ReH_9^{2-}

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ReH_9^{2-}

1992

11Д91. **Необычный дианион эннеагидридогената: ReH_9^{2-}.** The remarkable enneahydridorhenate dianion: ReH_9^{2-} / Shen M., Schaefer (III) H. F. // Mol. Phys. — 1992.— 76, № 4.— С. 995—1007.— Англ.

В релятивистском неэмпирич. приближении ССП с учетом всех электронов в широких базисах проведены расчеты необычного девятикоординированного иона ReH_9^{2-}. Определены параметры известной эксперим. структуры симметрии D_{3h}. Рассчитаны частоты гармонич. колебаний. Полученные результаты согласуются с экспериментом, хотя высказано предположение, что это может быть обусловлено случайной компенсацией релятивистских и корреляционных эффектов.

М.П.

Ф. 1992, N 11-12

ReH_9^{2-}

1992

117: 157978g The remarkable enneahydridorhenate dianion: ReH_9^{2-}. Shen, Mingzuo; Schaefer, Henry F., III; Partridge, Harry (Cent. Comput. Quantum Chem., Univ. Georgia, Athens, GA 30602 USA). *Mol. Phys.* 1992, 76(4), 995–1007 (Eng). All-electron, non-relativistic *ab initio* SCF (SCF) quantum mech. methods were applied to the unique enneahydridorhenate dianion (ReH_9^{2-}, D_{3h}). Three basis sets were constructed and used for rhenium: the (*20s14p11d7f*/*17s11p8d2f*) basis is loosely designated DZ; the (*23s17p14d9f*/*18s14p11d3f*) is similarly designated TZ; and TZ plus polarization plus diffuse is designated TZP+. The largest basis set, TZP+, has *24s20p15d10f* primitive Gaussian functions contracted to *19s17p11d4f*. Four basis sets were used for H: the (5/33) is designated TZ; (*5s2p*/*3s2p*) is designated TZ2P; (*6s2p*/*4s2p*) is designated QZ2P; and QZ2P plus one diffuse *s* function is designated QZ2P+. The well-known exptl. D_{3h} structure was investigated, with the three independent internal coordinates optimized using analytic gradient techniques. The larger basis sets were handled using the direct SCF approach. The largest basis set for which the geometry was optimized was TZP+ for Re and QZ2P+ for H (with 252 basis functions, where pure *5d* and *7f* sets of functions were used), and should approach closely the non-relativistic Hartree-Fock limit. Harmonic vibrational frequencies were obtained for two basis sets, the larger of which is TZ for Re and QZ2P for H (for a total of 221 basis functions). The mol. geometry seems to have approached the Hartree-Fock limit, and the six symmetry-equiv. prism Re-H bonds

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C.A. 1992,
117, N 16

are predicted to be longer than the three cap Re--H bonds by 0·06 Å. The predicted equil. geometry and harmonic vibrational frequencies generally agree with available exptl. data. The reason for the apparent agreement may be the accidental cancellation of relativistic effects and electron correlation effects.