Supporting Information: Fully numerical electronic structure calculations on diatomic molecules in weak and strong magnetic fields

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The total energy as a function of the magnetic field strength for all states obtained in the calculations with the finite-element (FEM) calculations with HelFEM, and the gauge-including Gaussian-type orbital (GTO) calculations with London are shown in Figs. 1 to 2 for H_2, in Figs. 3 to 4 for HeH^+, in Figs. 5 to 7 for LiH, in Figs. 8 to 10 for BeH^+, in Figs. 11 to 13 for BH, and in Figs. 14 to 16 for CH^+. The resulting ground-state configurations in the FEM and GTO calculations have been identified in table 1 for H_2, HeH^+, and LiH, and in tables 2, 3 and 4 for BeH^+, BH and CH^+, respectively.

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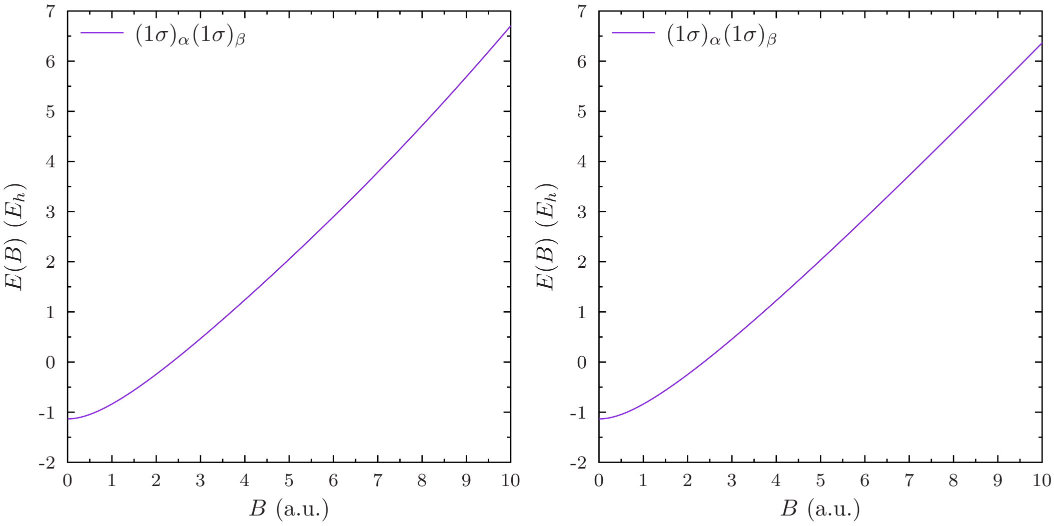
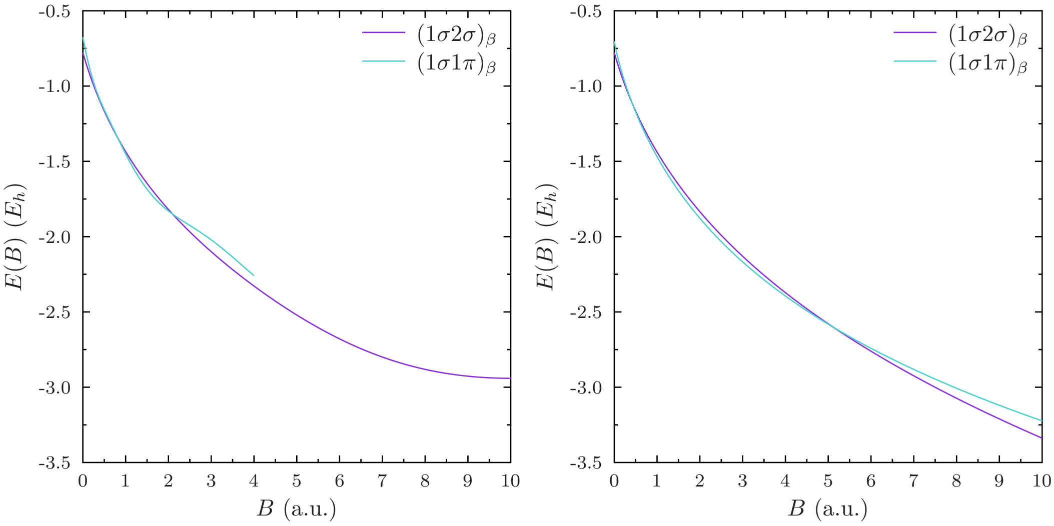


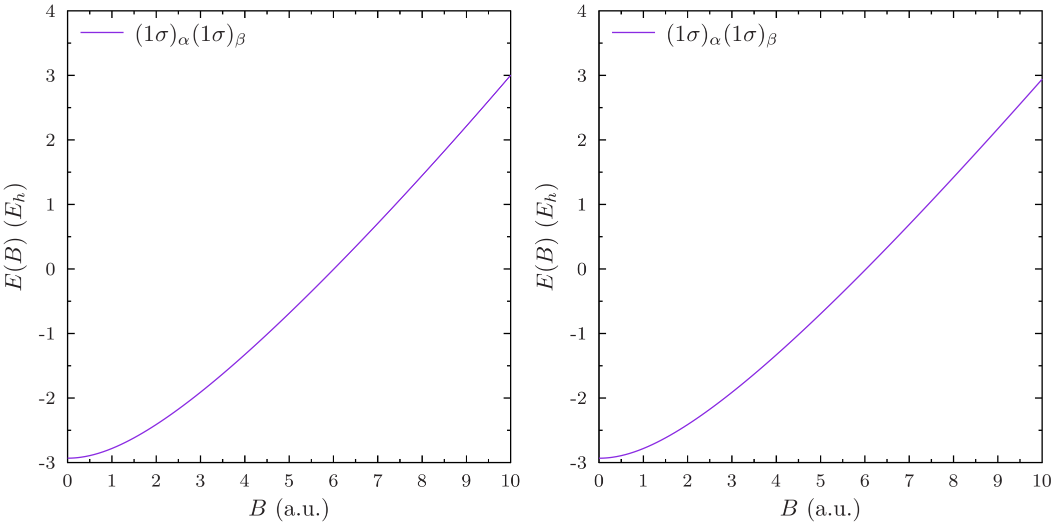
(a) GTO (b) FEM

Figure 1.: H_2 singlet.



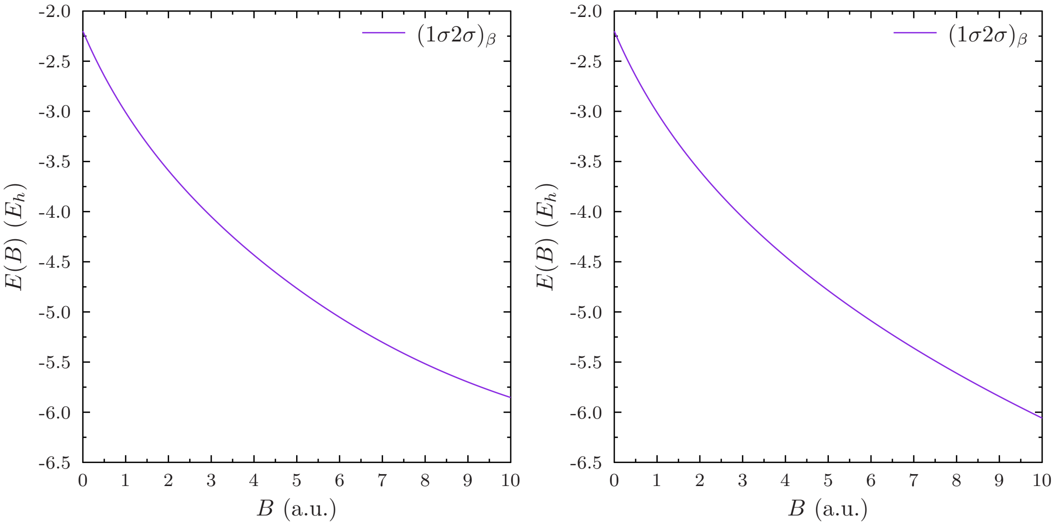
(a) GTO (b) FEM

Figure 2.: H_2 triplet.



