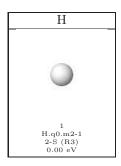
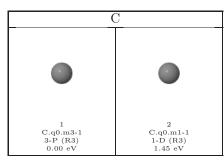
M3C-store

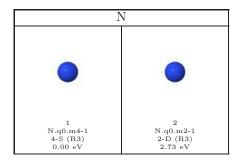
https://github.com/nfaguirrec/M3C-store

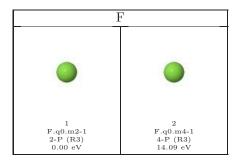
August 9, 2019

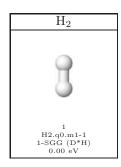
The latest release of M3C-store (version 1.2.0, released 2019-08-09) contains 1673 molecules including carbon clusters, hydrogenated and nitrogenated carbon clusters, and fragments from the furan molecule fragmentation. Its principal aim is to include the fragments necessary to describe the fragmentation of a given molecule. Each molecule is available at two levels of theory: B3LYP and CCSD(T), and two basis sets: 6-311++G(d,p) and 6-311++G(3df,2p). The files format is an extension of the popular .xyz format. Each molecule's file contains the energy, geometry, vibrational frequencies, symmetry and the symmetry of the electronic state. This database has been specially adapted as the starting point of an M3C calculation.

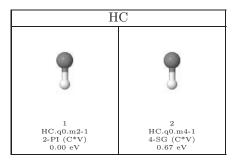


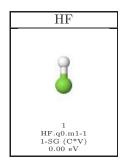


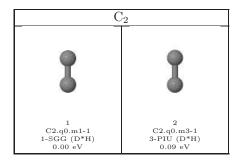


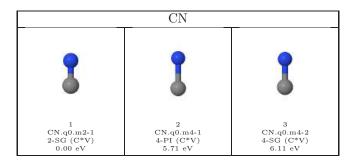


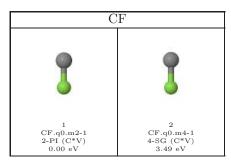


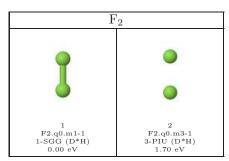


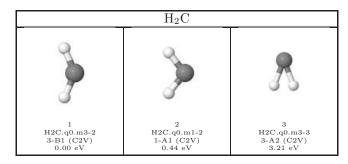


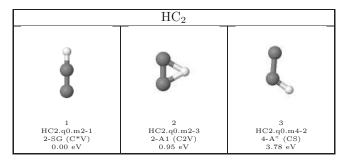


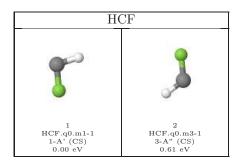




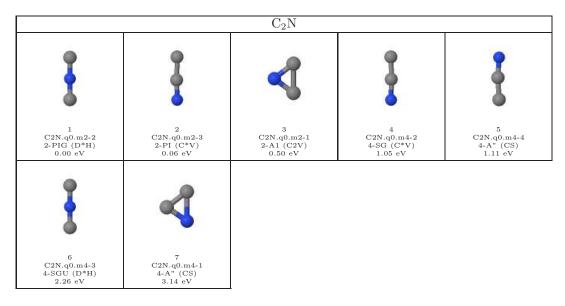


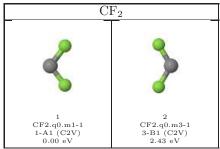


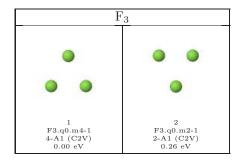


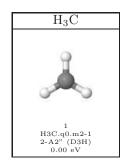


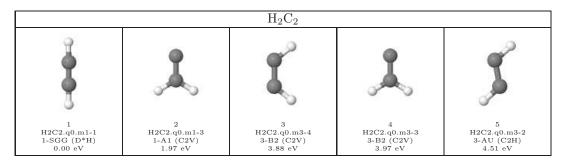
	C_3	
1	8	}
1 C3.q0.m1-1 1-SGG (D*H) 0.00 eV	2 C3.q0.m3-1 3-A1 ⁷ (D3H) 0.84 eV	3 C3.q0.m3-2 3-A" (CS) 2.22 eV

