TABLE IV. ____

Summary Comparison of Theoretical Methods[a] vs. Experiment

Quantity	HF/ 6-31G*	MP2/ 6-31G*	MP2/ TZP	"MP4SDQ/TZP"	LMP2/ cc-pVTZ(-f)	"LMP4/ cc-pVTZ(-f)"	GVB-LMP2/ cc-pVTZ(-f)
Number favoring the wrong conformer[b]	4	6	2	3	1	2	2
rms Dev.vs. Expt.[c]	0.72	0.70	0.45	0.38	0.35	0.32	0.32
Maximum Dev.[c]	2.23	2.00	1.04	0.90	0.92	0.91	0.81
Number of deviations:							
0.5 - 1.0 kcal/mol	6	3	8	7	7	5	4
> 1.0 kcal/mol	5	8	1	0	0	0	0

[a] The HF/6-31G* calculations used HF/6-31G*-optimized geometries; all others used MP2(FULL)/6-31G*-optimized geometries. See text for definitions of the composite "MP4SDQ/TZP" and "LMP4/cc-pVTZ(-f)" models.

[b] Number of cases in which the ab initio and experimental determinations disagree as to which conformer is lower in energy.

[c] In kcal/mol.

TABLE V. ____
Summary of Comparsions of Conformational Energies vs. Experiment and Ab Initio Data (Set 1).[a,b]

Quantity	MMFF 94	MMFF 94s	CFF 95	CVFF	MSI CHARMm	AMBER*	OPLS*	MM2 *	MM3*
Number of conformational comparisons	37	37	37	34	36	37	37	37	37
Number of ab initio conformers having no local force field minimum	0	0	0	3	1	0	0	0	0
Number favoring the wrong conformer	1	1	5	13	4	8	9	3	3
rms Dev.vs. Expt.	0.37	0.38	1.06	2.36	0.78	1.29	1.68	1.75	0.72
Maximum Dev.	0.99	0.99	4.80	6.11	2.07	4.60	5.64	7.47	2.57
rms Dev. vs. "MP4SDQ/TZP"	0.33	0.33	1.17	2.35	0.73	1.37	1.79	1.62	0.79
rms Dev. vs. GVB-LPM2/cc-pVTZ(-f)	0.28	0.27	1.13	2.32	0.72	1.35	1.70	1.62	0.76
Number of deviations:									
1 - 2 kcal/mol	0	0	4	14	4	7	6	2	4
2 - 3 kcal/mol	0	0	1	3	2	1	0	0	1
3 - 5 kcal/mol	0	0	1	4	0	2	4	0	0
5 - 7 kcal/mol	0	0	0	3	0	0	1	1	0
7 - 10 kcal/mol	0	0	0	0	0	0	0	1	0

[a] This table summarizes the detailed results in Table I of the manuscript. All energy quantities are in kcal/mol. The number of possible conformational comparisons is 37.

[b] The ab initio reference conformational energies are the "MP4SDQ/TZP" or GVB-LMP2/cc-pVTZ(-f) results shown in Table III of the manuscript.

TABLE VI. ____
Summary of Comparsions of Conformational Energies vs. Experiment (Set 2).[a]

Quantity	MMFF 94/94s	CFF 95	CVFF	MSI CHARMm	AMBER*	OPLS*	MM2*	MM3*
Number favoring the wrong conformer	4	7	7	4	5	7	2	2
rms Dev.vs. Expt.	0.74	2.21	2.86	0.70	1.03	1.28	0.68	0.78
Maximum Dev.	1.45	4.24	5.78	1.66	1.69	2.91	1.87	2.27
Number of deviations:								
1 - 2 kcal/mol	4	5	7	3	9	4	3	2
2 - 3 kcal/mol	0	1	4	0	0	3	0	1
3 - 5 kcal/mol	0	6	4	0	0	0	0	0
5 - 7 kcal/mol	0	0	1	0	0	0	0	0

[a] This table summarizes the detailed results in Table II of the manuscript. All energy quantities are in kcal/mol. The number of conformational comparisons is 19 for all force fields

TABLE VII. ____

Summary of Comparisons of Conformational Energies vs. "MP4/SDQTZP" Data.

Quantity	MMFF 94	MMFF 94s	CFF 95	MSI CHARMm	AMBER*	OPLS*	MM2*	MM3*
Number of conformational comparisons[a]	146	142	139	140	136	139	140	129
Number lacking parameters	0	0	0	0	0	0	0	12
Number of ab initio conformers having no local force field min.	1	5	8	7	11	8	7	6
Number favoring the wrong conformer	7	8	32	31	38	32	30	22
RMS Deviation	0.32	0.33	1.33	1.66	1.85	3.72	1.99	1.08
Maximum Deviation	1.56	1.56	5.37	6.24	11.55	20.45	11.07	3.96
Number of deviations:								
1 - 2 kcal/mol	2	2	21	23	26	22	14	25
2 - 3 kcal/mol	0	0	13	11	13	7	1	6
3 - 5 kcal/mol	0	0	5	6	4	5	13	3
5 - 7 kcal/mol	0	0	1	5	4	4	3	0
7 - 10 kcal/mol	0	0	0	0	0	5	1	0
> 10 kcal/mol	0	0	0	0	1	6	1	0

[a] The number of possible conformational comparisons is 147. Detailed results are given in Table SM-I of the Supplementary Material for the manuscript.