C63" "ca" 0 1 131072 73 6 -0.236128
"C64" "ca" 0 1 131072 74 6 -0.057606
"C65" "ca" 0 1 131072 75 6 -0.340798
"C66" "ca" 0 1 131072 76 6 0.415252
"N5" "nb" 0 1 131072 77 7 -0.396620
"C67" "ca" 0 1 131072 78 6 0.205203
"C68" "ca" 0 1 131072 79 6 -0.236128
"C69" "ca" 0 1 131072 80 6 -0.057606
"C70" "ca" 0 1 131072 81 6 -0.340798
"C71" "ca" 0 1 131072 82 6 0.415252
"N6" "nb" 0 1 131072 83 7 -0.396620
"C72" "ca" 0 1 131072 84 6 0.205203
"C73" "c3" 0 1 131072 85 6 -0.016153
"C74" "c3" 0 1 131072 86 6 -0.016153
"C75" "c3" 0 1 131072 87 6 -0.016153
"N7" "n3" 0 1 131072 88 7 0.002132
"H1" "hc" 0 1 131072 89 1 0.043257
"H2" "hc" 0 1 131072 90 1 0.043257
"H3" "hc" 0 1 131072 91 1 0.040063
"H4" "hc" 0 1 131072 92 1 0.032405
"H5" "hc" 0 1 131072 93 1 0.032405
"H6" "hc" 0 1 131072 94 1 0.043257
"H7" "hc" 0 1 131072 95 1 0.053750
"H8" "hc" 0 1 131072 96 1 0.043257
"H9" "hc" 0 1 131072 97 1 0.043257
"H10" "hc" 0 1 131072 98 1 0.032405
"H11" "hc" 0 1 131072 99 1 0.032405
"H12" "hc" 0 1 131072 100 1 0.043257
"H13" "hc" 0 1 131072 101 1 0.040063
"H14" "hc" 0 1 131072 102 1 0.032405
"H15" "hc" 0 1 131072 103 1 0.032405
"H16" "ha" 0 1 131072 104 1 0.156062
"H17" "ha" 0 1 131072 105 1 0.138653
"H18" "hc" 0 1 131072 106 1 0.040063
"H19" "ha" 0 1 131072 107 1 0.156062
"H20" "ha" 0 1 131072 108 1 0.138653
"H21" "hc" 0 1 131072 109 1 0.053750
"H22" "ha" 0 1 131072 110 1 0.156062
"H23" "ha" 0 1 131072 111 1 0.138653
"H24" "hc" 0 1 131072 112 1 0.053750
"H25" "ha" 0 1 131072 113 1 0.167135
"H26" "ha" 0 1 131072 114 1 0.171567
"H27" "ha" 0 1 131072 115 1 0.171567
"H28" "ha" 0 1 131072 116 1 0.167135
"H29" "ha" 0 1 131072 117 1 0.171567
"H30" "ha" 0 1 131072 118 1 0.167135
"H31" "h1" 0 1 131072 119 1 0.101396
"H32" "h1" 0 1 131072 120 1 0.101396
"H33" "h1" 0 1 131072 121 1 0.101396
"H34" "h1" 0 1 131072 122 1 0.101396
"H35" "h1" 0 1 131072 123 1 0.101396
"H36" "h1" 0 1 131072 124 1 0.101396
"H37" "ha" 0 1 131072 125 1 0.114672
"H38" "ha" 0 1 131072 126 1 0.156557
"H39" "ha" 0 1 131072 127 1 0.163475
"H40" "ha" 0 1 131072 128 1 0.114672
"H41" "ha" 0 1 131072 129 1 0.156557
"H42" "ha" 0 1 131072 130 1 0.163475
"H43" "ha" 0 1 131072 131 1 0.114672
"H44" "ha" 0 1 131072 132 1 0.156557
"H45" "ha" 0 1 131072 133 1 0.163475
"H46" "h1" 0 1 131072 134 1 0.043636

"H47" "h1" 0 1 131072 135 1 0.043636