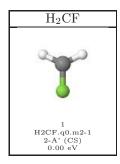


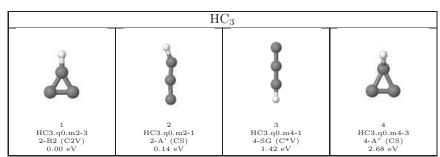


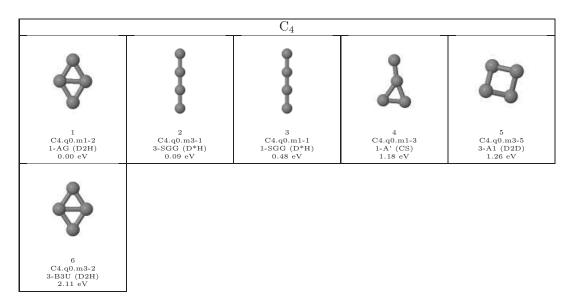


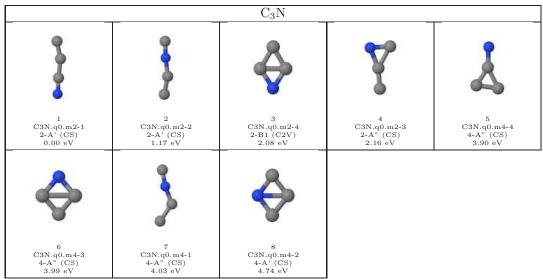


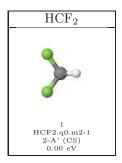


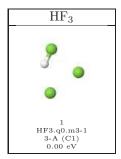


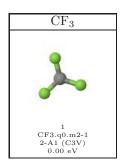


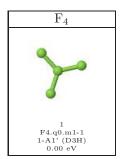


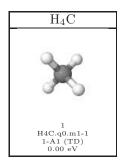


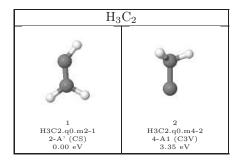


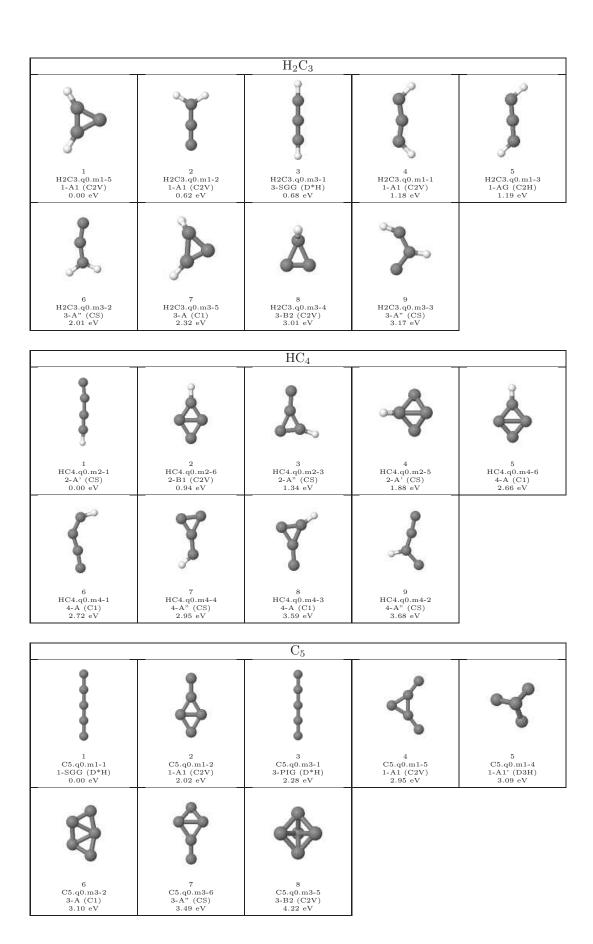




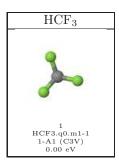


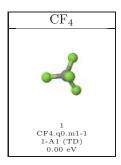


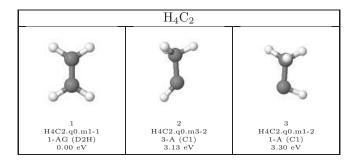


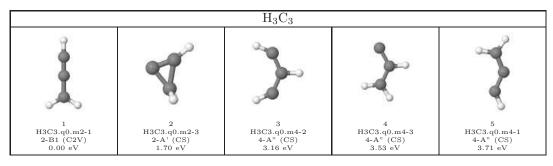


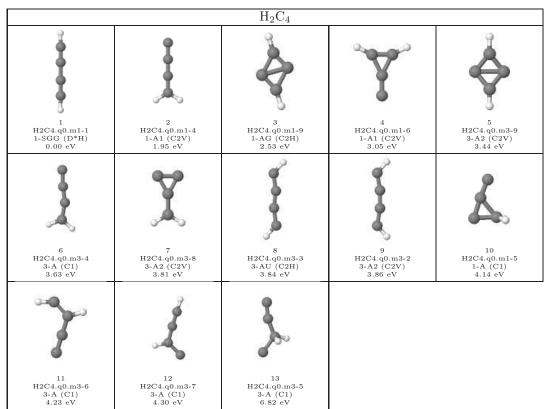
		$\mathrm{C_4N}$		
1 C4N.q0.m2-11 2-PI (C*V) 0.00 eV	2 C4N.q0.m2-6 2-B2 (C2V) 0.03 eV	3 C4N.q0.m2-7 2-B2 (C2V) 0.83 eV	4 C4N.q0.m2-3 2-PI (C*V) 1.00 eV	5 C4N.q0.m4-2 4-SG (C*V) 1.07 eV
7		0.000		\$
6 C4N.q0.m2-2 2-A' (CS) 1.57 eV	7 C4N.q0.m4-5 4-SG (C*V) 2.31 eV	8 C4N.q0.m2-1 2-PI (C*V) 2.69 eV	9 C4N.q0.m4-3 4-A (C1) 3.37 eV	10 C4N.q0.m4-8 4-A' (CS) 3.58 eV
		13	14	15
C4N.q0.m4-4 4-A" (CS) 3.60 eV	C4N.q0.m4-1 4-A" (CS) 3.62 eV	C4N.q0.m2-10 2-B2 (C2V) 4.14 eV	C4N.q0.m2-5 2-B2 (C2V) 4.29 eV	C4N.q0.m2-9 2-A' (CS) 4.41 eV
♦	\$	\$		\$
16 C4N.q0.m2-8 2-A1 (C3V) 4.49 eV	17 C4N.q0.m2-4 2-A' (CS) 4.49 eV	18 C4N.q0.m4-9 4-A" (CS) 5.74 eV	19 C4N.q0.m4-6 4-A1 (C2V) 5.75 eV	20 C4N.q0.m4-7 4-A' (CS) 6.30 eV





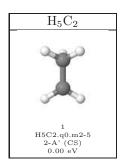


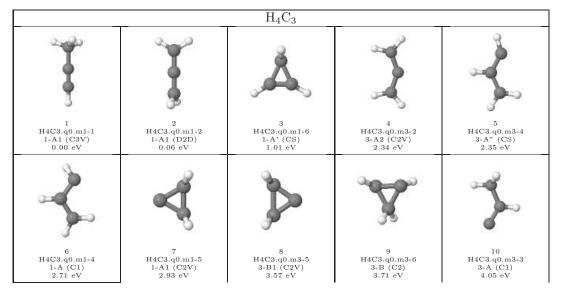




		HC_5		
		Å		*
1 HC5.q0.m2-1 2-PI (C*V) 0.00 eV	2 HC5.q0.m2-2 2-B2 (C2V) 0.10 eV	3 HC5.q0.m2-3 2-A' (CS) 0.91 eV	4 HC5.q0.m4-1 4-SG (C*V) 1.25 eV	5 HC5.q0.m2-11 2-A' (CS) 1.53 eV
N	>	*	Ø	*
6 HC5.q0.m2-8 2-A (C1) 2.01 eV	7 HC5.q0.m2-4 2-B2 (C2V) 2.18 eV	8 HC5.q0.m2-6 2-A' (CS) 2.20 eV	9 HC5.q0.m4-13 4-A" (CS) 2.65 eV	10 HC5.q0.m4-2 4-A" (CS) 2.71 eV
4	*	•		
11 HC5.q0.m2-15 2-A1 (C3V) 2.77 eV	12 HC5.q0.m2-14 2-B2 (C2V) 2.80 eV	13 HC5.q0.m4-6 4-A" (CS) 2.92 eV	14 HC5.q0.m2-9 2-A (C1) 2.98 eV	15 HC5.q0.m4-4 4-A2 (C2V) 3.16 eV
À	\$	•	*	
16 HC5.q0.m4-3 4-A" (CS) 3.25 eV	17 HC5.q0.m4-11 4-A (C1) 3.41 eV	18 HC5.q0.m2-10 2-A" (CS) 3.70 eV	19 HC5.q0.m4-12 4-A' (CS) 3.75 eV	20 HC5.q0.m4-5 4-A' (CS) 3.99 eV
\$	7		*	÷
21 HC5.q0.m4-9 4-A" (CS) 4.09 eV	22 HC5.q0.m4-7 4-A" (CS) 4.33 eV	23 HC5.q0.m4-15 4-A" (CS) 4.42 eV	24 HC5.q0.m4-14 4-A (C1) 4.90 eV	25 HC5.q0.m4-10 4-A' (CS) 5.46 eV

