

From Molecules with a Planar Tetracoordinate Carbon to an Astronomically Known C₅H₂ Carbene

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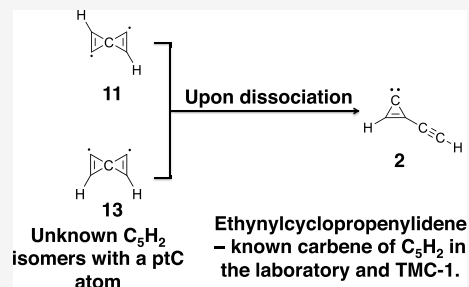


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Supporting Information

ABSTRACT: Ethynylcyclopropenylidene (**2**), an isomer of C₅H₂, is a known molecule in the laboratory and has recently been identified in Taurus Molecular Cloud-1 (TMC-1). Using high-level coupled-cluster methods up to the CCSDT(Q)/CBS level of theory, it is shown that two isomers of C₅H₂ with a planar tetracoordinate carbon (ptC) atom, (SP-4)-spiro[2.2]pent-1,4-dien-1,4-diyl (**11**) and (SP-4)-spiro[2.2]pent-1,4-dien-1,5-diyl (**13**), serve as the reactive intermediates for the formation of **2**. Here, a theoretical connection has been established between molecules containing ptC atoms (**11** and **13**) and a molecule (**2**) that is present nearly 430 light years away, thus providing evidence for the existence of ptC species in the interstellar medium. The reaction pathways connecting the transition states and the reactants and products have been confirmed by intrinsic reaction coordinate calculations at the CCSDT(Q)/CBS//B3LYP-D3BJ/cc-pVTZ level. While isomer **11** is non-polar ($\mu = 0$), isomers **2** and **13** are polar, with dipole moment values of 3.52 and 5.17 Debye at the CCSD(T)/cc-pVTZ level. Therefore, **13** is also a suitable candidate for both laboratory and radioastronomical studies.



INTRODUCTION

In 2021, two isomers of C₅H₂, ethynylcyclopropenylidene (**2**) and pentatetraenylidene (**3**) (see Figure 1), were identified in the Taurus Molecular Cloud-1 (TMC-1).^{1,2} To date, five isomers of C₅H₂ have been identified in the laboratory,^{3–12} including **2** and **3**. The other three isomers that have so far been identified in the laboratory alone are linear pentadiynylidene (**1**),^{4,8,9,12} ethynylpropadienylidene (**5**),⁷ and 2-cyclopropen-1-ylidenethenylidene (**8**).⁷ Among the five isomers that are identified in the laboratory, the linear triplet isomer, **1**, is a non-polar molecule and all other four carbene molecules (**2**, **3**, **5**, and **8**) have a permanent electric dipole ($\mu \neq 0$). The detection and spectral characterization of isomer **1**, which is an open-shell triplet ($\tilde{X}^3\Sigma_g^-$), was quite challenging for a long time.^{4,8,9} A detailed discussion related to this isomer was already reported by others^{9,13} and also in an earlier article by us, and therefore, it is not repeated here for brevity.¹⁴

Isomers **2**, **3**, **5**, and **8** of C₅H₂ were identified by Thaddeus, McCarthy, and co-workers using Fourier transform microwave (FTMW) spectroscopy in the Harvard Smithsonian Laboratory.^{3,6,7} Among the four isomers, the cumulene carbene isomer (**3**) was reported initially.³ Later, the laboratory detection of the three-membered ring-chain isomer (**2**) was reported with both a- and b-type rotational transitions as the inertial axis dipole moment components are in two directions for this molecule.⁶ Both **3** and **2** of C₅H₂ are higher homologues of propadienylidene (a cumulene carbene isomer of C₃H₂) and cyclopropenylidene (*c*-C₃H₂), respectively. Also, these two isomers of C₃H₂ and some of their isotopologues are known to exist in two starless cores (TMC-1C and