"H48" "h1" 0 1 131072 136 1 0.043636
"H49" "h1" 0 1 131072 137 1 0.043636
"H50" "h1" 0 1 131072 138 1 0.043636
"H51" "h1" 0 1 131072 139 1 0.043636

CCl_4 in empty B(+)
"C1" "c3" 0 1 131072 1 6 -0.511166
"Cl1" "cl" 0 1 131072 2 6 0.127791
"Cl2" "cl" 0 1 131072 3 6 0.127791
"Cl3" "cl" 0 1 131072 4 6 0.127791
"Cl4" "cl" 0 1 131072 5 6 0.127791

B(–)⊂CCl_4
"C1" "ca" 0 1 131072 1 6 -0.038420
"C2" "ca" 0 1 131072 2 6 -0.062457
"C3" "ca" 0 1 131072 3 6 -0.038420
"C4" "ca" 0 1 131072 4 6 -0.062457
"C5" "ca" 0 1 131072 5 6 -0.038420
"C6" "ca" 0 1 131072 6 6 -0.062457
"C7" "c3" 0 1 131072 7 6 0.011197
"C8" "c3" 0 1 131072 8 6 -0.011759
"C9" "c3" 0 1 131072 9 6 -0.074161
"C10" "c3" 0 1 131072 10 6 0.020432
"C11" "c3" 0 1 131072 11 6 0.011197
"C12" "c3" 0 1 131072 12 6 -0.011759
"C13" "c3" 0 1 131072 13 6 0.020432
"C14" "c3" 0 1 131072 14 6 0.011197
"C15" "c3" 0 1 131072 15 6 -0.011759
"C16" "c3" 0 1 131072 16 6 0.020432
"C17" "c3" 0 1 131072 17 6 -0.074161
"C18" "c3" 0 1 131072 18 6 -0.074161
"C19" "ca" 0 1 131072 19 6 0.059109
"C20" "ca" 0 1 131072 20 6 -0.235965
"C21" "ca" 0 1 131072 21 6 0.039268
"C22" "ca" 0 1 131072 22 6 0.008842
"C23" "ca" 0 1 131072 23 6 -0.220530
"C24" "ca" 0 1 131072 24 6 0.065460
"C25" "ca" 0 1 131072 25 6 0.065460
"C26" "ca" 0 1 131072 26 6 0.059109
"C27" "ca" 0 1 131072 27 6 -0.235965
"C28" "ca" 0 1 131072 28 6 0.039268
"C29" "ca" 0 1 131072 29 6 0.008842
"C30" "ca" 0 1 131072 30 6 -0.220530
"C31" "ca" 0 1 131072 31 6 0.065460
"C32" "ca" 0 1 131072 32 6 0.059109
"C33" "ca" 0 1 131072 33 6 -0.235965
"C34" "ca" 0 1 131072 34 6 0.039268
"C35" "ca" 0 1 131072 35 6 0.008842
"C36" "ca" 0 1 131072 36 6 -0.220530
"C37" "ca" 0 1 131072 37 6 -0.126988
"C38" "ca" 0 1 131072 38 6 -0.064658
"C39" "ca" 0 1 131072 39 6 -0.059446
"C40" "ca" 0 1 131072 40 6 -0.124351
"C41" "ca" 0 1 131072 41 6 -0.124351
"C42" "ca" 0 1 131072 42 6 -0.059446
"C43" "ca" 0 1 131072 43 6 -0.064658
"C44" "ca" 0 1 131072 44 6 -0.126988
"C45" "ca" 0 1 131072 45 6 -0.124351
"C46" "ca" 0 1 131072 46 6 -0.059446
"C47" "ca" 0 1 131072 47 6 -0.064658
"C48" "ca" 0 1 131072 48 6 -0.126988
"C49" "c" 0 1 131072 49 6 0.445430
"O1" "o" 0 1 131072 50 8 -0.516406
"N1" "n" 0 1 131072 51 7 -0.041762
"C50" "c" 0 1 131072 52 6 0.384770
"O2" "o" 0 1 131072 53 8 -0.494146
"C51" "c" 0 1 131072 54 6 0.384770