		C_6		
			\Diamond	į
1 C6.q0.m1-2 1-A1' (D3H) 0.00 eV	2 C6.q0.m3-1 3-SGG (D*H) 0.62 eV	3 C6.q0.m1-1 1-SGG (D*H) 0.77 eV	4 C6.q0.m3-2 3-B2 (C2V) 1.39 eV	5 C6.q0.m1-5 1-A1 (C2V) 1.45 eV
	7	8 8 5 5	9	10
C6.q0.m1-4 1-AG (D2H) 1.75 eV	C6.q0.m1-6 1-A' (CS) 2.51 eV	C6.q0.m3-5 3-B1 (C2V) 3.34 eV	C6.q0.m1-7 1-A1 (C2V) 3.89 eV	C6.q0.m3-3 3-A (C1) 4.58 eV
\$	~			
11 C6.q0.m3-4 3-A (C1) 5.10 eV	12 C6.q0.m3-6 3-A" (CS) 5.54 eV			

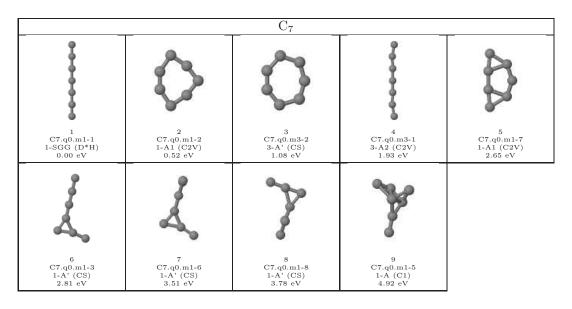


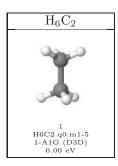


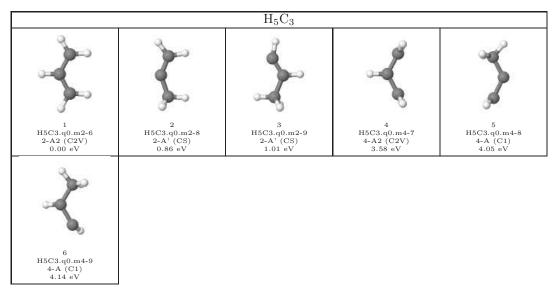
		$\mathrm{H_{3}C_{4}}$		
1	2	3	4	5
H3C4.q0.m2-2	H3C4.q0.m2-5	H3C4.q0.m2-13	H3C4.q0.m2-3	H3C4.q0.m2-7
2-B2 (C2V)	2-A' (CS)	2-A" (CS)	2-A (C1)	2-A (C1)
0.00 eV	0.42 eV	1.16 eV	1.18 eV	1.18 eV
6	7	8	9	10
H3C4.q0.m2-10	H3C4.q0.m2-12	H3C4.q0.m2-1	H3C4.q0.m2-14	H3C4.q0.m4-12
2-A (C1)	2-A" (CS)	2-A" (CS)	2-A (C1)	4-B2 (C2V)
1.40 eV	1.46 eV	1.60 eV	1.99 eV	2.25 eV
11	12	13	14	15
H3C4.q0.m4-2	H3C4.q0.m2-4	H3C4.q0.m2-8	H3C4.q0.m4-1	H3C4.q0.m4-5
4-A (C1)	2-A' (CS)	2-A (C1)	4-A1 (C3V)	4-A (C1)
2.35 eV 16 H3C4.q0.m4-14 4-A" (CS)	2.44 eV 17 H3C4.q0.m4-7 4-A" (CS)	2.70 eV 18 H3C4.q0.m4-3 4-A" (CS)	3.03 eV 19 H3C4.q0.m4-13 4-A (C1)	20 H3C4.q0.m4-8 4-A" (CS)
3.32 eV	3.56 eV	3.73 eV	3.75 eV	3.94 eV
H3C4.q0.m4-4	H3C4.q0.m4-10	H3C4.q0.m4-6	H3C4.q0.m4-9	
4-A" (CS)	4-A (C1)	4-A (C1)	4-A (C1)	
4.29 eV	4.30 eV	4.49 eV	4.68 eV	

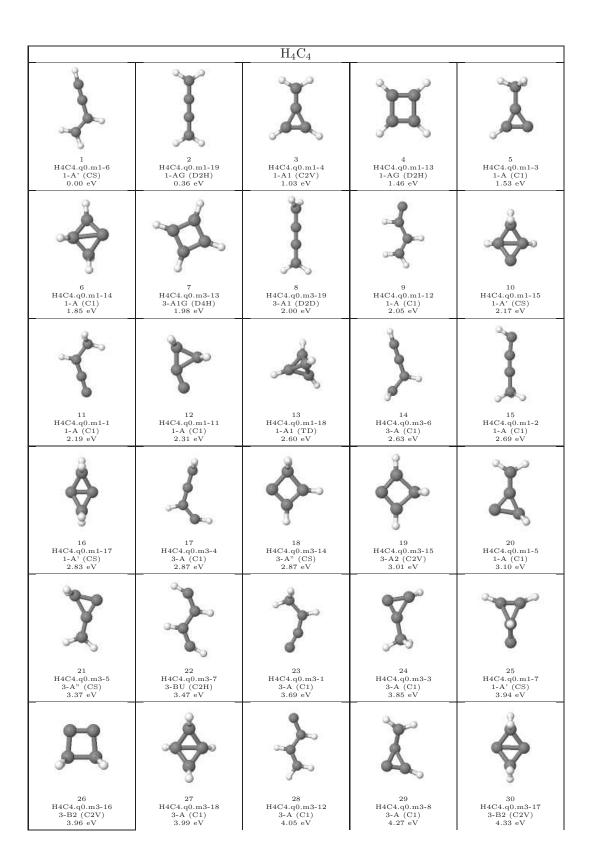
		$\mathrm{H_{2}C_{5}}$		
		3	4	5
H2C5.q0.m1-6 1-A' (CS) 0.00 eV	H2C5.q0.m3-1 3-SG (C*V) 0.21 eV	H2C5.q0.m1-2 1-A (C1) 0.61 eV	H2C5.q0.m1-14 1-A' (CS) 0.67 eV	H2C5.q0.m1-15 1-A1 (C2V) 0.77 eV
	*)	B	X
6 H2C5.q0.m1-4 1-A1 (C2V) 0.82 eV	7 H2C5.q0.m1-17 1-A1 (C2V) 0.99 eV	8 H2C5.q0.m3-2 3-A (C2) 1.72 eV	9 H2C5.q0.m1-29 1-A (C2) 1.84 eV	10 H2C5.q0.m1-12 1-A (C1) 1.86 eV
4		d	D	•
11 H2C5.q0.m1-30 1-A (C1) 1.89 eV	12 H2C5.q0.m3-14 3-A (C1) 1.91 eV	13 H2C5.q0.m1-28 1-A' (CS) 2.19 eV	14 H2C5.q0.m3-29 3-A2 (C2V) 2.30 eV	15 H2C5.q0.m1-25 1-A (C1) 2.44 eV
*	1		•	\$
16 H2C5.q0.m1-16 1-A (C1) 2.51 eV	17 H2C5.q0.m3-6 3-A" (CS) 2.64 eV	18 H2C5.q0.m1-31 1-A' (CS) 2.64 eV	19 H2C5.q0.m3-20 3-A (C1) 2.78 eV	20 H2C5.q0.m3-17 3-A" (CS) 2.83 eV
A	A		\$	2
21 H2C5.q0.m1-27 1-A (C1) 2.84 eV	22 H2C5.q0.m3-28 3-B2 (C2V) 2.87 eV	23 H2C5.q0.m3-4 3-A (C1) 2.89 eV	24 H2C5.q0.m1-26 1-A (C1) 2.91 eV	25 H2C5.q0.m3-10 3-A (C1) 2.95 eV
	4			
26 H2C5.q0.m3-8 3-A (C1) 3.05 eV	27 H2C5.q0.m1-13 1-A1 (C2V) 3.25 eV	28 H2C5.q0.m3-25 3-A" (CS) 3.42 eV	29 H2C5.q0.m3-3 3-A" (CS) 3.42 eV	30 H2C5.q0.m3-26 3-A" (CS) 3.52 eV

