Table VIII. Comparison of structural parameters resulting from different methods. The upper triangle is the *RMS*[a] between methods and the lower triangle represents the average difference[b] between structural parameters.

Meth.[c]	RHF/6d	MP2/6d	DMol	DG/L	DN/L	DN/N	Exp.[d]
RMS and average difference for bonds (in Å)							
RHF/6d		0.0151	0.0282	0.0246	0.0246	0.0250	0.0149
MP2/6d	0.0125		0.0171	0.0145	0.0147	0.0118	0.0064
DMol	0.0230	0.0105		0.0056	0.0060	0.0135	0.0152
DG/L	0.0200	0.0075	−0.0030		0.0011	0.0133	0.0133
DN/L	0.0195	0.0071	−0.0034	−0.0004		0.0140	0.0132
DN/N	0.0233	0.0108	0.0004	0.0034	0.0038		0.0124
Exp.[d]	0.0124	0.0000	−0.0096	−0.0076	−0.0071	−0.0107	
RMS and average difference for angles (in deg)							
RHF/6d		1.0820	1.7516	1.0992	1.0591	1.1269	1.1187
MP2/6d	−0.4245		0.8907	0.7592	0.8038	0.3213	0.7967
DMol	−0.6218	−0.1973		0.9566	1.0449	0.8117	0.9750
DG/L	−0.2952	0.1294	0.3266		0.2726	0.6366	1.1076
DN/L	−0.2595	0.1651	0.3623	0.0357		0.6854	1.0816
DN/N	−0.4255	−0.0010	0.1963	−0.1304	−0.1661		0.9614
Exp.[d]	−0.2614	0.0808	0.1018	−0.0345	−0.0339	0.0816	
RMS and average difference for torsion angles (in deg)							
RHF/6d		2.3898	3.8789	3.4424	2.9906	2.9531	
MP2/6d	−0.3471		1.6535	3.1353	2.2934	1.9975	
DMol	−0.4429	−0.0958		4.0184	3.2430	2.7053	
DG/L	0.9003	1.2474	1.3432		4.2688	2.0699	
DN/L	−1.0333	−0.6862	−0.5904	−1.9336		3.8109	
DN/N	0.2044	0.5515	0.6472	−0.6874	1.2376		

[a]root mean square difference, $RMS = \sqrt{\sum_{i=1}^{n_x}(x_i^{row} - x_i^{column})^2/n_x}$, where x_i^{row} and x_i^{column} are the structural parameters (i.e., bond length, angle or torsional angle), and n_x is the total number of structural parameters in all calculated molecules (53 bonds, 77 angles and 57 torsional angles).

[b]average difference, $\Delta = \sum_{i=1}^{n_x}(x_i^{row} - x_i^{column})/n_x$. For example: the DN/L calculated bond lengths were 0.0195 Å longer than RHF/6d calculated ones, while DMol calculated valence angles where on average 0.1018 degree smaller than the experimental values.

[c]for method description see Table I.

[d]Experimental data were compiled only for neutral molecules and consisted of 23 bond lengths and 31 valence angles.