"O3" "o" 0 1 131072 55 8 -0.494146
"C52" "c" 0 1 131072 56 6 0.445430
"O4" "o" 0 1 131072 57 8 -0.516406
"C53" "c" 0 1 131072 58 6 0.445430
"O5" "o" 0 1 131072 59 8 -0.516406
"C54" "c" 0 1 131072 60 6 0.384770
"O6" "o" 0 1 131072 61 8 -0.494146
"N2" "n" 0 1 131072 62 7 -0.041762
"N3" "n" 0 1 131072 63 7 -0.041762
"C55" "c3" 0 1 131072 64 6 -0.125963
"C56" "c3" 0 1 131072 65 6 -0.125963
"C57" "c3" 0 1 131072 66 6 -0.125963
"C58" "ca" 0 1 131072 67 6 -0.225330
"C59" "ca" 0 1 131072 68 6 -0.074663
"C60" "ca" 0 1 131072 69 6 -0.322344
"C61" "ca" 0 1 131072 70 6 0.397826
"N4" "nb" 0 1 131072 71 7 -0.387242
"C62" "ca" 0 1 131072 72 6 0.202719
"C63" "ca" 0 1 131072 73 6 -0.225330
"C64" "ca" 0 1 131072 74 6 -0.074663
"C65" "ca" 0 1 131072 75 6 -0.322344
"C66" "ca" 0 1 131072 76 6 0.397826
"N5" "nb" 0 1 131072 77 7 -0.387242
"C67" "ca" 0 1 131072 78 6 0.202719
"C68" "ca" 0 1 131072 79 6 -0.225330
"C69" "ca" 0 1 131072 80 6 -0.074663
"C70" "ca" 0 1 131072 81 6 -0.322344
"C71" "ca" 0 1 131072 82 6 0.397826
"N6" "nb" 0 1 131072 83 7 -0.387242
"C72" "ca" 0 1 131072 84 6 0.202719
"C73" "c3" 0 1 131072 85 6 -0.021967
"C74" "c3" 0 1 131072 86 6 -0.021967
"C75" "c3" 0 1 131072 87 6 -0.021967
"N7" "n3" 0 1 131072 88 7 0.027067
"H1" "hc" 0 1 131072 89 1 0.044767
"H2" "hc" 0 1 131072 90 1 0.044767
"H3" "hc" 0 1 131072 91 1 0.043715
"H4" "hc" 0 1 131072 92 1 0.039467
"H5" "hc" 0 1 131072 93 1 0.039467
"H6" "hc" 0 1 131072 94 1 0.044767

"H7" "hc" 0 1 131072 95 1 0.050913
"H8" "hc" 0 1 131072 96 1 0.044767
"H9" "hc" 0 1 131072 97 1 0.044767
"H10" "hc" 0 1 131072 98 1 0.039467
"H11" "hc" 0 1 131072 99 1 0.039467
"H12" "hc" 0 1 131072 100 1 0.044767
"H13" "hc" 0 1 131072 101 1 0.043715
"H14" "hc" 0 1 131072 102 1 0.039467
"H15" "hc" 0 1 131072 103 1 0.039467
"H16" "ha" 0 1 131072 104 1 0.151798
"H17" "ha" 0 1 131072 105 1 0.143145
"H18" "hc" 0 1 131072 106 1 0.043715
"H19" "ha" 0 1 131072 107 1 0.151798
"H20" "ha" 0 1 131072 108 1 0.143145
"H21" "hc" 0 1 131072 109 1 0.050913
"H22" "ha" 0 1 131072 110 1 0.151798
"H23" "ha" 0 1 131072 111 1 0.143145
"H24" "hc" 0 1 131072 112 1 0.050913
"H25" "ha" 0 1 131072 113 1 0.165749
"H26" "ha" 0 1 131072 114 1 0.163582
"H27" "ha" 0 1 131072 115 1 0.163582
"H28" "ha" 0 1 131072 116 1 0.165749
"H29" "ha" 0 1 131072 117 1 0.163582