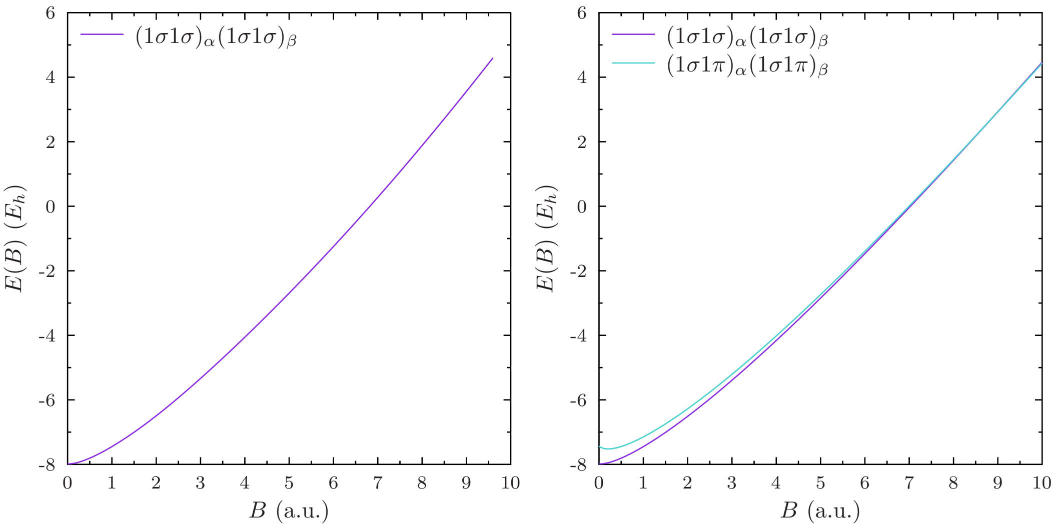
(a) GTO (b) FEM

Figure 3.: HeH^+ singlet.



(a) GTO (b) FEM

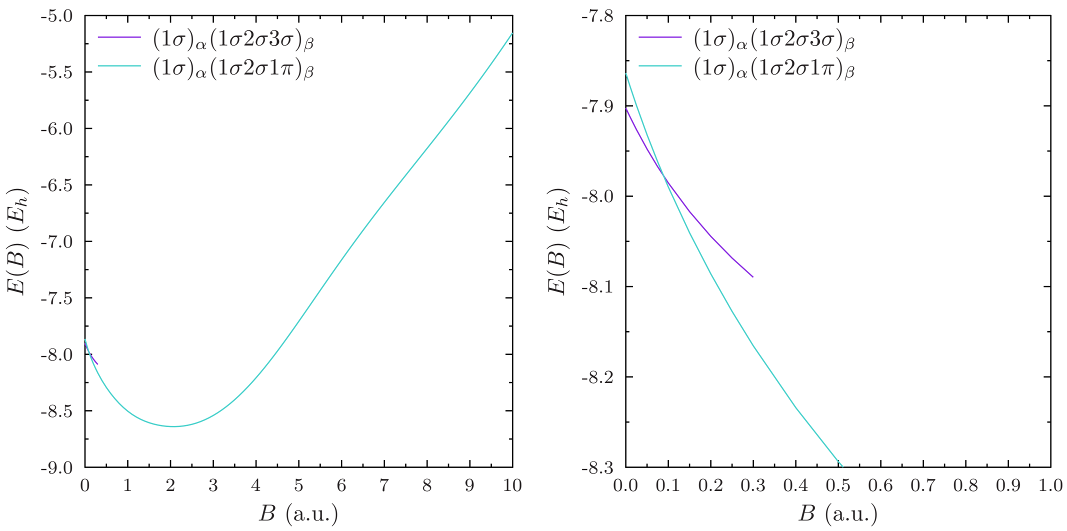
Figure 4.: HeH^+ triplet.



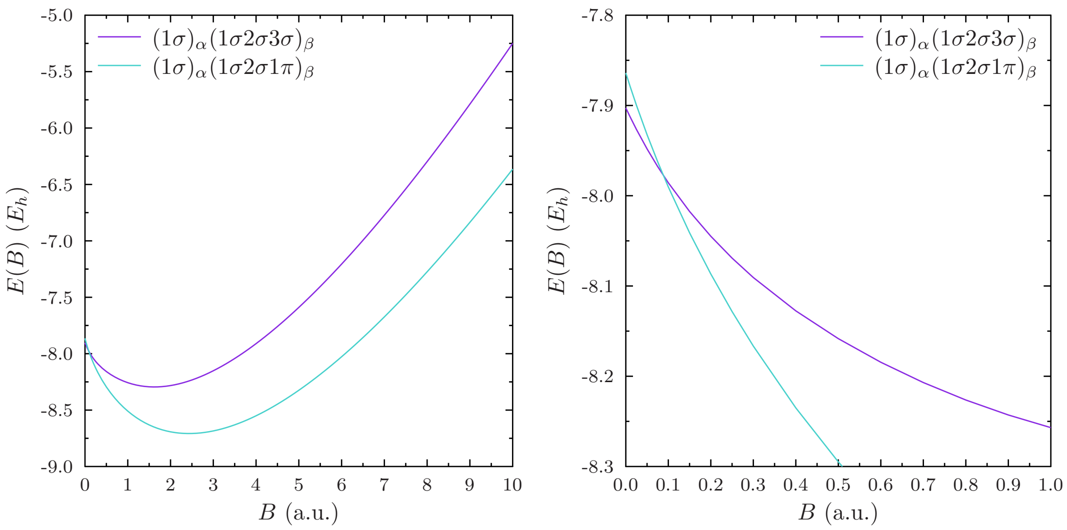
(a) GTO

(b) FEM

Figure 5.: LiH singlet.