L1544).^{15–20} The laboratory detection of C₃H₂ isomers was undoubtedly very helpful in the identification of the same in the ISM.^{15,21} Stanton and co-workers predicted that isomers **5** and **8** are also low-lying isomers from the thermodynamic perspective (lying within 1 eV) based on the relative energies of C₅H₂ isomers computed using coupled-cluster theory.¹³ Bowie and co-workers had detected not only **5** but also **1** and **3** via the corresponding anion using the charge reversal and neutralization reionization mass spectra.¹⁰ Both of these theoretically suggested carbenes (**5** and **8**), which are highly polar with dipole moments of 4.79 and 8.16 Debye, respectively, at the all-electron-(ae)-CCSD(T)/cc-pVTZ level of theory,¹³ were also identified later using FTMW spectroscopy.⁷ In 2019, Hemberger and co-workers characterized isomers **1** and **8** of C₅H₂ using mass-selective threshold photoelectron spectroscopy.¹¹ They also determined an adiabatic ionization energy of 8.36 ± 0.03 and 8.60 ± 0.03 eV, respectively, for these two isomers.¹¹ Despite all these experimental evidence, our recent theoretical studies have predicted that three singlet polar carbenes, bent-pentadienylidene (**4**), buta-1,3-diynylcarbene (**6**), and 2-methylenebicyclo[1.1.0]but-1(3)-en-4-ylidene (**9**), are yet to

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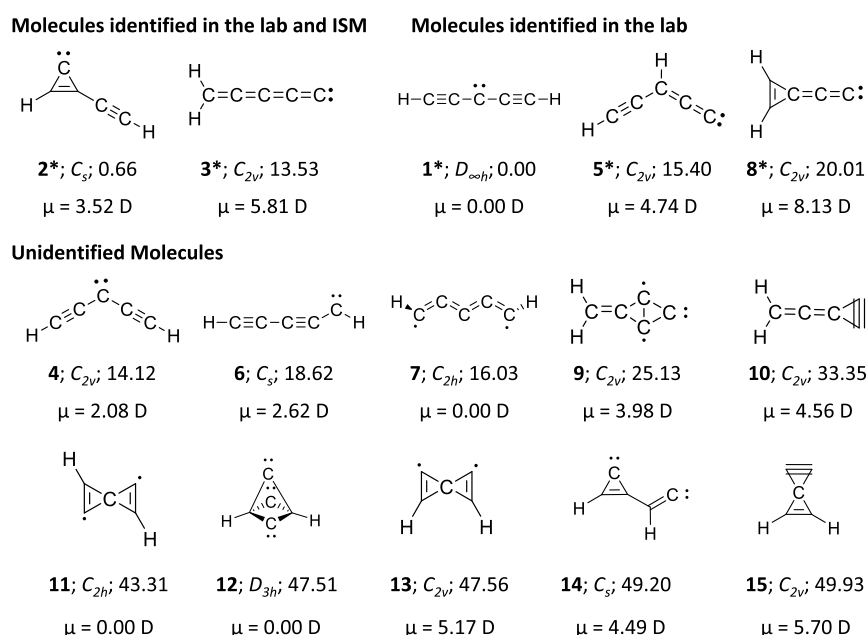


Figure 1. Fifteen different C_5H_2 isomers that are considered in the present work. Relative energies (ZPVE inclusive) are calculated at the CCSDT(Q)/CBS level of theory (in kcal mol⁻¹). ZPVEs and dipole moments (in Debye) are computed at the fc-CCSD(T)/cc-pVTZ level of theory. At the latter level, isomer 7 is a second-order saddle point, **10** and **15** are transition states, and all others are minima. It is also noted here that isomer **1** is a triplet ($\tilde{X}^3\Sigma_g^-$), and all others are singlets. Molecules identified in the laboratory are marked with an asterisk. Both **2** and **3** have been recently identified in TMC-1.^{1,2}

be identified in the laboratory.^{14,22} Thus, further theoretical exploration of C_5H_2 isomers became a natural prerequisite. Here, our prime focus is on two molecules, (SP-4)-spiro[2.2]pent-1,4-dien-1,4-diyl (**11**) and (SP-4)-spiro[2.2]pent-1,4-dien-1,5-diyl (**13**), that contain a planar tetracoordinate carbon (ptC) atom.^{23–26} Though molecules with a ptC atom deviate from the traditional aspects of the tetrahedral tetracoordinate nature of carbon, which is one of the cornerstones of organic chemistry, tremendous interest has been paid by both experimentalists^{27–31} and theoreticians^{32–42} in this new class of molecules as they could potentially be used as new materials. With respect to C_5H_2 , the relevance of isomers **11** and **13** in the formation of **2** is theoretically established here. Moreover, for **11** and **13**, high-level coupled-cluster calculations including spectroscopic parameters such as rotational and centrifugal distortion constants are still missing in the literature.^{8–11,13,14,43–55} Moreover, isomers **2** and **3** of C_5H_2 have been recently confirmed in TMC-1.^{1,2} Therefore, it is worth investigating the isomerization processes within C_5H_2 isomers, which leads to these two carbenes.

