

# Supporting Information

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## Explicitly correlated coupled cluster calculations for propadienylidene ( $\text{H}_2\text{CCC}$ )

6 tables

**TABLE S1:** Equilibrium geometrical parameters for H<sub>2</sub>CCC ( $\tilde{X}^1A_1$ ) from different CCSD(T)-F12x methods and two basis sets<sup>a</sup>

Geometrical parameter	VTZ-F12				VQZ-F12			
	F12a	F12a(*) <sup>b</sup>	F12b	F12b(*) <sup>b</sup>	F12a	F12a(*) <sup>b</sup>	F12b	F12b(*) <sup>b</sup>
$r_e$ (C <sub>(1)</sub> H)	1.08506	1.08511	1.08503	1.08508	1.08483	1.08486	1.08481	1.08484
$\alpha_e$ (HC <sub>(1)</sub> H)	117.549	117.551	117.546	117.548	117.544	117.45	117.543	117.544
$R_{1e}$ (C <sub>(1)</sub> C <sub>(2)</sub> )	1.33069	1.33119	1.33059	1.33109	1.33031	1.33057	1.33026	1.33052
$R_{2e}$ (C <sub>(2)</sub> C <sub>(3)</sub> )	1.29030	1.29048	1.29019	1.29037	1.28987	1.28997	1.28983	1.28993
$V_e$ (+115) /E <sub>h</sub>	-0.161273	-0.163300	-0.154398	-0.156425	-0.162799	-0.163837	-0.158672	-0.159711

<sup>a</sup> Equilibrium bond lengths in Å, bond angle in degrees. Valence electrons are correlated.

<sup>b</sup> (\*) denotes scaling of connected triple substitutions.

**TABLE S2:** Equilibrium geometrical parameters from all-electron CCSD(T) calculations

	VTZ <sup>b</sup>	CVTZ <sup>b</sup>	VQZ <sup>b</sup>	CVQZ <sup>b</sup>	V5Z <sup>c</sup>	CV5Z <sup>c</sup>	V6Z <sup>c</sup>	CV6Z <sup>c</sup>
$r_e$ (C <sub>(1)</sub> H) <sup>a</sup>	1.0812	1.0848	1.0825	1.0837	1.0814	1.0833	1.0822	1.0833
$\alpha_e$ (HC <sub>(1)</sub> H) <sup>a</sup>	117.40	117.40	117.40	117.46	117.48	117.52	117.52	117.53
$R_{1e}$ (C <sub>(1)</sub> C <sub>(2)</sub> ) <sup>a</sup>	1.3274	1.3312	1.3276	1.3281	1.3261	1.3274	1.3258	1.3273
$R_{2e}$ (C <sub>(2)</sub> C <sub>(3)</sub> ) <sup>a</sup>	1.2894	1.2918	1.2876	1.2879	1.2854	1.2869	1.2853	1.2867

<sup>a</sup> Bond lengths in Å, bond angle in degrees.

<sup>b</sup> Ref 9.

<sup>c</sup> Present work.

**TABLE S3:** Harmonic vibrational wavenumbers (in  $\text{cm}^{-1}$ ) for  $\text{H}_2\text{CCC}$  from different CCSD(T)-F12x methods and two basis sets

Vibration	VTZ-F12				VQZ-F12			
	F12a	F12a(*) <sup>a</sup>	F12b	F12b(*) <sup>a</sup>	F12a	F12a(*) <sup>a</sup>	F12b	F12b(*) <sup>a</sup>
$\omega_1$ ( $a_1$ )	3118.4	3117.4	3118.7	3117.6	3119.4	3119.0	3119.6	3119.1
$\omega_2$ ( $a_1$ )	1996.7	1994.5	1997.5	1995.4	1998.3	1997.1	1998.9	1997.7
$\omega_3$ ( $a_1$ )	1487.6	1486.6	1488.4	1487.6	1487.8	1487.2	1487.9	1487.6
$\omega_4$ ( $a_1$ )	1117.8	1116.2	1118.2	1116.7	1118.6	1117.6	1118.8	1118.0
$\omega_5$ ( $b_1$ )	1013.7	1012.6	1014.2	1013.0	1015.7	1015.4	1015.5	1015.0
$\omega_6$ ( $b_1$ )	203.2	202.3	202.7	202.0	206.0	205.5	205.8	205.2
$\omega_7$ ( $b_2$ )	3208.8	3207.8	3208.8	3207.8	3209.9	3209.5	3210.0	3209.5
$\omega_8$ ( $b_2$ )	1048.6	1047.8	1049.5	1048.7	1048.9	1048.5	1049.0	1048.8
$\omega_9$ ( $b_2$ )	268.4	267.1	268.2	267.3	270.2	269.2	269.8	269.3

<sup>a</sup> (\*) denotes scaling of connected triple substitutions.

**TABLE S4:** Harmonic vibrational wavenumbers and zero-point energies (in  $\text{cm}^{-1}$ ) from all-electron CCSD(T) calculations

	VTZ <sup>a</sup>	CVTZ <sup>a</sup>	VQZ <sup>b</sup>	CVQZ <sup>b</sup>	V5Z <sup>b</sup>	CV5Z <sup>b</sup>
$\omega_1$ (a <sub>1</sub> )	3148.0	3123.2	3132.6	3126.1	3137.1	3126.3
$\omega_2$ (a <sub>1</sub> )	2019.4	1997.9	2011.8	2004.8	2013.6	2007.7
$\omega_3$ (a <sub>1</sub> )	1503.5	1495.2	1495.7	1491.9	1496.8	1490.7
$\omega_4$ (a <sub>1</sub> )	1124.9	1118.5	1127.0	1122.3	1125.6	1122.7
$\omega_5$ (b <sub>1</sub> )	1048.4	1020.4	1030.8	1022.5	1025.6	1021.0
$\omega_6$ (b <sub>1</sub> )	239.5	216.9	228.0	210.9	203.8	210.2
$\omega_7$ (b <sub>2</sub> )	3211.4	3212.0	3220.9	3215.6	3224.7	3216.3
$\omega_8$ (b <sub>2</sub> )	1056.6	1052.0	1054.2	1051.5	1054.0	1052.0
$\omega_9$ (b <sub>2</sub> )	275.3	275.3	278.0	274.1	267.9	272.8
ZPE (harm)	6814	6756	6790	6760	6774	6760

<sup>a</sup> Ref 9.