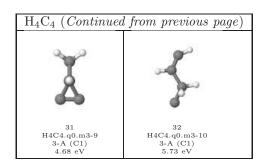
	H ₂ C ₅ (<i>Ca</i>	ontinued from preva	ious page)	
31	32	33	34	35
H2C5.q0.m3-19 3-A (C1) 3.62 eV	H2C5.q0.m3-16 3-A" (CS) 3.65 eV	H2C5.q0.m1-21 1-A' (CS) 3.70 eV	H2C5.q0.m3-30 3-A' (CS) 3.84 eV	H2C5.q0.m3-5 3-A (C1) 3.84 eV
Q	*	7	\$	A
36 H2C5.q0.m3-27 3-A (C1) 3.94 eV	37 H2C5.q0.m3-18 3-A" (CS) 4.05 eV	38 H2C5.q0.m3-12 3-A (C1) 4.09 eV	39 H2C5.q0.m3-21 3-A" (CS) 4.11 eV	40 H2C5.q0.m3-31 3-A" (CS) 4.14 eV
4	*	3	♦	Å
41 H2C5.q0.m3-13 3-A (C1) 4.21 eV	42 H2C5.q0.m1-18 1-A (C1) 4.39 eV	43 H2C5.q0.m3-22 3-A (C1) 4.47 eV	44 H2C5.q0.m3-24 3-A' (CS) 4.89 eV	45 H2C5.q0.m3-7 3-A (C1) 5.09 eV
1	*			
46 H2C5.q0.m3-9 3-A (C1) 5.26 eV	47 H2C5.q0.m3-23 3-A (C1) 5.70 eV			