COMPUTATIONAL DETAILS

The C_5H_2 isomers (**1**–**15**) reported here (see Figure 1) are initially optimized using second-order Møller–Plesset perturbation theory (MP2).⁵⁷ Further, both geometry optimization and frequency calculations were also done using density functional theory (DFT) and coupled-cluster (CC) methods. The CC methods considered for the geometry optimizations are CC with singles and doubles (CCSD)^{58,59} and CCSD with perturbative triple excitations [CCSD(T)].^{60–62} We have used Dunning's correlation consistent polarized valence double and triple zeta (cc-pVnZ; n = D and T) basis sets⁶³ in these calculations. Frozen-core approximation is utilized (i.e., the carbon 1s orbitals are frozen) in the post-Hartree–Fock (HF) calculations. We note that the CCSD(T)/cc-pVTZ level of

theory has been found to give accurate equilibrium geometries with a mean-absolute deviation of only 0.003 Å relative to CCSD(T)/CBS bond distances for a wide and diverse set of the 122 species with up to five non-hydrogen atoms.⁶⁴ Harmonic vibrational frequencies were computed at the same levels of theory by the analytic calculation of second derivatives for all stationary points.⁶⁵ All MP2, CCSD, and CCSD(T) calculations were carried out with the CFOUR program package.⁶⁶ All DFT calculations were carried out at the B3LYP-D3BJ^{67–72}/def2-TZVP⁷³ level of theory. It is worthwhile to examine the effect of using a B3LYP-D3BJ/def2-TZVP or a CCSD(T)/cc-pVTZ reference geometry on the final W3-F12 energies. These results are presented in Table S1 of the Supporting Information for isomers **2**, **11**, **13**, and **14**. Inspection of Table S1 reveals that there is some reshuffling between the SCF and valence CCSD(T) correlation energies due to the structural changes. In particular, the SCF energy obtained with the B3LYP-D3BJ reference geometry deviates by 1.3–1.7 kcal mol⁻¹ from the CCSD(T) geometry, whereas the CCSD(T) correlation component obtained with the B3LYP-D3BJ geometry deviates by 1.2–1.5 kcal mol⁻¹ from that obtained with the CCSD(T) geometry. However, as is often the case when using DFT and CCSD(T) reference structures,^{74–76} the changes in the SCF and CCSD(T) correlation energies have opposite signs and cancel each other out to a large extent. The two reference geometries affect the core–valence component by about 0.2 kcal mol⁻¹ (Table S1). As expected, the difference in geometries has practically no effect on the post-CCSD(T) contributions. Overall, the differences in the all-electron CCSDT(Q)/CBS energies between the B3LYP-D3BJ and CCSD(T) structures are relatively small and amount to 0.11 (**2**), 0.17 (**11**), 0.17 (**13**), and –0.24 (**14**) kcal mol⁻¹. These differences are consistent with a recent study that examined the effect of the reference geometry on W1-F12 energies and obtained a mean-

Table 1. Component Breakdown of the W2-F12 and W3-F12 Relative Energies along with the Final W2-F12 and W3-F12 Values at the Bottom of the Well (ΔE_e) and at 0 K (ΔE_0)^a