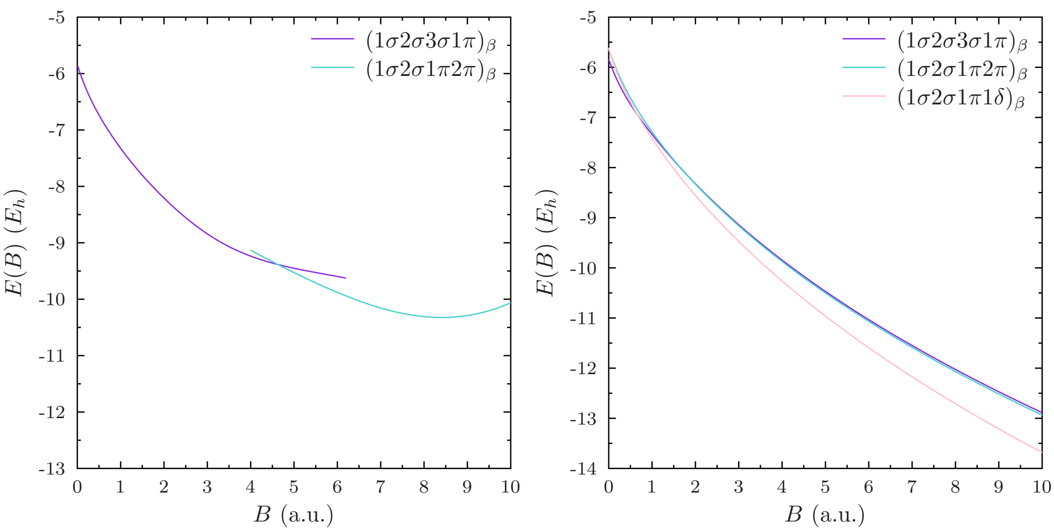


(a) GTO



(b) FEM

Figure 6.: LiH triplet.



(a) GTO

(b) FEM

Figure 7.: LiH quintet.

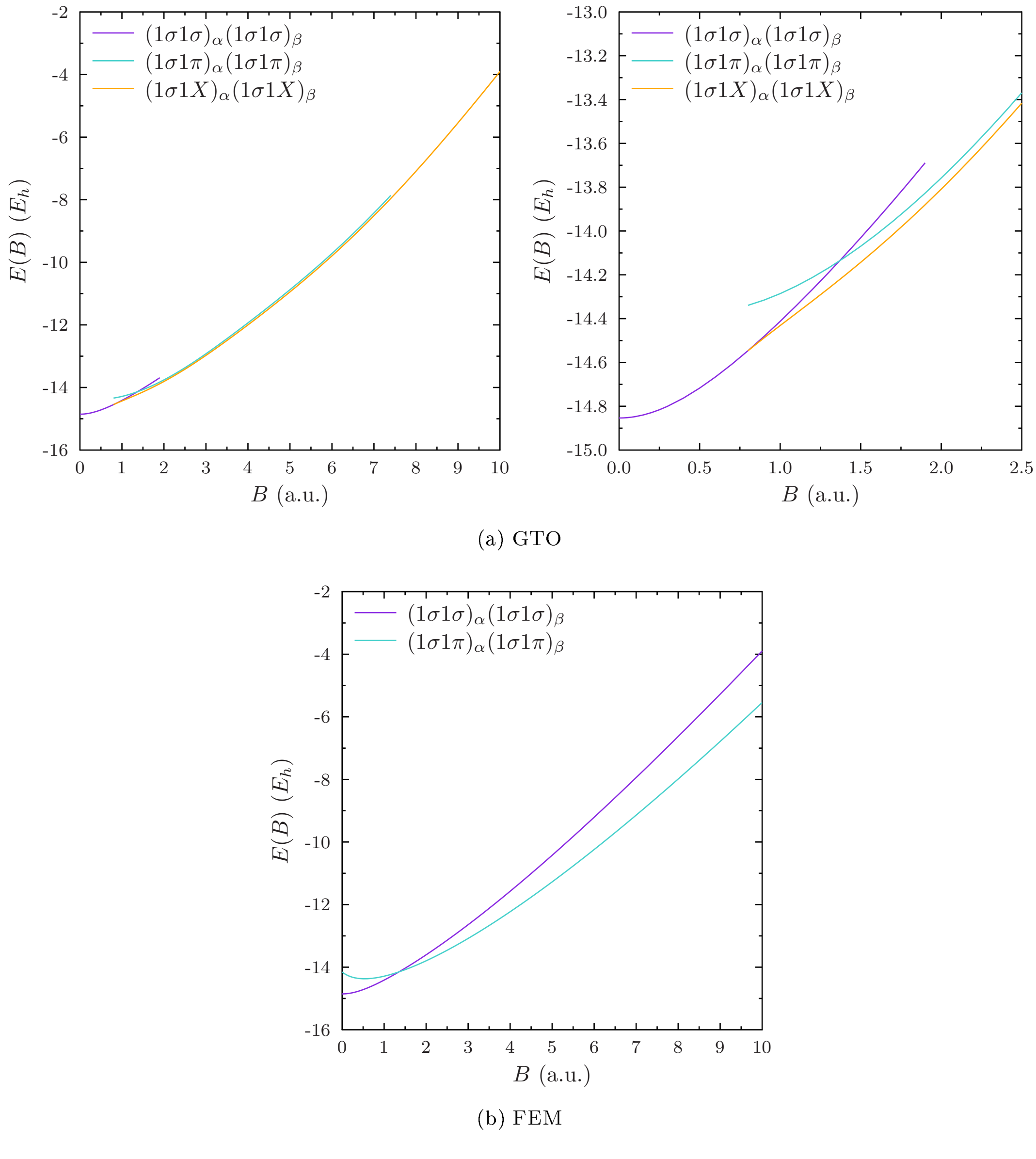
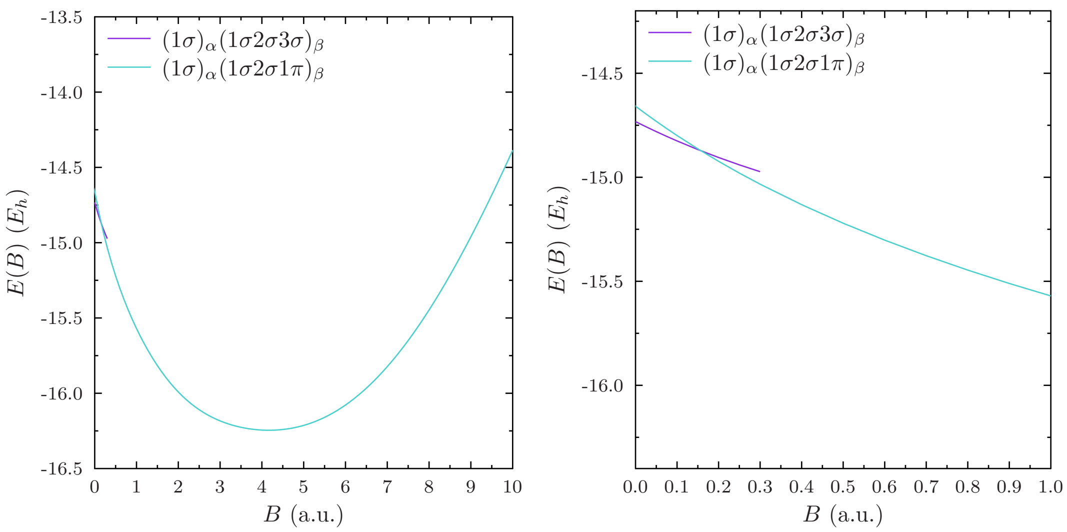
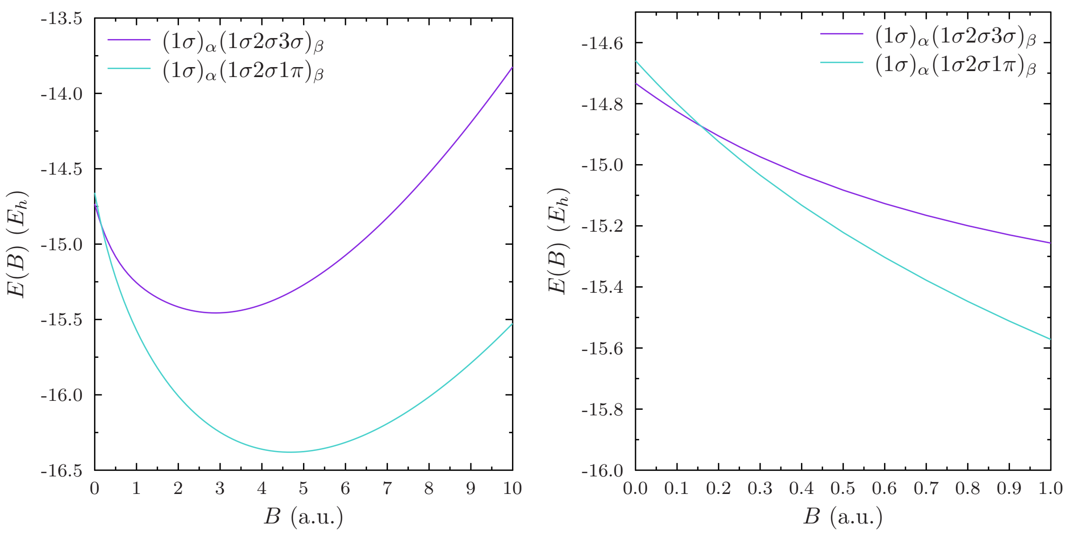