"H30" "ha" 0 1 131072 118 1 0.165749
"H31" "h1" 0 1 131072 119 1 0.094161
"H32" "h1" 0 1 131072 120 1 0.094161
"H33" "h1" 0 1 131072 121 1 0.094161
"H34" "h1" 0 1 131072 122 1 0.094161
"H35" "h1" 0 1 131072 123 1 0.094161
"H36" "h1" 0 1 131072 124 1 0.094161
"H37" "ha" 0 1 131072 125 1 0.112078
"H38" "ha" 0 1 131072 126 1 0.159017
"H39" "ha" 0 1 131072 127 1 0.156477
"H40" "ha" 0 1 131072 128 1 0.112078
"H41" "ha" 0 1 131072 129 1 0.159017
"H42" "ha" 0 1 131072 130 1 0.156477
"H43" "ha" 0 1 131072 131 1 0.112078
"H44" "ha" 0 1 131072 132 1 0.159017
"H45" "ha" 0 1 131072 133 1 0.156477
"H46" "h1" 0 1 131072 134 1 0.040609
"H47" "h1" 0 1 131072 135 1 0.040609
"H48" "h1" 0 1 131072 136 1 0.040609
"H49" "h1" 0 1 131072 137 1 0.040609
"H50" "h1" 0 1 131072 138 1 0.040609
"H51" "h1" 0 1 131072 139 1 0.040609

CCl_4 in empty B(–)
"C1" "c3" 0 1 131072 1 6 -0.504724
"Cl1" "cl" 0 1 131072 2 6 0.126181
"Cl2" "cl" 0 1 131072 3 6 0.126181
"Cl3" "cl" 0 1 131072 4 6 0.126181
"Cl4" "cl" 0 1 131072 5 6 0.126181

B(+)⊂CBr_4
"C1" "ca" 0 1 131072 1 6 -0.036689
"C2" "ca" 0 1 131072 2 6 -0.066867
"C3" "ca" 0 1 131072 3 6 -0.036689
"C4" "ca" 0 1 131072 4 6 -0.066867
"C5" "ca" 0 1 131072 5 6 -0.036689
"C6" "ca" 0 1 131072 6 6 -0.066867
"C7" "c3" 0 1 131072 7 6 0.015139
"C8" "c3" 0 1 131072 8 6 -0.007334
"C9" "c3" 0 1 131072 9 6 -0.070214
"C10" "c3" 0 1 131072 10 6 0.016630
"C11" "c3" 0 1 131072 11 6 0.015139
"C12" "c3" 0 1 131072 12 6 -0.007334
"C13" "c3" 0 1 131072 13 6 0.016630
"C14" "c3" 0 1 131072 14 6 0.015139
"C15" "c3" 0 1 131072 15 6 -0.007334
"C16" "c3" 0 1 131072 16 6 0.016630
"C17" "c3" 0 1 131072 17 6 -0.070214
"C18" "c3" 0 1 131072 18 6 -0.070214
"C19" "ca" 0 1 131072 19 6 0.064632
"C20" "ca" 0 1 131072 20 6 -0.227083
"C21" "ca" 0 1 131072 21 6 0.026529
"C22" "ca" 0 1 131072 22 6 0.009650
"C23" "ca" 0 1 131072 23 6 -0.209498
"C24" "ca" 0 1 131072 24 6 0.053260
"C25" "ca" 0 1 131072 25 6 0.053260
"C26" "ca" 0 1 131072 26 6 0.064632
"C27" "ca" 0 1 131072 27 6 -0.227083
"C28" "ca" 0 1 131072 28 6 0.026529
"C29" "ca" 0 1 131072 29 6 0.009650
"C30" "ca" 0 1 131072 30 6 -0.209498
"C31" "ca" 0 1 131072 31 6 0.053260
"C32" "ca" 0 1 131072 32 6 0.064632
"C33" "ca" 0 1 131072 33 6 -0.227083
"C34" "ca" 0 1 131072 34 6 0.026529
"C35" "ca" 0 1 131072 35 6 0.009650
"C36" "ca" 0 1 131072 36 6 -0.209498