theory ^g	comp.	2	3	4	5	6	7	8	9	10	11	12	13	14	15
W2-F12	HF	-18.77	4.88	2.66	1.89	6.48	11.91	1.98	20.01	29.59	30.38	55.68	34.05	19.11	36.87
W2-F12	CCSD	13.77	9.01	11.40	10.87	11.10	9.17	13.75	2.77	4.80	10.64	-8.09	11.17	23.25	10.27
W2-F12	(T)	1.73	-2.74	-0.65	-0.32	-1.55	-3.08	0.11	-2.50	-3.41	-0.93	-5.72	-0.76	3.50	-0.54
W2-F12	inner-shell	0.60	0.84	0.51	0.86	0.48	0.42	0.76	1.58	1.28	1.43	2.08	1.48	1.38	1.34
W2-F12	scalar rel.	-0.06	-0.11	-0.07	-0.12	-0.06	-0.05	-0.07	-0.17	-0.14	-0.15	-0.19	-0.15	-0.15	-0.12
W3.2	T-(T)	-0.06	-0.38	-0.59	-0.35	4.01	-0.96	-0.12	0.40	0.02	0.09	1.07	-0.01	-0.64	0.13
W3.2	(Q)	0.48	-0.33	-0.22	0.15	-2.26	-1.03	0.36	-0.08	-0.32	0.32	-0.78	0.35	0.83	0.42
W2-F12	CCSD(T)/CBS ^b	-2.73	11.89	13.85	13.19	16.45	18.37	16.53	21.71	32.12	41.37	43.76	45.79	47.09	47.82
W3-F12	CCSDT(Q)/CBS ^c	-2.31	11.18	13.04	12.99	18.20	16.38	16.77	22.03	31.83	41.77	44.05	46.14	47.28	48.37
W2-F12	ZPVE ^d	2.97	2.35	1.08	2.46	0.42	-0.35	3.24	3.10	1.52	1.54	3.46	1.42	1.92	1.56
W2-F12	CCSD(T)/CBS ^e	0.24	14.24	14.94	15.64	16.87	18.02	19.77	24.81	33.64	42.91	47.22	47.21	49.02	49.38
W3-F12	CCSDT(Q)/CBS ^f	0.66	13.53	14.12	15.44	18.62	16.03	20.01	25.13	33.35	43.31	47.51	47.56	49.20	49.93
other ^g	ae-CCSD(T)/cc-pVTZ ^h	2.01	13.82		16.78			21.14							
other ^g	M06-2X/cc-pVTZ	-0.60	18.02		20.67			17.78							
other ^g	CCSD(T)/cc-pVQZ ^k	-1.50	11.90	13.80	13.50	15.50		17.70							

^aAll values are given relative to isomer **1** in kcal mol⁻¹. ^bRelativistic, all-electron CCSD(T)/CBS relative energies at the bottom of the well (ΔE_e). ^cRelativistic, all-electron CCSDT(Q)/CBS relative energies at the bottom of the well (ΔE_e). ^dcc-CCSD(T)/cc-pVTZ harmonic ZPVEs scaled by a factor of 0.9868. ^eRelativistic, all-electron CCSD(T)/CBS relative energies at 0 K (ΔE_0). ^fRelativistic, all-electron CCSDT(Q)/CBS relative energies at 0 K (ΔE_0). ^gNon-relativistic, all-electron CCSD(T)/cc-pVTZ relative energies at 0 K (ΔE_0). ^hNote that the ZPVEs were calculated at the ae-CCSD/DZP level of theory. ⁱRelative energies at 0 K (ΔE_0) taken from ref 9. ^jRelative energies at 0 K (ΔE_0) taken from ref 48. ^kGeometries and ZPVEs calculated at the B3LYP/6-311G(d,p) level of theory. ^lValues for isomers **1**–**10** are from ref 22

absolute deviation of $0.29 \text{ kcal mol}^{-1}$ between B3LYP/def2-TZVPP and CCSD(T)/CBS structures for a wide and diverse set of 122 organic molecules.⁷⁶

All the transition states corresponding to the dissociation of C–C bonds connected to the ptC atom were obtained at the latter level, including intrinsic reaction coordinate (IRC) calculations.^{77,78} These calculations were done with the Gaussian 16 program suite.⁷⁹ We use the W3-F12 thermochemical protocol to obtain highly accurate relative energies for isomers 1–15 in Figure 1. The W3-F12 theory represents layered extrapolations to the relativistic, all-electron CCSDT(Q)/CBS limit and can achieve near-benchmark accuracy for challenging atomization and isomerization reactions.^{80–83} The valence CCSDT(Q) energy is extrapolated to the complete basis set (CBS) limit with basis sets of up to cc-VQZ-F12 quality. Inner-shell and scalar relativistic effects are calculated at the CCSD(T)/CBS level (for further details, see refs 80 and 83). All the W3-F12 single-point energy calculations were carried out using the fc-CCSD(T)/cc-pVTZ equilibrium geometries. Zero-point vibrational energies (ZPVEs) are calculated at the same level of theory and scaled by a scaling factor of 0.9868, as recommended elsewhere.⁵⁶ All the CCSD(T) energy calculations involved in the W3-F12 energies were computed using the Molpro program package,⁸⁴ while the post-CCSD(T) calculations were carried out with the MRCC program.^{85,86}

