1 Introduction

Butyrylcholinesterase (BChE) is a prophylactic therapeutic glycoprotein for organophosphorus (OP) nerve agents [1]. OP nerve agents are toxic because they inhibit acetylcholinesterase (AChE) [2], the hydrolyzing enzyme of neurotransmitter acetylcholine [3]. According to Raveh et al, OP nerve agents have "traditionally been attributed to inhibition of AChE because the pathophysiological effects of these compounds" [1]. Some examples of OP nerve agents include sarin, somen and tabun. BChE must be administered within two minutes of an OP exposure in humans, which inactivates the OP before local AChE is affected [4]. For a comprehensive review of OP nerve agents and their treatment, the reader is referred to reference number [5].

2 Methodology

Relative potential energies were computed at MP2.5 [6, 7, 8] and CCSD(T) [9] theory levels by performing a single self-consistent field evaluation upon the fully optimized geometries. Extrapolations to the complete-basis-set (CBS) limit was done using the two-point scheme of Helgaker and coworkers [10]; the two basis sets used in the extrapolation are presented within square brackets. All constraint optimization associated with rPE surfaces were computed using the Gamess program (v. 1 MAY 2013 (R1)) [11]. All other calculations were performed using the Psi4 program (v. 1.1a2.dev170) [12].

3 Results

Table 1: Selected internal coordinate values for unique methanol minima and first-order transition states. Average values for bond and angles are also given as a function of theory level, as computed by the conformations given.

Method	r_{CO}	r_{OH}	ϕ_{COH}	δ_{HCOH}
Minimum: t				
Exp.[a]	1.427	0.956	108.52	
Exp.[b]	1.427	0.953	108.24	
Exp.[c]	1.428	0.960	109	
HF/6-31G(d)[d]	1.400	0.946	109.45	61.2
MP2/aV5Z	1.419	0.958	108.22	61.4
CCSD(T)/6-311G(3df,2p)[d]	1.417	0.958	107.9	61.5
CCSD(T)/DPZ[e]	1.429	0.964	107.6	61.5
CCSD(T)/aVTZ[f]	1.425	0.961		

a. Reference [13]
b. Reference [14]
c. Reference [15]
d. Reference [16]
e. Reference [17]; note that the COH angle appears to be mislabeled in Table XII as COH_3.
f. Reference [18]; note that the aVTZ basis sets was modified by removing the highest spin functions.

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