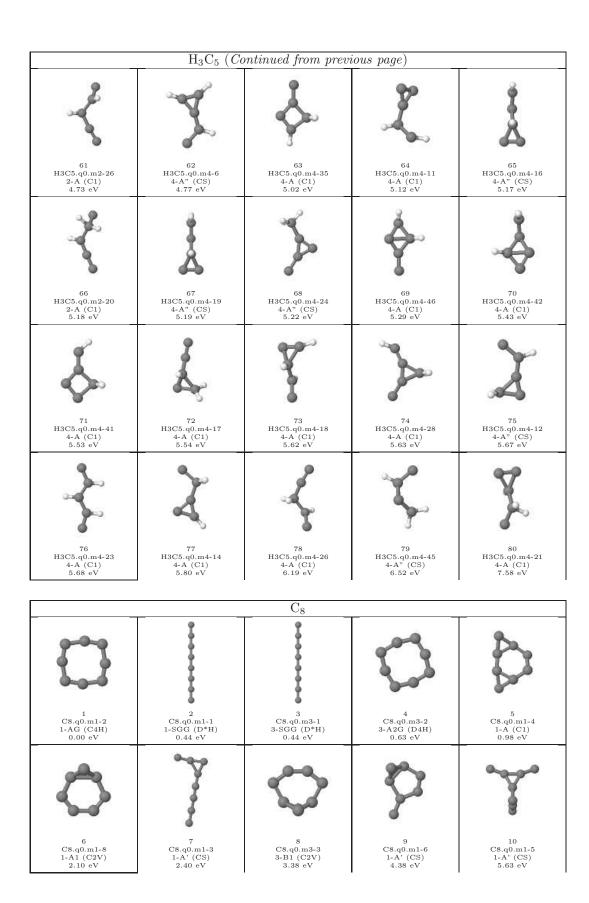




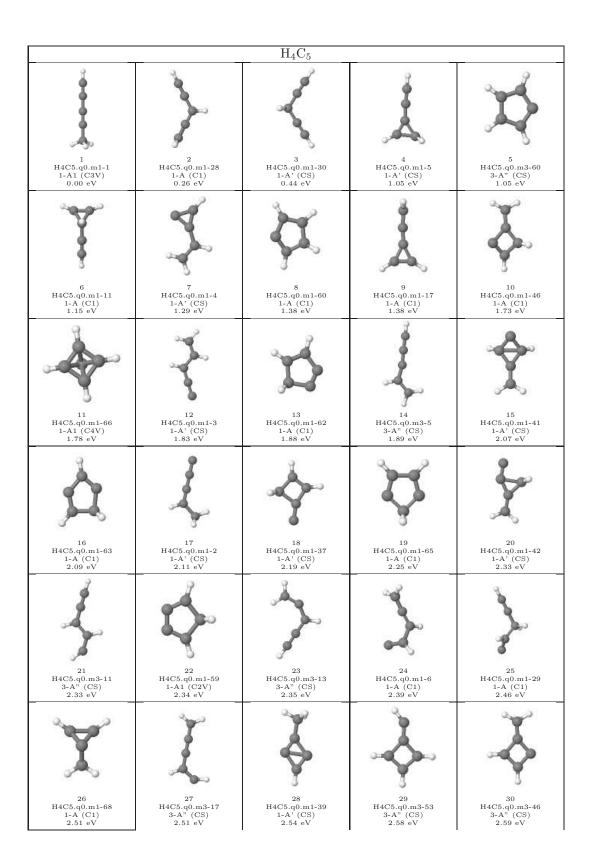


		$\mathrm{H_{3}C_{5}}$		
	>	Å	*	
H3C5.q0.m2-2 2-A (C1) 0.00 eV	H3C5.q0.m2-27 2-B1 (C2V) 0.04 eV	H3C5.q0.m2-50 2-A" (CS) 1.42 eV	H3C5.q0.m2-37 2-A" (CS) 1.60 eV	5 H3C5.q0.m2-1 2-A (C1) 1.70 eV
T		I	>	
6 H3C5.q0.m2-9 2-A' (CS) 1.76 eV	7 H3C5.q0.m2-3 2-A" (CS) 1.81 eV	8 H3C5.q0.m2-10 2-A (C1) 1.93 eV	9 H3C5.q0.m2-22 2-A (C1) 1.93 eV	10 H3C5.q0.m2-8 2-A" (CS) 2.08 eV
Å	P		X	-
11 H3C5.q0.m4-50 4-B2 (C2V) 2.09 eV	12 H3C5.q0.m4-49 4-A2 (C2V) 2.16 eV	13 H3C5.q0.m2-28 2-A (C1) 2.21 eV	14 H3C5.q0.m2-5 2-A' (CS) 2.23 eV	15 H3C5.q0.m2-32 2-A" (CS) 2.30 eV
-	*	B	*	*
16 H3C5.q0.m2-25 2-A (C1) 2.45 eV	17 H3C5.q0.m2-33 2-A (C1) 2.49 eV	18 H3C5.q0.m2-47 2-A (C1) 2.64 eV	19 H3C5.q0.m2-36 2-A (C1) 2.69 eV	20 H3C5.q0.m4-7 4-A (C1) 2.71 eV
	*	d		X
21 H3C5.q0.m2-51 2-B1 (C2V) 2.75 eV	22 H3C5.q0.m2-4 2-A' (CS) 2.77 eV	23 H3C5.q0.m2-48 2-A' (CS) 2.84 eV	24 H3C5.q0.m4-2 4-A (C1) 2.90 eV	25 H3C5.q0.m2-6 2-A' (CS) 2.91 eV
\$	>	*		*
26 H3C5.q0.m2-40 2-A (C1) 2.97 eV	27 H3C5.q0.m2-24 2-A (C1) 3.03 eV	28 H3C5.q0.m2-35 2-A' (CS) 3.19 eV	29 H3C5.q0.m4-3 4-A" (CS) 3.25 eV	30 H3C5.q0.m4-36 4-A" (CS) 3.49 eV

H ₃ C ₅ (Continued from previous page)				
\$	X			7
31 H3C5.q0.m2-39 2-A (C1) 3.50 eV	32 H3C5.q0.m2-53 2-A' (CS) 3.54 eV	33 H3C5.q0.m2-34 2-A (C1) 3.59 eV	34 H3C5.q0.m4-40 4-A" (CS) 3.60 eV	35 H3C5.q0.m4-8 4-A" (CS) 3.61 eV
-	\$	P		
36 H3C5.q0.m4-31 4-A" (CS) 3.63 eV	37 H3C5.q0.m4-33 4-A" (CS) 3.65 eV	38 H3C5.q0.m4-48 4-A" (CS) 3.79 eV	39 H3C5.q0.m4-13 4-A (C1) 3.84 eV	40 H3C5.q0.m2-18 2-A (C1) 3.90 eV
	-			a
41 H3C5.q0.m2-46 2-A (C1) 3.92 eV	42 H3C5.q0.m4-32 4-A' (CS) 3.94 eV	43 H3C5.q0.m2-12 2-A (C1) 3.95 eV	44 H3C5.q0.m4-27 4-A2 (C2V) 3.97 eV	45 H3C5.q0.m4-47 4-A (C1) 3.99 eV
*		4		-
46 H3C5.q0.m4-25 4-A" (CS) 4.00 eV	47 H3C5.q0.m4-4 4-A" (CS) 4.00 eV	48 H3C5.q0.m4-37 4-A" (CS) 4.04 eV	49 H3C5.q0.m4-22 4-A" (CS) 4.06 eV	50 H3C5.q0.m2-38 2-A' (CS) 4.16 eV
300	\$	1	3	7
51 H3C5.q0.m2-23 2-A" (CS) 4.17 eV	52 H3C5.q0.m4-39 4-A (C1) 4.18 eV	53 H3C5.q0.m4-5 4-A" (CS) 4.31 eV	54 H3C5.q0.m4-1 4-A" (CS) 4.41 eV	55 H3C5.q0.m4-10 4-A" (CS) 4.44 eV
7	1	*		
56 H3C5.q0.m4-9 4-A" (CS) 4.48 eV	57 H3C5.q0.m2-14 2-A (C1) 4.55 eV	58 H3C5.q0.m4-38 4-A (C1) 4.65 eV	59 H3C5.q0.m4-15 4-A" (CS) 4.70 eV	60 H3C5.q0.m4-43 4-A" (CS) 4.72 eV



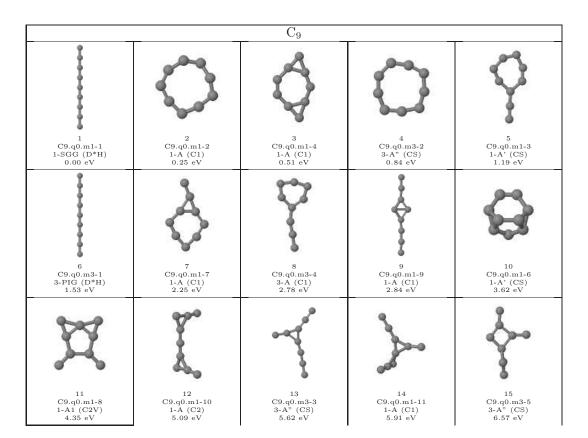
	$\mathrm{H_6C_3}$	
	~	
1 H6C3.q0.m1-4 1-A (C1) 0.00 eV	2 H6C3.q0.m1-3 1-A1' (D3H) 0.32 eV	3 H6C3.q0.m3-4 3-A (C1) 2.95 eV



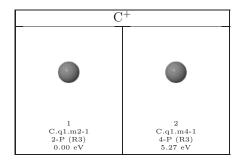
	$\mathrm{H_4C_5}$ (Continued from previous page)				
*	*	A		a	
31 H4C5.q0.m1-45 1-A (C1) 2.60 eV	32 H4C5.q0.m1-47 1-A' (CS) 2.63 eV	33 H4C5.q0.m3-59 3-B2 (C2V) 2.64 eV	34 H4C5.q0.m1-14 1-A1 (C2V) 2.65 eV	35 H4C5.q0.m3-65 3-A (C1) 2.68 eV	
-	A	\$		*	
36 H4C5.q0.m1-67 1-A' (CS) 2.69 eV	37 H4C5.q0.m3-63 3-A (C1) 2.69 eV	38 H4C5.q0.m3-41 3-A2 (C2V) 2.73 eV	39 H4C5.q0.m1-53 1-A (C1) 2.86 eV	40 H4C5.q0.m1-25 1-A' (CS) 2.95 eV	
*			7	*	
41 H4C5.q0.m1-40 1-A (C1) 2.97 eV	42 H4C5.q0.m3-32 3-B1 (C2V) 3.05 eV	43 H4C5.q0.m1-38 1-A (C1) 3.09 eV	44 H4C5.q0.m1-16 1-A' (CS) 3.09 eV	45 H4C5.q0.m1-10 1-A' (CS) 3.10 eV	
		a gray	A	*	
46 H4C5.q0.m3-28 3-A" (CS) 3.16 eV	47 H4C5.q0.m1-13 1-A (C1) 3.17 eV	48 H4C5.q0.m3-3 3-A" (CS) 3.21 eV	49 H4C5.q0.m1-61 1-A' (CS) 3.35 eV	50 H4C5.q0.m3-47 3-A (C1) 3.39 eV	
*	P	7	\$		
51 H4C5.q0.m3-39 3-A" (CS) 3.42 eV	52 H4C5.q0.m3-62 3-A" (CS) 3.43 eV	53 H4C5.q0.m3-4 3-A" (CS) 3.45 eV	54 H4C5.q0.m3-52 3-A' (CS) 3.54 eV	55 H4C5.q0.m1-70 1-A1 (C2V) 3.55 eV	
*	4	*		\$	
56 H4C5.q0.m3-10 3-A" (CS) 3.55 eV	57 H4C5.q0.m3-50 3-A' (CS) 3.59 eV	58 H4C5.q0.m3-16 3-A" (CS) 3.63 eV	59 H4C5.q0.m3-2 3-A (C1) 3.63 eV	60 H4C5.q0.m3-42 3-A (C1) 3.73 eV	