"C37" "ca" 0 1 131072 37 6 -0.122791
"C38" "ca" 0 1 131072 38 6 -0.025985
"C39" "ca" 0 1 131072 39 6 -0.093800
"C40" "ca" 0 1 131072 40 6 -0.137795
"C41" "ca" 0 1 131072 41 6 -0.137795
"C42" "ca" 0 1 131072 42 6 -0.093800
"C43" "ca" 0 1 131072 43 6 -0.025985
"C44" "ca" 0 1 131072 44 6 -0.122791
"C45" "ca" 0 1 131072 45 6 -0.137795
"C46" "ca" 0 1 131072 46 6 -0.093800
"C47" "ca" 0 1 131072 47 6 -0.025985
"C48" "ca" 0 1 131072 48 6 -0.122791
"C49" "c" 0 1 131072 49 6 0.338108
"O1" "o" 0 1 131072 50 8 -0.485642
"N1" "n" 0 1 131072 51 7 -0.007247
"C50" "c" 0 1 131072 52 6 0.488266
"O2" "o" 0 1 131072 53 8 -0.532438
"C51" "c" 0 1 131072 54 6 0.488266

"O3" "o" 0 1 131072 55 8 -0.532438
"C52" "c" 0 1 131072 56 6 0.338108
"O4" "o" 0 1 131072 57 8 -0.485642
"C53" "c" 0 1 131072 58 6 0.338108
"O5" "o" 0 1 131072 59 8 -0.485642
"C54" "c" 0 1 131072 60 6 0.488266
"O6" "o" 0 1 131072 61 8 -0.532438
"N2" "n" 0 1 131072 62 7 -0.007247
"N3" "n" 0 1 131072 63 7 -0.007247
"C55" "c3" 0 1 131072 64 6 -0.199511
"C56" "c3" 0 1 131072 65 6 -0.199511
"C57" "c3" 0 1 131072 66 6 -0.199511
"C58" "ca" 0 1 131072 67 6 -0.172398
"C59" "ca" 0 1 131072 68 6 -0.095979
"C60" "ca" 0 1 131072 69 6 -0.331076
"C61" "ca" 0 1 131072 70 6 0.427428
"N4" "nb" 0 1 131072 71 7 -0.396633
"C62" "ca" 0 1 131072 72 6 0.180024
"C63" "ca" 0 1 131072 73 6 -0.172398
"C64" "ca" 0 1 131072 74 6 -0.095979
"C65" "ca" 0 1 131072 75 6 -0.331076
"C66" "ca" 0 1 131072 76 6 0.427428
"N5" "nb" 0 1 131072 77 7 -0.396633
"C67" "ca" 0 1 131072 78 6 0.180024
"C68" "ca" 0 1 131072 79 6 -0.172398
"C69" "ca" 0 1 131072 80 6 -0.095979
"C70" "ca" 0 1 131072 81 6 -0.331076
"C71" "ca" 0 1 131072 82 6 0.427428
"N6" "nb" 0 1 131072 83 7 -0.396633
"C72" "ca" 0 1 131072 84 6 0.180024
"C73" "c3" 0 1 131072 85 6 -0.043922
"C74" "c3" 0 1 131072 86 6 -0.043922
"C75" "c3" 0 1 131072 87 6 -0.043922
"N7" "n3" 0 1 131072 88 7 -0.115223
"H1" "hc" 0 1 131072 89 1 0.045017
"H2" "hc" 0 1 131072 90 1 0.045017
"H3" "hc" 0 1 131072 91 1 0.042024
"H4" "hc" 0 1 131072 92 1 0.038142
"H5" "hc" 0 1 131072 93 1 0.038142
"H6" "hc" 0 1 131072 94 1 0.045017
"H7" "hc" 0 1 131072 95 1 0.053391
"H8" "hc" 0 1 131072 96 1 0.045017
"H9" "hc" 0 1 131072 97 1 0.045017
"H10" "hc" 0 1 131072 98 1 0.038142
"H11" "hc" 0 1 131072 99 1 0.038142
"H12" "hc" 0 1 131072 100 1 0.045017