Figure 8.: BeH^+ singlet.

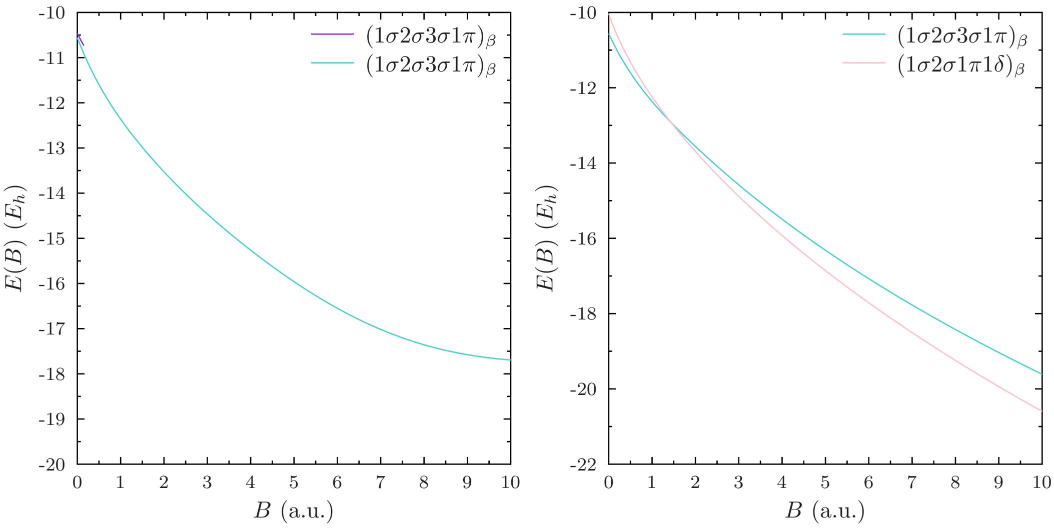


(a) GTO



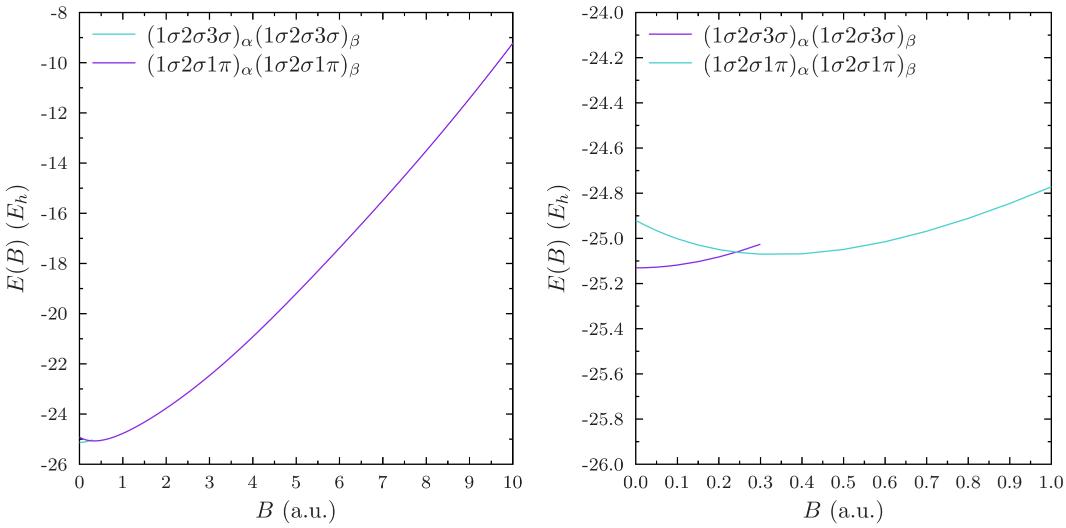
(b) FEM

Figure 9.: BeH^+ triplet.

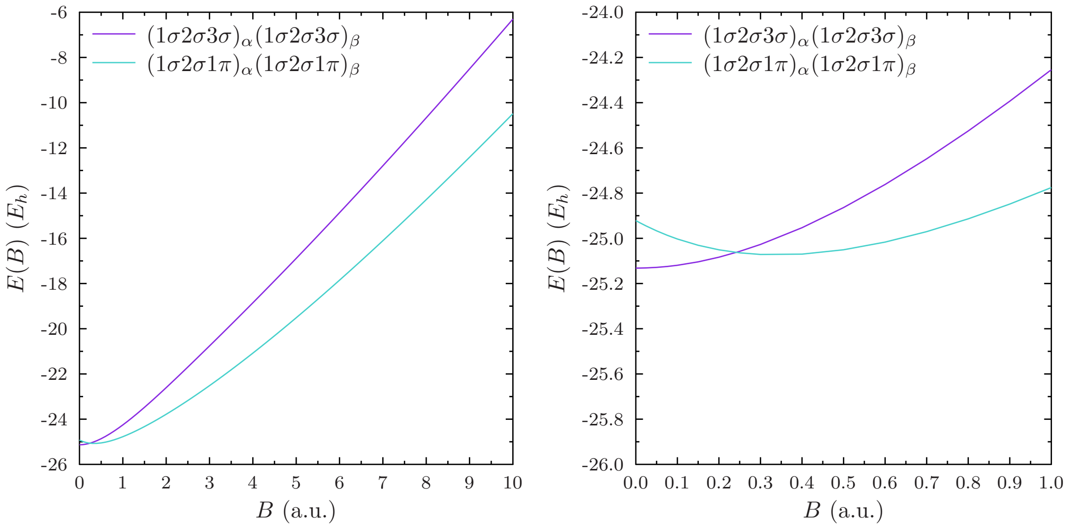


(a) GTO (b) FEM

Figure 10.: BeH^+ quintet.



(a) GTO



(b) FEM

Figure 11.: BH singlet.