RESULTS AND DISCUSSION

Energetics. In Table 1, we have collected the component breakdown of the W3-F12 energies for 15 different C_5H_2 isomers. Relative energies including ZPVE corrections obtained from previous theoretical reports at different levels^{9,13,48} are also given for comparison. The parenthetical connected triple excitations [CCSD(T)–CCSD] make significant contributions to the relative energies of up to $-5.72 \text{ kcal mol}^{-1}$ (12). This also indicates that post-CCSD(T) contributions are likely to be important and cannot be neglected for chemical accuracy. Indeed, the higher-order triple contributions [CCSDT–CCSD(T)] reach up to $+4.01 \text{ kcal mol}^{-1}$, and the parenthetical connected quadruple excitations [CCSDT(Q)–CCSDT] reach up to $-2.26 \text{ kcal mol}^{-1}$ (both for 6). Overall, the post-CCSD(T) contributions approach or exceed 1 kcal mol^{-1} for four species, namely, -0.71 (3), -0.81 (4), $+1.75$ (6), and -1.99 (7) kcal mol^{-1} . For the rest of the species, post-CCSD(T) contributions range between $+0.19$ (14) and $+0.55$ (15) kcal mol^{-1} . Core–valence effects make significant contributions to the relative energies of up to $2.08 \text{ kcal mol}^{-1}$ (12) and likewise cannot be neglected for chemical accuracy. Finally, we note that as expected, scalar relativistic effects are relatively modest and do not exceed $0.19 \text{ kcal mol}^{-1}$.

Isomerization Pathways. Schematic reaction profile diagrams connecting reactants 11 and 13 and their isomerization products through the relevant transition states are shown in Figures 2 and 3, respectively. For isomer 11, two different transition states are identified with respect to the breaking of the C–C single bond connected to the ptC atom. The activation energy calculated for pathways A and B are 4.88 and $12.39 \text{ kcal mol}^{-1}$, respectively, at the W3-F12 level of theory. To reach to product 2 through transition-state A, a 1,2-hydrogen shift takes place, whereas to reach to 2 via transition-state B, a C–C bond breaking takes place followed by realignment of the molecule (to be planar), which justifies a

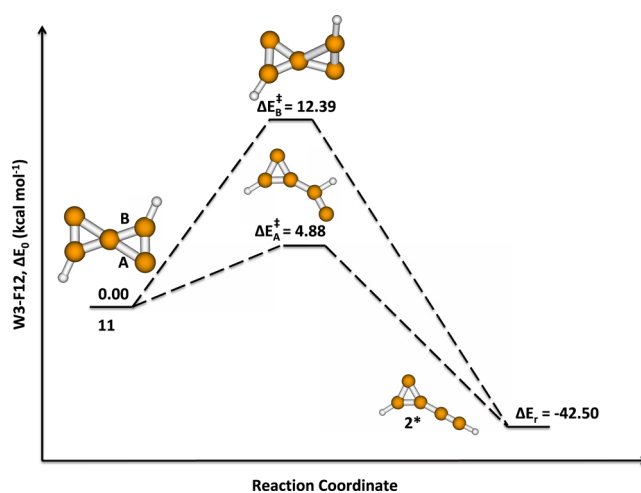


Figure 2. Schematic reaction profile for isomer 11 and its isomerization pathways connected to the ptC atom. Relative energy differences were calculated at the W3-F12 level of theory.

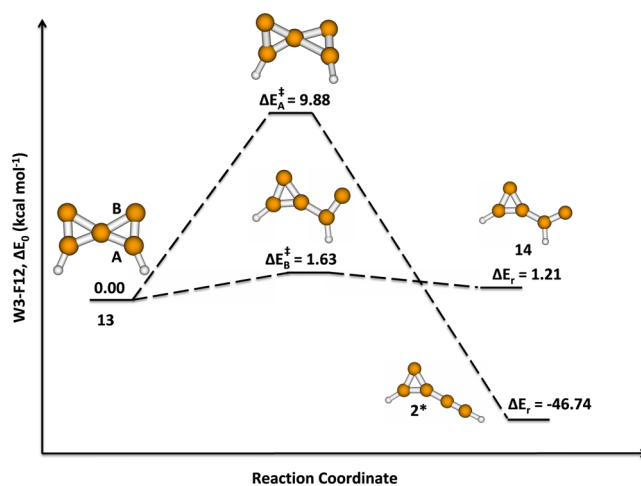


Figure 3. Schematic reaction profile for isomer 13 and its isomerization pathways connected to the ptC atom. Relative energy differences were calculated at the W3-F12 level of theory.

higher activation energy. The calculated reaction energy of $-42.50 \text{ kcal mol}^{-1}$ (energy difference between 2 and 11) for isomer 11 indicates the exothermic nature of the minimum-energy pathway in the formation of isomer 2.