"H13" "hc" 0 1 131072 101 1 0.042024
"H14" "hc" 0 1 131072 102 1 0.038142
"H15" "hc" 0 1 131072 103 1 0.038142
"H16" "ha" 0 1 131072 104 1 0.152040
"H17" "ha" 0 1 131072 105 1 0.137073
"H18" "hc" 0 1 131072 106 1 0.042024
"H19" "ha" 0 1 131072 107 1 0.152040
"H20" "ha" 0 1 131072 108 1 0.137073
"H21" "hc" 0 1 131072 109 1 0.053391
"H22" "ha" 0 1 131072 110 1 0.152040
"H23" "ha" 0 1 131072 111 1 0.137073
"H24" "hc" 0 1 131072 112 1 0.053391
"H25" "ha" 0 1 131072 113 1 0.166682
"H26" "ha" 0 1 131072 114 1 0.167539
"H27" "ha" 0 1 131072 115 1 0.167539
"H28" "ha" 0 1 131072 116 1 0.166682
"H29" "ha" 0 1 131072 117 1 0.167539
"H30" "ha" 0 1 131072 118 1 0.166682
"H31" "h1" 0 1 131072 119 1 0.110667
"H32" "h1" 0 1 131072 120 1 0.110667
"H33" "h1" 0 1 131072 121 1 0.110667
"H34" "h1" 0 1 131072 122 1 0.110667
"H35" "h1" 0 1 131072 123 1 0.110667
"H36" "h1" 0 1 131072 124 1 0.110667
"H37" "ha" 0 1 131072 125 1 0.108825
"H38" "ha" 0 1 131072 126 1 0.162727
"H39" "ha" 0 1 131072 127 1 0.165144
"H40" "ha" 0 1 131072 128 1 0.108825
"H41" "ha" 0 1 131072 129 1 0.162727
"H42" "ha" 0 1 131072 130 1 0.165144
"H43" "ha" 0 1 131072 131 1 0.108825
"H44" "ha" 0 1 131072 132 1 0.162727
"H45" "ha" 0 1 131072 133 1 0.165144
"H46" "h1" 0 1 131072 134 1 0.069273
"H47" "h1" 0 1 131072 135 1 0.069273
"H48" "h1" 0 1 131072 136 1 0.069273
"H49" "h1" 0 1 131072 137 1 0.069273
"H50" "h1" 0 1 131072 138 1 0.069273
"H51" "h1" 0 1 131072 139 1 0.069273

CBr_4 in empty B(+)
"C1" "c3" 0 1 131072 1 6 -1.097090
"Br1" "br" 0 1 131072 2 5 0.274273
"Br2" "br" 0 1 131072 3 5 0.274273
"Br3" "br" 0 1 131072 4 5 0.274273
"Br4" "br" 0 1 131072 5 5 0.274273

B(–)⊂CBr_4
"C1" "ca" 0 1 131072 1 6 -0.037729
"C2" "ca" 0 1 131072 2 6 -0.068818
"C3" "ca" 0 1 131072 3 6 -0.037729
"C4" "ca" 0 1 131072 4 6 -0.068818
"C5" "ca" 0 1 131072 5 6 -0.037729
"C6" "ca" 0 1 131072 6 6 -0.068818
"C7" "c3" 0 1 131072 7 6 0.020664
"C8" "c3" 0 1 131072 8 6 -0.012499
"C9" "c3" 0 1 131072 9 6 -0.063680
"C10" "c3" 0 1 131072 10 6 0.027035
"C11" "c3" 0 1 131072 11 6 0.020664
"C12" "c3" 0 1 131072 12 6 -0.012499
"C13" "c3" 0 1 131072 13 6 0.027035
"C14" "c3" 0 1 131072 14 6 0.020664

"C15" "c3" 0 1 131072 15 6 -0.012499
"C16" "c3" 0 1 131072 16 6 0.027035
"C17" "c3" 0 1 131072 17 6 -0.063680
"C18" "c3" 0 1 131072 18 6 -0.063680