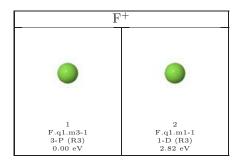
$\mathrm{H_4C_5}$ (Continued from previous page)				
No.	2	X	a face	•
61 H4C5.q0.m1-71 1-A (C1) 3.76 eV	62 H4C5.q0.m3-18 3-A (C1) 3.84 eV	63 H4C5.q0.m1-15 1-A1 (C2V) 3.85 eV	64 H4C5.q0.m3-35 3-A (C1) 3.89 eV	65 H4C5.q0.m3-44 3-A (C1) 3.93 eV
7	\langle	*		4
66 H4C5.q0.m3-22 3-A (C1) 3.93 eV	67 H4C5.q0.m1-69 1-A1 (C2V) 3.99 eV	68 H4C5.q0.m3-37 3-A (C1) 4.03 eV	69 H4C5.q0.m3-30 3-B (C2) 4.04 eV	70 H4C5.q0.m1-23 1-A (C1) 4.14 eV
*	Ž		7	7
71 H4C5.q0.m3-54 3-A (C1) 4.21 eV	72 H4C5.q0.m3-6 3-A (C1) 4.24 eV	73 H4C5.q0.m3-27 3-A" (CS) 4.30 eV	74 H4C5.q0.m3-9 3-A (C1) 4.34 eV	75 H4C5.q0.m3-8 3-A" (CS) 4.37 eV
A	X		L	Y
76 H4C5.q0.m3-61 3-B1 (C2V) 4.37 eV	77 H4C5.q0.m1-31 1-A' (CS) 4.37 eV	78 H4C5.q0.m3-29 3-A (C1) 4.37 eV	79 H4C5.q0.m3-19 3-A (C1) 4.38 eV	80 H4C5.q0.m3-25 3-A (C1) 4.38 eV
	2		*	\$
81 H4C5.q0.m3-40 3-A (C1) 4.39 eV	82 H4C5.q0.m3-15 3-A (C1) 4.39 eV	83 H4C5.q0.m3-38 3-A" (CS) 4.40 eV	84 H4C5.q0.m1-34 1-A (C2) 4.50 eV	85 H4C5.q0.m3-45 3-A (C1) 4.50 eV
>		1	*	*
86 H4C5.q0.m3-26 3-A (C1) 4.56 eV	87 H4C5.q0.m1-49 1-A' (CS) 4.59 eV	88 H4C5.q0.m3-7 3-A (C1) 4.67 eV	89 H4C5.q0.m3-43 3-A (C1) 4.70 eV	90 H4C5.q0.m3-33 3-A (C1) 4.74 eV

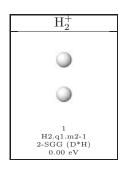
$\mathrm{H_4C_5}$ (Continued from previous page)							
.	\$	*	\darphi				
91 H4C5.q0.m3-69 3-A' (CS) 4.75 eV	92 H4C5.q0.m1-48 1-A' (CS) 4.76 eV	93 H4C5.q0.m3-70 3-B1 (C2V) 4.76 eV	94 H4C5.q0.m3-66 3-A' (CS) 4.81 eV	95 H4C5.q0.m1-7 1-A (C1) 4.82 eV			
\frac{1}{2}	Q	D	7	*			
96 H4C5.q0.m3-48 3-A" (CS) 4.93 eV	97 H4C5.q0.m3-64 3-A" (CS) 4.96 eV	98 H4C5.q0.m1-64 1-A' (CS) 5.07 eV	99 H4C5.q0.m3-24 3-A (C1) 5.08 eV	100 H4C5.q0.m3-71 3-A (C1) 5.14 eV			
*	\$	*		\$			
101 H4C5.q0.m1-12 1-A (C1) 5.26 eV	102 H4C5.q0.m3-68 3-B1 (C2V) 5.47 eV	103 H4C5.q0.m3-51 3-A (C1) 5.59 eV	104 H4C5.q0.m3-49 3-A" (CS) 5.67 eV	105 H4C5.q0.m3-58 3-A (C1) 5.80 eV			
X	T	À	the				
106 H4C5.q0.m3-31 3-A (C1) 6.22 eV	107 H4C5.q0.m3-23 3-A (C1) 6.29 eV	108 H4C5.q0.m3-21 3-A (C1) 6.62 eV	109 H4C5.q0.m3-20 3-A (C1) 7.05 eV				

