PCCP

SUPPORTING INFORMATION

Designing Precise and Efficient Computational Methods for Molecular Structure Prediction

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Contents

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S1 Vibrational corrections to the rotational constants at the HPCS2 level of theory

S1.1 Cis-hexatriene

Table 1 Vibrational corrections (in MHz) to the rotational constants of the different isotopic species of cis-hexatriene at the HPCS2 level of theory. Refer to the main text for atom numbering.

Isotopic species	ΔA	ΔB	ΔC
Parent	161.0757	7.9863	7.4784
^{13}C1	160.9740	7.7378	7.2658
^{13}C2	159.4494	7.9052	7.3956
^{13}C3	156.9418	7.9184	7.4182
$D1_c$, $D1_t$	145.7559	7.3542	6.8147
$D1_c$	154.6372	7.6639	7.0937
$D1_t$	153.6667	7.5749	7.1258
D2	158.6416	7.5274	7.1048
D3	133.2740	8.2721	7.5597

S1.2 Azulene

Table 2 Vibrational corrections (in MHz) to the rotational constants of the different isotopic species of azulene at the HPCS2 level of theory. Refer to the main text for atom numbering.

Isotopic species	ΔA	ΔB	ΔC
Parent	20.1461	7.6747	5.4262
^{13}C1	19.9362	7.6147	5.3663
^{13}C2	20.1161	7.5548	5.3363
^{13}C4	19.7263	7.7047	5.3963
^{13}C5	19.8762	7.6147	5.3663
^{13}C6	19.9962	7.6147	5.3363
^{13}C9	19.9662	7.6447	5.3663
C1-D1	19.3666	7.6447	5.3063
C2-D1	20.0861	7.4349	5.2763
C4-D1	18.8569	7.7946	5.3363
C5-D1	19.4266	7.5847	5.3063
C6-D1	20.1760	7.4049	5.2763
C1,3-D2	18.7370	7.4648	5.1864
C4,8-D2	17.7477	7.8246	5.2464
C5,7-D2	18.7370	7.4648	5.1564

S1.3 t-Butyl isocyanide

Table 3 Vibrational corrections (in MHz) to the rotational constants of the different isotopic species of 1,4-dihydronaphthalene at the HPCS2 level of theory. Refer to the main text for atom numbering.

Isotopic species	ΔA	ΔB	ΔC
Parent	51.1989	18.8773	18.8773
C1	51.0948	17.9744	17.9744
N1	50.7238	18.6047	18.6047
C2	51.2553	18.6882	18.6882
C3	50.0131	18.7157	18.6309

S1.4 1,4-Dihydronaphthalene

Table 4 Vibrational corrections (in MHz) to the rotational constants of the different isotopic species of 1,4-dihydronaphthalene at the HPCS2 level of theory. Refer to the main text for atom numbering.

Isotopic species	ΔA	ΔB	ΔC
Parent	19.9987	7.5938	4.5728
^{13}C2/9	19.9493	7.4558	4.5109
^{13}C1/10	19.5252	7.5523	4.5200
^{13}C4/7	19.8417	7.5622	4.5437
^{13}C5/6	19.7518	7.5352	4.5343
^{13}C3/8	19.9060	7.4616	4.5151

S1.5 Proline II$_a$

Table 5 Vibrational corrections (in MHz) to the rotational constants of the different isotopic species of Proline II$_a$ at the HPCS2 level of theory. Refer to the main text for atom numbering.

Isotopic species	ΔA	ΔB	ΔC
Parent	44.3693	7.7047	7.1950
^{13}C1	44.3693	7.5548	6.8952
^{13}C2	42.4506	8.2143	7.2850
^{13}C3	42.4506	8.1544	7.2250
^{13}C4	43.5898	7.8546	7.1051
^{13}C5	45.3286	7.0151	6.7154
^{15}N	42.6904	8.1544	7.2550
ND	39.9623	8.6940	7.9745
OD	43.1401	7.5847	6.6854