"C19" "ca" 0 1 131072 19 6 0.045865
"C20" "ca" 0 1 131072 20 6 -0.223525
"C21" "ca" 0 1 131072 21 6 0.023701
"C22" "ca" 0 1 131072 22 6 0.010625
"C23" "ca" 0 1 131072 23 6 -0.215268
"C24" "ca" 0 1 131072 24 6 0.068436
"C25" "ca" 0 1 131072 25 6 0.068436
"C26" "ca" 0 1 131072 26 6 0.045865
"C27" "ca" 0 1 131072 27 6 -0.223525
"C28" "ca" 0 1 131072 28 6 0.023701
"C29" "ca" 0 1 131072 29 6 0.010625
"C30" "ca" 0 1 131072 30 6 -0.215268
"C31" "ca" 0 1 131072 31 6 0.068436
"C32" "ca" 0 1 131072 32 6 0.045865
"C33" "ca" 0 1 131072 33 6 -0.223525
"C34" "ca" 0 1 131072 34 6 0.023701
"C35" "ca" 0 1 131072 35 6 0.010625
"C36" "ca" 0 1 131072 36 6 -0.215268
"C37" "ca" 0 1 131072 37 6 -0.123345
"C38" "ca" 0 1 131072 38 6 -0.080150
"C39" "ca" 0 1 131072 39 6 -0.048023
"C40" "ca" 0 1 131072 40 6 -0.117735
"C41" "ca" 0 1 131072 41 6 -0.117735
"C42" "ca" 0 1 131072 42 6 -0.048023
"C43" "ca" 0 1 131072 43 6 -0.080150
"C44" "ca" 0 1 131072 44 6 -0.123345
"C45" "ca" 0 1 131072 45 6 -0.117735
"C46" "ca" 0 1 131072 46 6 -0.048023
"C47" "ca" 0 1 131072 47 6 -0.080150
"C48" "ca" 0 1 131072 48 6 -0.123345
"C49" "c" 0 1 131072 49 6 0.441880
"O1" "o" 0 1 131072 50 8 -0.514632
"N1" "n" 0 1 131072 51 7 -0.027666
"C50" "c" 0 1 131072 52 6 0.377978
"O2" "o" 0 1 131072 53 8 -0.493879
"C51" "c" 0 1 131072 54 6 0.377978
"O3" "o" 0 1 131072 55 8 -0.493879
"C52" "c" 0 1 131072 56 6 0.441880
"O4" "o" 0 1 131072 57 8 -0.514632
"C53" "c" 0 1 131072 58 6 0.441880
"O5" "o" 0 1 131072 59 8 -0.514632
"C54" "c" 0 1 131072 60 6 0.377978
"O6" "o" 0 1 131072 61 8 -0.493879
"N2" "n" 0 1 131072 62 7 -0.027666
"N3" "n" 0 1 131072 63 7 -0.027666
"C55" "c3" 0 1 131072 64 6 -0.125355
"C56" "c3" 0 1 131072 65 6 -0.125355
"C57" "c3" 0 1 131072 66 6 -0.125355
"C58" "ca" 0 1 131072 67 6 -0.226187
"C59" "ca" 0 1 131072 68 6 -0.074839
"C60" "ca" 0 1 131072 69 6 -0.336381
"C61" "ca" 0 1 131072 70 6 0.413522
"N4" "nb" 0 1 131072 71 7 -0.428489
"C62" "ca" 0 1 131072 72 6 0.265152
"C63" "ca" 0 1 131072 73 6 -0.226187
"C64" "ca" 0 1 131072 74 6 -0.074839
"C65" "ca" 0 1 131072 75 6 -0.336381
"C66" "ca" 0 1 131072 76 6 0.413522
"N5" "nb" 0 1 131072 77 7 -0.428489
"C67" "ca" 0 1 131072 78 6 0.265152
"C68" "ca" 0 1 131072 79 6 -0.226187
"C69" "ca" 0 1 131072 80 6 -0.074839
"C70" "ca" 0 1 131072 81 6 -0.336381