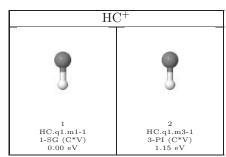


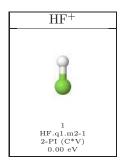


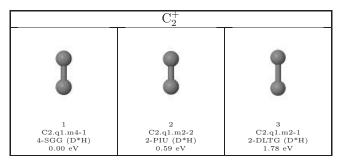


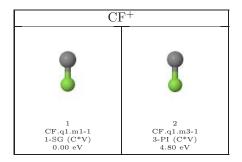


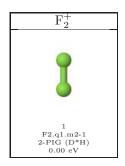


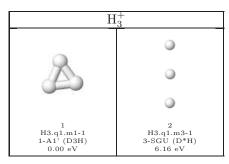


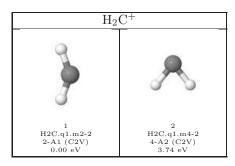


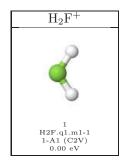


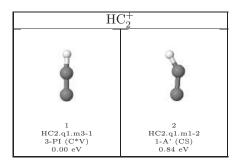


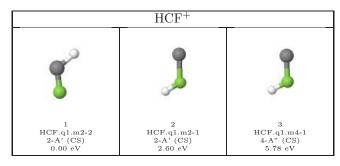


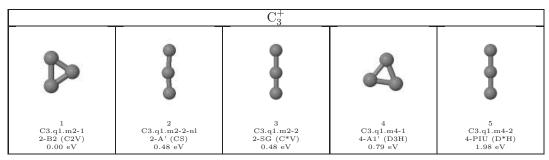


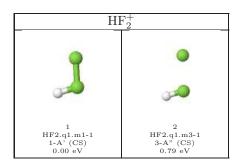


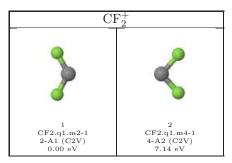


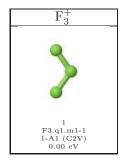


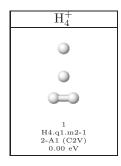


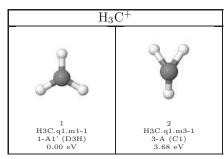


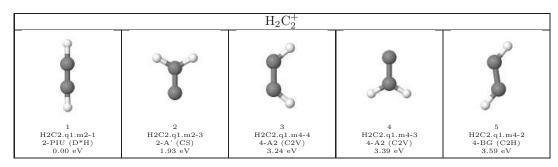


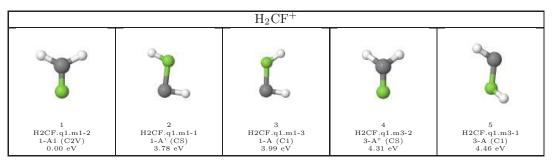


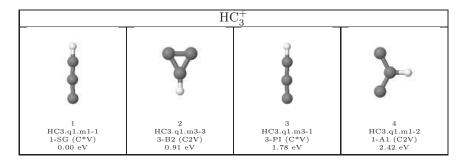


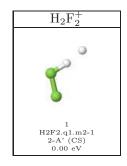


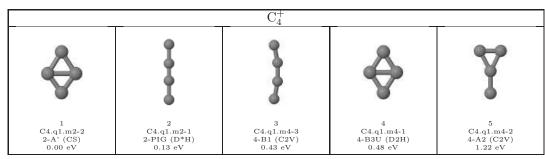


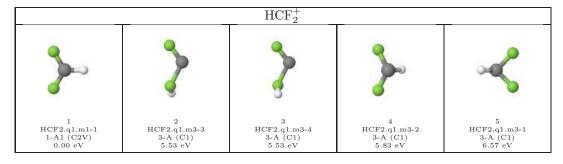


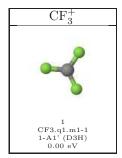


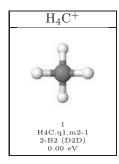


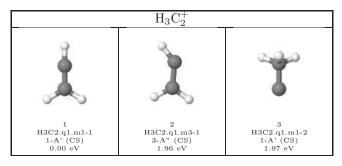


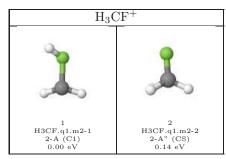


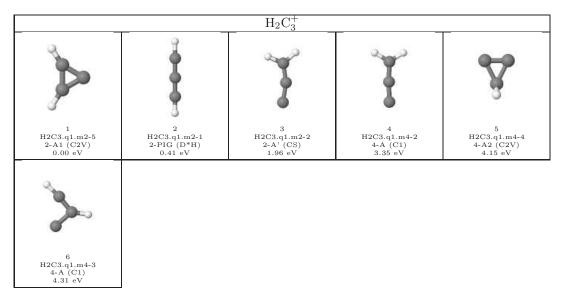




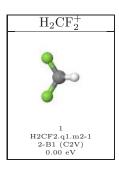


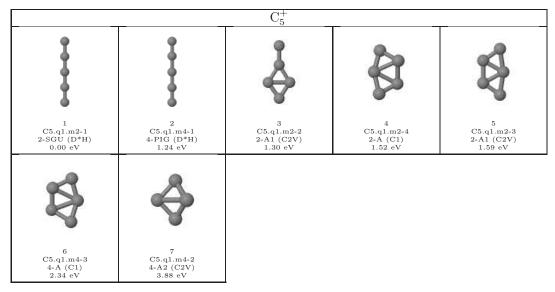


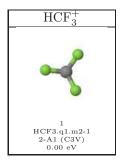


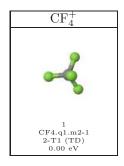


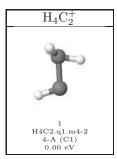
HC_4^+						
	\$		4	\$		
1 HC4.q1.m3-1 3-A" (CS) 0.00 eV	2 HC4.q1.m1-6 1-A1 (C2V) 0.08 eV	3 HC4.q1.m1-1 1-PI (C*V) 0.53 eV	4 HC4.q1.m1-5 1-A1 (C2V) 1.16 eV	5 HC4.q1.m3-5 3-A" (CS) 1.23 eV		
7	Å	7				
6 HC4.q1.m1-3 1-A' (CS) 1.25 eV	7 HC4.q1.m3-3 3-A" (CS) 1.30 eV	8 HC4.q1.m3-4 3-A2 (C2V) 1.72 eV				

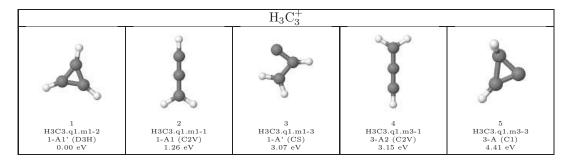








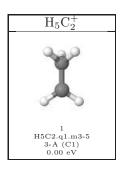




$\mathrm{H_2C_4^+}$						
1 H2C4.q1.m2-1 2-PIG (D*H)	2 H2C4.q1.m2-9 2-B2G (D2H)	3 H2C4.q1.m2-4 2-B2 (C2V)	4 H2C4.q1.m2-7 2-A" (CS)	5 H2C4.q1.m4-2 4-B1 (C2V)		
0.00 eV	0.76 eV	1.71 eV	1.89 eV	2.83 eV		
X		♦	*			
6 H2C4.q1.m4-8 4-A2 (C2V) 3.19 eV	7 H2C4.q1.m4-4 4-A2 (C2V) 3.22 eV	8 H2C4.q1.m4-9 4-A2 (C2V) 3.52 eV	9 H2C4.q1.m4-7 4-A" (CS) 3.60 eV	10 H2C4.q1.m4-6 4-A" (CS) 3.97 eV		
11 H2C4.q1.m4-5 4-A (C1) 6.92 eV						

_		HC_5^+		
	Å		\$	7
1 HC5.q1.m1-1 1-SG (C*V) 0.00 eV	2 HC5.q1.m3-2 3-B2 (C2V) 1.49 eV	3 HC5.q1.m3-1 3-PI (C*V) 1.69 eV	4 HC5.q1.m1-12 1-A1 (C2V) 1.93 eV	5 HC5.q1.m3-3 3-A' (CS) 2.13 eV
1	*	*	S.	T)
6 HC5.q1.m1-3 1-A (C1) 2.49 eV	7 HC5.q1.m3-11 3-B2 (C2V) 2.86 eV	8 HC5.q1.m3-12 3-B2 (C2V) 2.96 eV	9 HC5.q1.m3-8 3-A (C1) 3.01 eV	10 HC5.q1.m1-8 1-A (C1) 3.21 eV
4	} ~	A		
11 HC5.q1.m1-5 1-A' (CS) 3.34 eV	12 HC5.q1.m1-16 1-A1 (C2V) 3.72 eV	13 HC5.q1.m3-6 3-A' (CS) 3.74 eV	14 HC5.q1.m1-4 1-A1 (C2V) 3.76 eV	15 HC5.q1.m3-4 3-B2 (C2V) 3.85 eV
*	4	*		\$
16 HC5.q1.m1-9 1-A (C1) 3.94 eV	17 HC5.q1.m3-9 3-A (C1) 4.39 eV	18 HC5.q1.m3-15 3-A (C1) 4.75 eV	19 HC5.q1.m3-14 3-A" (CS) 5.02 eV	20 HC5.q1.m3-10 3-A" (CS) 5.18 eV