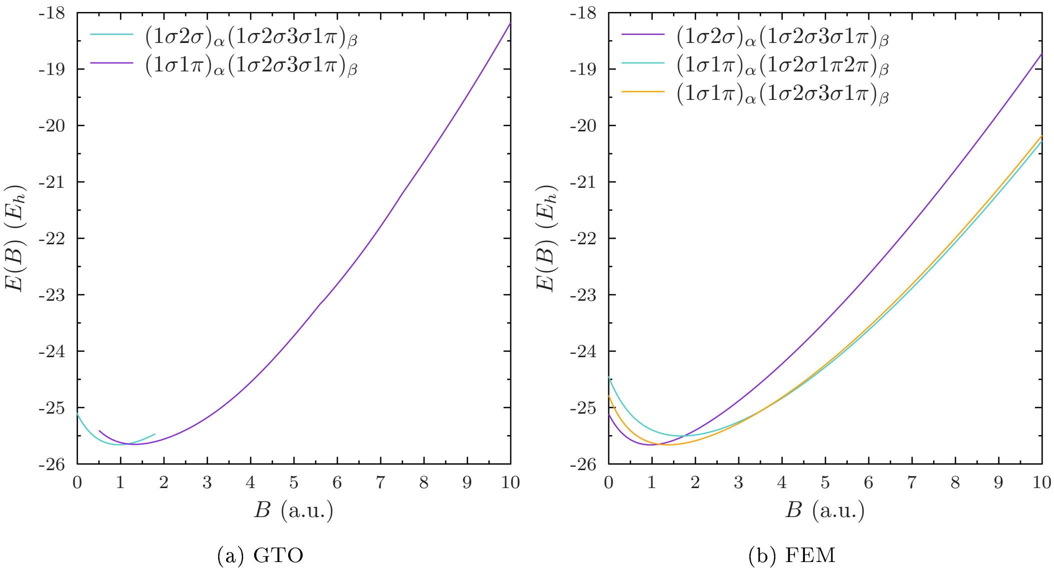
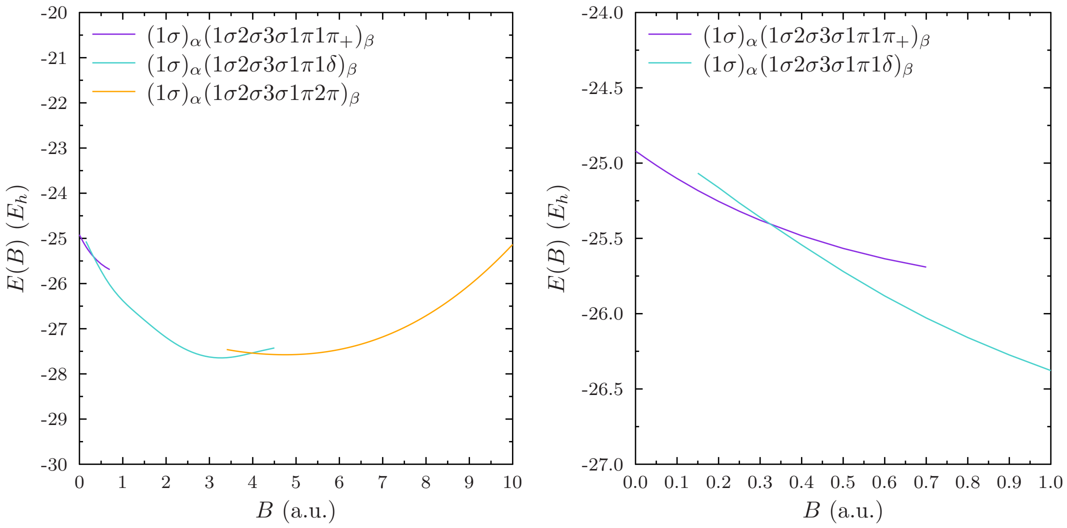
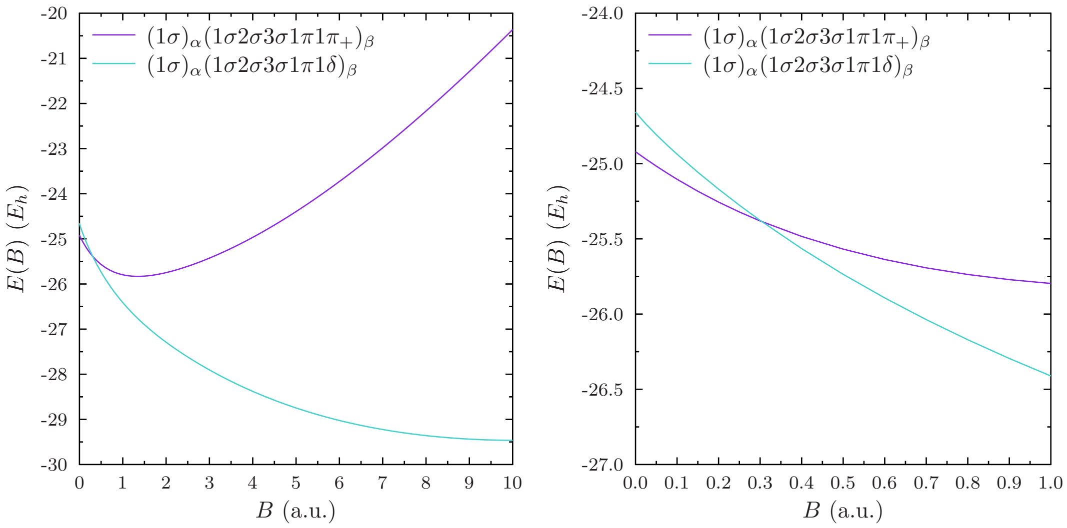


Figure 12.: BH triplet.