With respect to isomer 13, we have located two different transition states as well as two different products (14 and 2) unlike isomer 11, where only a single product was formed. The activation energy calculated for pathways A and B in this case (see Figure 3) are 9.88 and $1.63 \text{ kcal mol}^{-1}$, respectively, at the W3-F12 level of theory. The lowest activation energy path (pathway B) leads to a bicarbene structure, 14, whose geometry is very similar to that of 13, except that one of the C–C bond connected to the ptC atom is broken. One can also arrive at isomer 11 from this bicarbene structure by the internal rotation of its C–C bond connected to the three-membered ring. It is noted here that in terms of relative energy, isomer 13 is slightly more stable than isomer 14. Though pathway B has the lowest activation energy compared to pathway A, thermodynamically the reactant (13) is more stable than the product (14), and therefore, pathway B is endothermic in nature. Moreover, isomer 13 is quite polar [$\mu =$

5.17 Debye at the CCSD(T)/cc-pVTZ level] like the other carbenes identified in the laboratory.^{3,6,7} Therefore, isomer **13** is also a potential candidate for both laboratory and astronomical observations though it lies 47.56 kcal mol⁻¹ above **1** at the CCSDT(Q)/CBS level of theory (see Figure 1). For brevity, the rotational and centrifugal distortion constants of isomers **13** and **14** are given in the Supporting Information (Table S21). It is worth noting here that thermodynamically high-lying isomers are found both in the laboratory and in the ISM. The case of cumulene carbenes, C_nH₂ (*n* = 3–6), is unequivocally one of the best known examples till date.^{2,3,16,87,88} For example, the longer chain isomer among the astronomically known cumulene carbenes is hexapentaenylidene, which lies at 50.30 kcal mol⁻¹ above the most stable triacetylene (HC₆H) molecule at the CCSD(T)/cc-pVTZ level of theory.⁸⁹ Also, in the laboratory, the case of 1-azulenylcarbene (C₁₁H₈), which lies 60.23 kcal mol⁻¹ above its global minimum isomer cyclopenta[*cd*]indene at the B3LYP/6-311+G(d,p) level of theory, is another good example.^{90,91} Back to C₅H₂ isomers, through pathway **A** of isomer **13**, one could also reach to isomer **2**. The calculated reaction energy of -46.74 kcal mol⁻¹ (energy difference between **2** and **13**) at the W3-F12 level for isomer **13** indicates the exothermic nature of the minimum energy pathway in arriving at **2**. All in all, both the ptC isomers that are minima are connected to the astronomically known molecule. Isomer **15**, (SP-4)-spiro[2.2]pent-1-en-4-yne, also contains a ptC atom. However, at all levels, it was identified to be a transition state. IRC calculations of isomer **15** reveal that it reaches to isomer **8** in both forward and reverse directions. It is noted here that **8** is a known molecule in the laboratory, and the presence of **5** and **8** is yet to be verified in the ISM though laboratory data are available.⁷

CONCLUSIONS

In conclusion, in this work, 15 different isomers of C₅H₂ are theoretically studied at the CCSDT(Q)/CBS level of theory. Among them, three isomers of C₅H₂ contain a ptC atom. While two are minima (**11** and **13**), one structure is a transition state (**15**). Isomerization pathways of C–C single bonds connected to the ptC atom in isomers **11** and **13** reveal that they both serve as reactive intermediates for the formation of isomer **2**, which is a known molecule not only in the laboratory but also in TMC-1, which is 430 light years away. It is believed that the current theoretical work carried out here may assist and encourage further experimental and observational studies in identifying isomer **13** in the laboratory as well as in the ISM, respectively.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/acs.jpca.2c01261>.

Cartesian coordinates of the optimized geometries, total electronic energies, ZPVEs, ZPVE-corrected total energies, harmonic vibrational frequencies, IR intensities, and rotational and centrifugal distortion constants of C₅H₂ isomers calculated at different levels (PDF)

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Notes

The authors declare no competing financial interest.

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