<sup>b</sup> Present work.

**TABLE S5:** CCSD(T\*)-F12a/VQZ-F12 potential energy function (PEF) for the totally symmetric stretching vibrations of H<sub>2</sub>CCC

PEF term <sup>a</sup>				coefficient	PEF term <sup>a</sup>				coefficient
i	j	k	l	(a.u.)	i	j	k	l	(a.u.)
2	0	0	0	0.1776164	2	0	0	1	-0.0008492
3	0	0	0	-0.1271142	1	0	0	2	-0.0004061
4	0	0	0	0.0605114	2	2	0	0	0.0030314
5	0	0	0	-0.0248780	3	1	0	0	0.0001417
6	0	0	0	0.0070326	1	3	0	0	-0.0022304
0	2	0	0	0.0529956	0	2	2	0	0.0006254
0	3	0	0	0.0072258	0	3	1	0	0.0017544
0	4	0	0	0.0007077	0	1	3	0	0.0020230
0	5	0	0	0.0005206	0	0	2	2	0.0096868
0	6	0	0	-0.0001080	0	0	3	1	0.0089642
0	0	2	0	0.2904105	0	0	1	3	-0.0014076
0	0	3	0	-0.2909171	2	0	2	0	0.0038788
0	0	4	0	0.1857793	3	0	1	0	-0.0023784
0	0	5	0	-0.1016448	1	0	3	0	0.0032870
0	0	6	0	0.0392399	0	2	0	2	-0.0006306
0	0	0	2	0.3311562	0	3	0	1	-0.0008771
0	0	0	3	-0.3587094	0	1	0	3	-0.0003089
0	0	0	4	0.2334716	2	0	0	2	0.0068696
0	0	0	5	-0.1254794	3	0	0	1	0.0004173
0	0	0	6	0.0541677	1	0	0	3	0.0012486
1	1	0	0	-0.0107735	1	1	1	0	-0.0064017
2	1	0	0	0.0042664	1	1	0	1	-0.0010548
1	2	0	0	-0.0149471	1	0	1	1	0.0026437
0	1	1	0	0.0289800	0	1	1	1	0.0004306
0	2	1	0	-0.0057685	2	1	1	0	0.0001558
0	1	2	0	-0.0080080	1	2	1	0	0.0018173
0	0	1	1	0.0124444	1	1	2	0	-0.0008164
0	0	2	1	-0.0251801	2	1	0	1	-0.0008152
0	0	1	2	0.0055749	1	2	0	1	0.0001443
1	0	1	0	0.0125278	1	1	0	2	0.0009253
2	0	1	0	0.0049007	2	0	1	1	0.0007964
1	0	2	0	-0.0110693	1	0	2	1	-0.0010949
0	1	0	1	0.0020614	1	0	1	2	-0.0014654
0	2	0	1	-0.0028195	0	2	1	1	0.0051243
0	1	0	2	0.0005378	0	1	2	1	0.0006540
1	0	0	1	-0.0006752	0	1	1	2	-0.0025801
					1	1	1	1	-0.0006243

<sup>a</sup> See eqs 2a-2d and eq 3 for definition.

**TABLE S6:** CCSD(T\*)-F12a/VQZ-F12 electric dipole moment function (EDMF) for the totally symmetric vibrations of H<sub>2</sub>CCC

EDMF term <sup>a</sup>				coefficient	EDMF term <sup>a</sup>				coefficient
i	j	k	l	(a.u.)	i	j	k	l	(a.u.)
0	0	0	0	-1.65275	1	1	0	0	0.02510
1	0	0	0	0.02858	2	1	0	0	-0.02869
2	0	0	0	0.07311	1	2	0	0	-0.03784
3	0	0	0	0.00138	0	1	1	0	0.00093
4	0	0	0	0.00446	0	2	1	0	0.05304
0	1	0	0	-0.07706	0	1	2	0	0.06076
0	2	0	0	0.01168	0	0	1	1	0.40682
0	3	0	0	-0.05784	0	0	2	1	-0.44257
0	4	0	0	-0.01372	0	0	1	2	0.01015
0	0	1	0	-0.49070	1	0	1	0	-0.22187
0	0	2	0	0.07631	2	0	1	0	-0.10995
0	0	3	0	0.24019	1	0	2	0	0.04386
0	0	4	0	-0.10298	0	1	0	1	0.05803
0	0	0	1	0.98566	0	2	0	1	-0.00478
0	0	0	2	-0.16655	0	1	0	2	-0.15436
0	0	0	3	0.06082	1	0	0	1	0.02703
0	0	0	4	-0.04715	2	0	0	1	0.04075
					1	0	0	2	-0.11665
					1	1	1	0	-0.17015
					1	1	0	1	0.07453
					1	0	1	1	0.13530
					0	1	1	1	0.11594

<sup>a</sup> Defined in an analogous way as PEF terms.