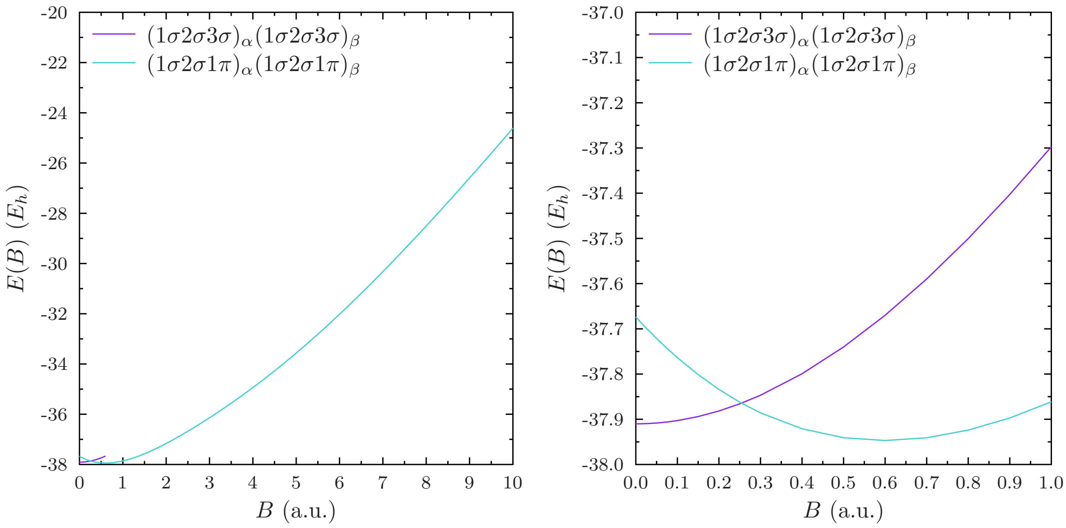


(a) GTO

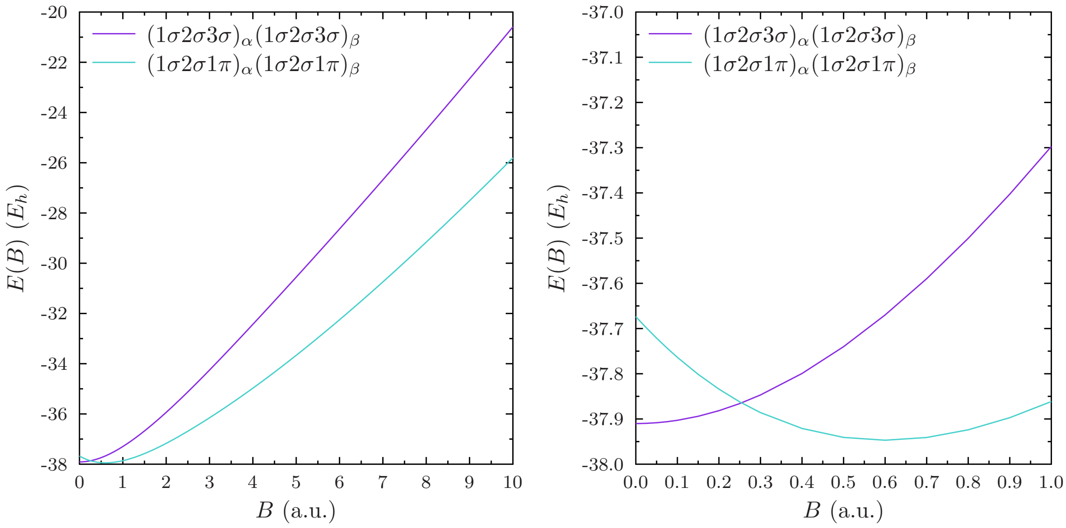


(b) FEM

Figure 13.: BH quintet.

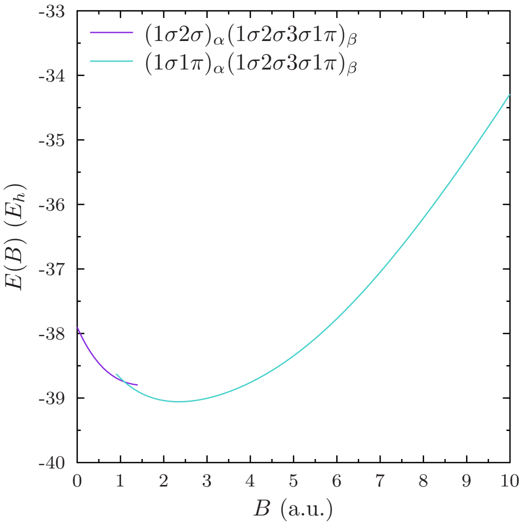


(a) GTO

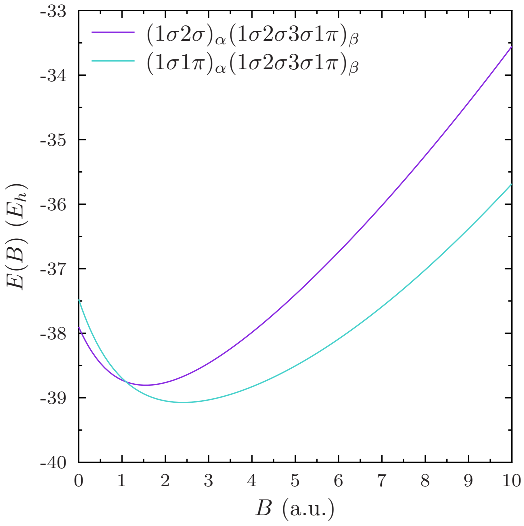


(b) FEM

Figure 14.: CH^+ singlet.

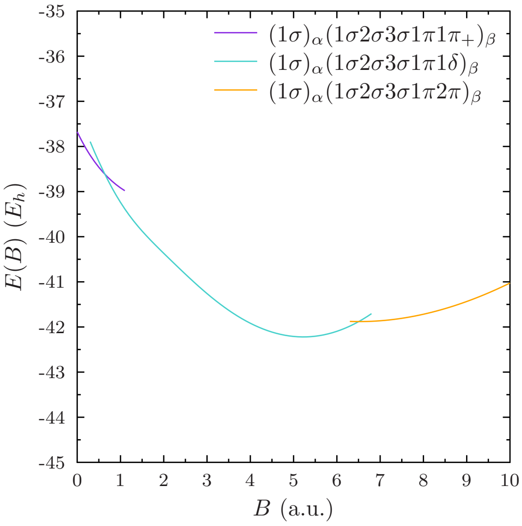


(a) GTO

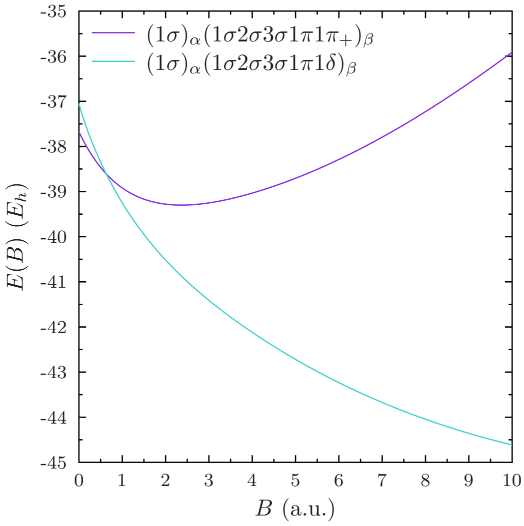


(b) FEM

Figure 15.: CH^+ triplet.



(a) GTO



(b) FEM

Figure 16.: CH^+ quintet.

Table 1.: Ground-state configurations for H_2, HeH^+, LiH, and BeH^+ as a function of the magnetic field strength calculated at the Hartree–Fock level using gauge-including Gaussian-type orbitals (GTO) and finite element (FEM) basis sets. The label X refers to symmetry-broken orbitals. Note that the orbitals are not sorted according to their energies.