"C71" "ca" 0 1 131072 82 6 0.413522
"N6" "nb" 0 1 131072 83 7 -0.428489
"C72" "ca" 0 1 131072 84 6 0.265152
"C73" "c3" 0 1 131072 85 6 -0.056284
"C74" "c3" 0 1 131072 86 6 -0.056284
"C75" "c3" 0 1 131072 87 6 -0.056284
"N7" "n3" 0 1 131072 88 7 -0.106308
"H1" "hc" 0 1 131072 89 1 0.043668
"H2" "hc" 0 1 131072 90 1 0.043668
"H3" "hc" 0 1 131072 91 1 0.043943
"H4" "hc" 0 1 131072 92 1 0.035453
"H5" "hc" 0 1 131072 93 1 0.035453
"H6" "hc" 0 1 131072 94 1 0.043668
"H7" "hc" 0 1 131072 95 1 0.047518
"H8" "hc" 0 1 131072 96 1 0.043668
"H9" "hc" 0 1 131072 97 1 0.043668
"H10" "hc" 0 1 131072 98 1 0.035453
"H11" "hc" 0 1 131072 99 1 0.035453
"H12" "hc" 0 1 131072 100 1 0.043668
"H13" "hc" 0 1 131072 101 1 0.043943
"H14" "hc" 0 1 131072 102 1 0.035453
"H15" "hc" 0 1 131072 103 1 0.035453
"H16" "ha" 0 1 131072 104 1 0.150195
"H17" "ha" 0 1 131072 105 1 0.140002
"H18" "hc" 0 1 131072 106 1 0.043943
"H19" "ha" 0 1 131072 107 1 0.150195
"H20" "ha" 0 1 131072 108 1 0.140002
"H21" "hc" 0 1 131072 109 1 0.047518
"H22" "ha" 0 1 131072 110 1 0.150195
"H23" "ha" 0 1 131072 111 1 0.140002
"H24" "hc" 0 1 131072 112 1 0.047518
"H25" "ha" 0 1 131072 113 1 0.163242
"H26" "ha" 0 1 131072 114 1 0.164649
"H27" "ha" 0 1 131072 115 1 0.164649
"H28" "ha" 0 1 131072 116 1 0.163242
"H29" "ha" 0 1 131072 117 1 0.164649
"H30" "ha" 0 1 131072 118 1 0.163242
"H31" "h1" 0 1 131072 119 1 0.092938
"H32" "h1" 0 1 131072 120 1 0.092938
"H33" "h1" 0 1 131072 121 1 0.092938
"H34" "h1" 0 1 131072 122 1 0.092938

"H35" "h1" 0 1 131072 123 1 0.092938
"H36" "h1" 0 1 131072 124 1 0.092938
"H37" "ha" 0 1 131072 125 1 0.114495
"H38" "ha" 0 1 131072 126 1 0.160456
"H39" "ha" 0 1 131072 127 1 0.159513
"H40" "ha" 0 1 131072 128 1 0.114495
"H41" "ha" 0 1 131072 129 1 0.160456
"H42" "ha" 0 1 131072 130 1 0.159513
"H43" "ha" 0 1 131072 131 1 0.114495
"H44" "ha" 0 1 131072 132 1 0.160456
"H45" "ha" 0 1 131072 133 1 0.159513
"H46" "h1" 0 1 131072 134 1 0.063466
"H47" "h1" 0 1 131072 135 1 0.063466
"H48" "h1" 0 1 131072 136 1 0.063466
"H49" "h1" 0 1 131072 137 1 0.063466
"H50" "h1" 0 1 131072 138 1 0.063466
"H51" "h1" 0 1 131072 139 1 0.063466

CBr_4 in empty B(–)
"C1" "c3" 0 1 131072 1 6 -1.096339
"Br1" "br" 0 1 131072 2 5 0.274085
"Br2" "br" 0 1 131072 3 5 0.274085
"Br3" "br" 0 1 131072 4 5 0.274085
"Br4" "br" 0 1 131072 5 5 0.274085