Molecule	spin state	basis	configuration	field strength (B_0)
H_2	singlet	FEM	$1\sigma_\alpha 1\sigma_\beta$	$0 \leq B \leq 10$
		GTO	$1\sigma_\alpha 1\sigma_\beta$	$0 \leq B \leq 10$
	triplet	FEM	$(1\sigma 2\sigma)_\beta$	$0 \leq B < 0.5$
			$(1\sigma 1\pi)_\beta$	$0.5 \leq B < 5.2$
			$(1\sigma 2\sigma)_\beta$	$5.2 \leq B \leq 10$
		GTO	$(1\sigma 2\sigma)_\beta$	$0 \leq B < 0.9$
			$(1\sigma 1\pi)_\beta$	$0.9 \leq B < 2.2$
			$(1\sigma 2\sigma)_\beta$	$2.2 \leq B \leq 10$
HeH^+	singlet	FEM	$1\sigma_\alpha 1\sigma_\beta$	$0 \leq B \leq 10$
		GTO	$1\sigma_\alpha 1\sigma_\beta$	$0 \leq B \leq 10$
	triplet	FEM	$(1\sigma 2\sigma)_\beta$	$0 \leq B \leq 10$
		GTO	$(1\sigma 2\sigma)_\beta$	$0 \leq B \leq 10$
LiH	singlet	FEM	$(1\sigma 2\sigma)_\alpha(1\sigma 2\sigma)_\beta$	$0 \leq B < 8.8$
			$(1\sigma 1\pi)_\alpha(1\sigma 1\pi)_\beta$	$8.8 \leq B \leq 10$
		GTO	$(1\sigma 2\sigma)_\alpha(1\sigma 2\sigma)_\beta$	$0 \leq B < 9.6$
			$(1\sigma X)_\alpha(1\sigma X)_\beta$	$9.6 \leq B \leq 10$
	triplet	FEM	$1\sigma_\alpha(1\sigma 2\sigma 3\sigma)_\beta$	$0 \leq B < 0.1$
			$1\sigma_\alpha(1\sigma 2\sigma 3\sigma)_\beta$	$0.1 \leq B \leq 10$
		GTO	$1\sigma_\alpha(1\sigma 2\sigma 3\sigma)_\beta$	$0 \leq B < 0.1$
			$1\sigma_\alpha(1\sigma 2\sigma 1\pi)_\beta$	$0.1 \leq B \leq 10$
	quintet	FEM	$(1\sigma 2\sigma 3\sigma 1\pi)_\beta$	$0 \leq B < 0.1$
			$(1\sigma 2\sigma 1\pi 3\sigma)_\beta$	$0.1 \leq B < 0.7$
			$(1\sigma 2\sigma 1\pi 1\delta)_\beta$	$0.7 \leq B < 2.0$
			$(1\sigma 1\pi 2\sigma 1\delta)_\beta$	$2.0 \leq B \leq 10$
		GTO	$(1\sigma 2\sigma 3\sigma 4\sigma)_\beta$	$0 \leq B < 0.01$
			$(1\sigma 2\sigma 3\sigma 1\pi)_\beta$	$0.01 \leq B < 4.7$
			$(1\sigma 2\sigma 1\pi 2\pi)_\beta$	$4.7 \leq B < 9.7$
			$(1\sigma 2\sigma 3\sigma 1\pi)_\beta$	$9.7 \leq B \leq 10$

Table 2.: Ground-state configurations for BeH^+ as a function of the magnetic field strength calculated at the Hartree–Fock level using gauge-including Gaussian-type orbitals (GTO) and finite element (FEM) basis sets.

Spin state	basis	configuration	field strength (B_0)
singlet	FEM	$(1\sigma 2\sigma)_\alpha(1\sigma 2\sigma)_\beta$	$0 \le B < 1.4$
		$(1\sigma 1\pi)_\alpha(1\sigma 1\pi)_\beta$	$1.4 \le B < 10$
	GTO	$(1\sigma 2\sigma)_\alpha(1\sigma 2\sigma)_\beta$	$0 \le B < 1.4$
		$(1\sigma 1\pi)_\alpha(1\sigma 1\pi)_\beta$	$1.4 \le B \le 10$
triplet	FEM	$1\sigma_\alpha(1\sigma 2\sigma 3\sigma)_\beta$	$0 \le B < 0.2$
		$1\sigma_\alpha(1\sigma 2\sigma 1\pi)_\beta$	$0.2 \le B < 2.0$
		$1\sigma_\alpha(1\sigma 1\pi 2\sigma)_\beta$	$2.0 \le B < 10$
	GTO	$1\sigma_\alpha(1\sigma 2\sigma 3\sigma)_\beta$	$0 \le B < 0.2$
		$1\sigma_\alpha(1\sigma 2\sigma 1\pi)_\beta$	$0.2 \le B < 2.1$
		$1\sigma_\alpha(1\sigma 1\pi 2\sigma)_\beta$	$2.1 \le B \le 10$
quintet	FEM	$(1\sigma 2\sigma 3\sigma 1\pi)_\beta$	$0 \le B \le 0.1$
		$(1\sigma 2\sigma 1\pi 3\sigma)_\beta$	$0.1 < B < 1.3$
		$(1\sigma 1\pi 2\sigma 3\sigma)_\beta$	$1.3 \le B < 1.5$
		$(1\sigma 1\pi 2\sigma 1\delta)_\beta$	$1.5 \le B < 5.8$
		$(1\sigma 1\pi 1\delta 2\sigma)_\beta$	$5.8 \le B \le 10$
	GTO	$(1\sigma 2\sigma 3\sigma 1\pi)_\beta$	$0 \le B < 0.2$
		$(1\sigma 2\sigma 1\pi 3\sigma)_\beta$	$0.2 \le B < 1.3$
		$(1\sigma 1\pi 2\sigma 3\sigma)_\beta$	$1.3 \le B \le 10$

Table 3.: Ground-state configurations for BH as a function of the magnetic field strength calculated at the Hartree–Fock level using gauge-including Gaussian-type orbitals (GTO) and finite element (FEM) basis sets. π_+ orbitals have a higher energy in the presence of the magnetic field than at zero field.

Spin state	basis	configuration	field strength (B_0)
singlet	FEM	$(1\sigma2\sigma3\sigma)_\alpha(1\sigma2\sigma3\sigma)_\beta$	$0 \leq B < 0.3$
		$(1\sigma2\sigma1\pi)_\alpha(1\sigma2\sigma1\pi)_\beta$	$0.3 \leq B < 0.9$
		$(1\sigma1\pi2\sigma)_\alpha(1\sigma1\pi2\sigma)_\beta$	$0.9 \leq B \leq 10$
	GTO	$(1\sigma2\sigma3\sigma)_\alpha(1\sigma2\sigma3\sigma)_\beta$	$0 \leq B < 0.3$
		$(1\sigma2\sigma1\pi)_\alpha(1\sigma2\sigma1\pi)_\beta$	$0.3 \leq B < 0.7$
		$(1\sigma1\pi2\sigma)_\alpha(1\sigma1\pi2\sigma)_\beta$	$0.7 \leq B \leq 10$
triplet	FEM	$(1\sigma2\sigma)_\alpha(1\sigma2\sigma3\sigma1\pi)_\beta$	$0 \leq B < 0.3$
		$(1\sigma2\sigma)_\alpha(1\sigma2\sigma1\pi3\sigma)_\beta$	$0.3 \leq B < 0.9$
		$(1\sigma2\sigma)_\alpha(1\sigma1\pi2\sigma3\sigma)_\beta$	$0.9 \leq B < 1.2$
		$(1\sigma1\pi)_\alpha(1\sigma2\sigma1\pi3\sigma)_\beta$	$1.2 \leq B < 2.7$
		$(1\sigma1\pi)_\alpha(1\sigma1\pi2\sigma3\sigma)_\beta$	$2.7 \leq B < 3.6$
		$(1\sigma1\pi)_\alpha(1\sigma1\pi2\sigma2\pi)_\beta$	$3.6 \leq B \leq 10$
	GTO	$(1\sigma2\sigma)_\alpha(1\sigma2\sigma3\sigma1\pi)_\beta$	$0 \leq B < 0.3$
		$(1\sigma2\sigma)_\alpha(1\sigma2\sigma1\pi3\sigma)_\beta$	$0.3 \leq B < 0.9$
		$(1\sigma2\sigma)_\alpha(1\sigma1\pi2\sigma3\sigma)_\beta$	$0.9 \leq B < 1.5$
		$(1\sigma1\pi)_\alpha(1\sigma2\sigma1\pi3\sigma)_\beta$	$1.5 \leq B < 3.3$
		$(1\sigma1\pi)_\alpha(1\sigma1\pi2\sigma3\sigma)_\beta$	$3.3 \leq B \leq 10$
quintet	FEM	$1\sigma_\alpha(1\sigma2\sigma3\sigma1\pi1\pi_+)_\beta$	$0 \leq B < 0.3$
		$1\sigma_\alpha(1\sigma2\sigma1\pi3\sigma1\pi_+)_\beta$	$B = 0.3$
		$1\sigma_\alpha(1\sigma2\sigma1\pi3\sigma1\delta)_\beta$	$0.4 \leq B < 1.5$
		$1\sigma_\alpha(1\sigma1\pi2\sigma3\sigma1\delta)_\beta$	$1.5 \leq B < 1.8$
		$1\sigma_\alpha(1\sigma1\pi2\sigma1\delta3\sigma)_\beta$	$1.8 \leq B \leq 10$
	GTO	$1\sigma_\alpha(1\sigma2\sigma3\sigma1\pi1\pi_+)_\beta$	$0 \leq B < 0.4$
		$1\sigma_\alpha(1\sigma2\sigma3\sigma4\sigma1\pi)_\beta$	$0.4 \leq B < 0.7$
		$1\sigma_\alpha(1\sigma2\sigma3\sigma1\pi2\pi)_\beta$	$0.7 \leq B < 1.5$
		$1\sigma_\alpha(1\sigma1\pi2\sigma3\sigma1\delta)_\beta$	$1.5 \leq B < 2.0$
		$1\sigma_\alpha(1\sigma1\pi2\sigma1\delta3\sigma)_\beta$	$2.0 \leq B < 3.3$
		$1\sigma_\alpha(1\sigma1\pi2\sigma3\sigma1\delta)_\beta$	$3.3 \leq B < 4.0$
		$1\sigma_\alpha(1\sigma2\sigma3\sigma4\sigma1\pi)_\beta$	$4.0 \leq B \leq 10$

Table 4.: Ground-state configurations for CH^+ as a function of the magnetic field strength calculated at the Hartree–Fock level using gauge-including Gaussian-type orbitals (GTO) and finite element (FEM) basis sets. π_+ orbitals have a higher energy in the presence of the magnetic field than at zero field.

Spin state	basis	configuration	field strength (B_0)
singlet	FEM	$(1\sigma 2\sigma 3\sigma)_\alpha(1\sigma 2\sigma 3\sigma)_\beta$	$0 \leq B < 0.3$
		$(1\sigma 2\sigma 1\pi)_\alpha(1\sigma 2\sigma 1\pi)_\beta$	$0.3 \leq B < 1.0$
		$(1\sigma 1\pi 2\sigma)_\alpha(1\sigma 1\pi 2\sigma)_\beta$	$1.0 \leq B \leq 10$
	GTO	$(1\sigma 2\sigma 3\sigma)_\alpha(1\sigma 2\sigma 3\sigma)_\beta$	$0 \leq B < 0.3$
		$(1\sigma 2\sigma 1\pi)_\alpha(1\sigma 2\sigma 1\pi)_\beta$	$0.3 \leq B < 1.0$
		$(1\sigma 1\pi 2\sigma)_\alpha(1\sigma 1\pi 2\sigma)_\beta$	$1.0 \leq B \leq 10$
triplet	FEM	$(1\sigma 2\sigma)_\alpha(1\sigma 2\sigma 3\sigma 1\pi)_\beta$	$0 \leq B < 0.3$
		$(1\sigma 2\sigma)_\alpha(1\sigma 2\sigma 1\pi 3\sigma)_\beta$	$0.3 \leq B < 1.0$
		$(1\sigma 2\sigma)_\alpha(1\sigma 1\pi 2\sigma 3\sigma)_\beta$	$B = 1.0$
		$(1\sigma 1\pi)_\alpha(1\sigma 2\sigma 1\pi 3\sigma)_\beta$	$1.1 \leq B < 1.5$
		$(1\sigma 1\pi)_\alpha(1\sigma 1\pi 2\sigma 3\sigma)_\beta$	$1.5 \leq B \leq 10$
	GTO	$(1\sigma 2\sigma)_\alpha(1\sigma 2\sigma 3\sigma 1\pi)_\beta$	$0 \leq B < 0.3$
		$(1\sigma 2\sigma)_\alpha(1\sigma 2\sigma 1\pi 3\sigma)_\beta$	$0.3 \leq B < 1.0$
		$(1\sigma 2\sigma)_\alpha(1\sigma 1\pi 2\sigma 3\sigma)_\beta$	$1.0 \leq B < 1.3$
		$(1\sigma 1\pi)_\alpha(1\sigma 2\sigma 1\pi 3\sigma)_\beta$	$1.3 \leq B < 1.5$
		$(1\sigma 1\pi)_\alpha(1\sigma 1\pi 2\sigma 3\sigma)_\beta$	$1.5 \leq B \leq 10$
quintet	FEM	$1\sigma_\alpha(1\sigma 2\sigma 3\sigma 1\pi 1\pi_+)_\beta$	$0 \leq B < 0.3$
		$1\sigma_\alpha(1\sigma 2\sigma 1\pi 3\sigma 1\pi_+)_\beta$	$0.3 \leq B < 0.7$
		$1\sigma_\alpha(1\sigma 2\sigma 1\pi 3\sigma 1\delta)_\beta$	$0.7 \leq B < 1.2$
		$1\sigma_\alpha(1\sigma 1\pi 2\sigma 3\sigma 1\delta)_\beta$	$1.2 \leq B < 3.0$
		$1\sigma_\alpha(1\sigma 1\pi 2\sigma 1\delta 3\sigma)_\beta$	$3.0 \leq B < 6.6$
		$1\sigma_\alpha(1\sigma 1\pi 1\delta 2\sigma 3\sigma)_\beta$	$6.6 \leq B \leq 10$
	GTO	$1\sigma_\alpha(1\sigma 2\sigma 3\sigma 1\pi 1\pi_+)_\beta$	$0 \leq B < 0.3$
		$1\sigma_\alpha(1\sigma 2\sigma 1\pi 3\sigma 1\pi_+)_\beta$	$0.3 \leq B < 0.7$
		$1\sigma_\alpha(1\sigma 2\sigma 1\pi 3\sigma 1\delta)_\beta$	$0.7 \leq B < 1.2$
		$1\sigma_\alpha(1\sigma 1\pi 2\sigma 3\sigma 1\delta)_\beta$	$1.2 \leq B < 3.4$
		$1\sigma_\alpha(1\sigma 1\pi 2\sigma 1\delta 3\sigma)_\beta$	$3.4 \leq B < 6.5$
		$1\sigma_\alpha(1\sigma 2\sigma 3\sigma 4\sigma 1\pi)_\beta$	$6.5 \leq B \leq 10$