		C_6^+		
	\$	\Diamond	7	\$
1 C6.q1.m2-10 2-PIU (D*H) 0.00 eV	2 C6.q1.m2-7 2-AG (D2H) 0.69 eV	3 C6.q1.m4-11 4-B1 (C2V) 1.35 eV	4 C6.q1.m4-8 4-A" (CS) 1.47 eV	5 C6.q1.m2-3 2-B3G (D2H) 1.51 eV
*	*	♦	A	4
6 C6.q1.m4-1 4-A' (CS) 1.69 eV	7 C6.q1.m2-1 2-A1 (C2V) 2.30 eV	8 C6.q1.m2-9 2-A (C1) 2.80 eV	9 C6.q1.m2-6 2-A (C1) 3.22 eV	10 C6.q1.m2-12 2-A (C1) 3.24 eV
D	Ħ	Z.	ئ	
11 C6.q1.m4-6 4-A (C1) 3.71 eV	12 C6.q1.m4-2 4-A (C1) 3.76 eV	13 C6.q1.m4-12 4-A (C1) 3.78 eV	14 C6.q1.m4-5 4-A (C1) 4.10 eV	



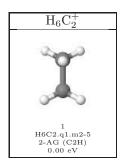
		$\mathrm{H_4C_3^+}$		
I			Å	*
1 H4C3.q1.m2-2 2-B2 (D2) 0.00 eV	2 H4C3.q1.m2-1 2-A (C1) 0.61 eV	3 H4C3.q1.m2-4 2-A (C1) 0.91 eV	4 H4C3.q1.m2-6 2-A (C1) 0.93 eV	5 H4C3.q1.m2-3 2-A (C1) 2.78 eV
7				
6 H4C3.q1.m4-2 4-B1 (C2V) 3.16 eV	7 H4C3.q1.m4-4 4-A (C1) 3.29 eV	8 H4C3.q1.m4-6 4-A (C1) 4.00 eV	9 H4C3.q1.m4-1 4-A" (CS) 4.11 eV	10 H4C3.q1.m4-3 4-A" (CS) 4.12 eV
11 H4C3.q1.m4-5 4-A" (CS) 4.23 eV				

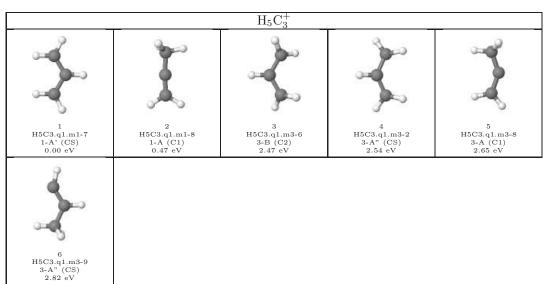
		$\mathrm{H_{3}C_{4}^{+}}$	-	-
	\$	Å		Å
1 H3C4.q1.m1-2 1-A1 (C2V) 0.00 eV	2 H3C4.q1.m1-13 1-A1 (C2V) 0.43 eV	3 H3C4.q1.m1-5 1-A' (CS) 0.76 eV	4 H3C4.q1.m1-15 1-A' (CS) 1.04 eV	5 H3C4.q1.m1-7 1-A' (CS) 1.24 eV
À			I	A
6 H3C4.q1.m3-5 3-A" (CS) 1.53 eV	7 H3C4.q1.m3-2 3-A2 (C2V) 1.61 eV	8 H3C4.q1.m1-1 1-A1 (C3V) 1.83 eV	9 H3C4.q1.m3-7 3-A" (CS) 1.89 eV	10 H3C4.q1.m3-12 3-A" (CS) 2.11 eV
مگر			\rightarrow	\$
11 H3C4.q1.m1-3 1-A' (CS) 2.78 eV	12 H3C4.q1.m3-3 3-A" (CS) 2.98 eV	13 H3C4.q1.m3-10 3-A (C1) 3.05 eV	14 H3C4.q1.m3-13 3-A" (CS) 3.18 eV	15 H3C4.q1.m3-14 3-A (C1) 3.23 eV
		· Second		K
16 H3C4.q1.m3-15 3-A' (CS) 3.63 eV	17 H3C4.q1.m3-1 3-A" (CS) 3.73 eV	18 H3C4.q1.m3-4 3-A" (CS) 4.18 eV	19 H3C4.q1.m3-11 3-A (C1) 4.24 eV	20 H3C4.q1.m1-11 1-A (C1) 4.75 eV
7	*			
21 H3C4.q1.m1-10 1-A (C1) 4.83 eV	22 H3C4.q1.m3-8 3-A (C1) 5.02 eV			

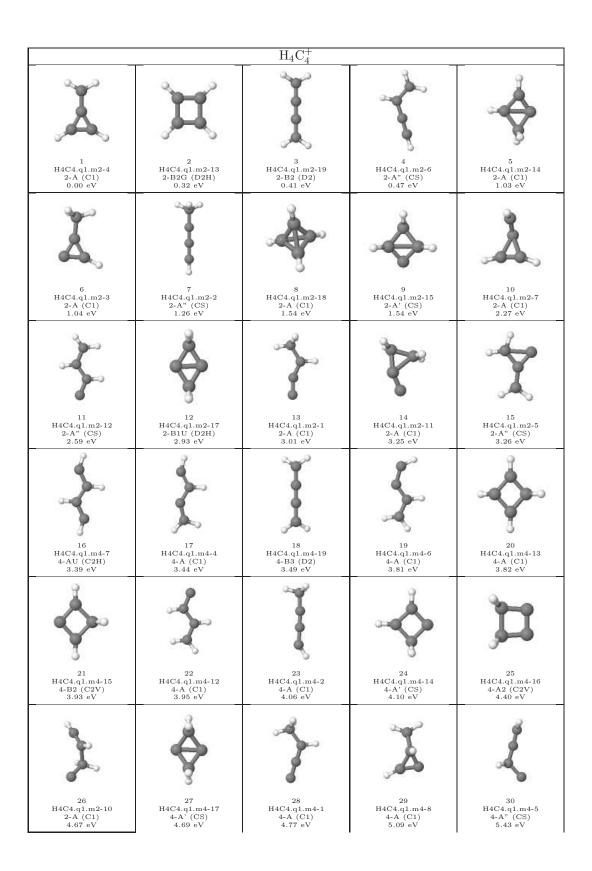
$\mathrm{H_2C_5^+}$				
		•		N
1 H2C5.q1.m2-6 2-A (C1) 0.00 eV	2 H2C5.q1.m2-4 2-A1 (C2V) 0.76 eV	3 H2C5.q1.m2-20 2-A' (CS) 1.20 eV	4 H2C5.q1.m2-2 2-B1 (C2V) 1.30 eV	5 H2C5.q1.m2-29 2-B (C2) 1.48 eV
>	A	*		1
6 H2C5.q1.m2-14 2-A' (CS) 1.72 eV	7 H2C5.q1.m2-28 2-A1 (C2V) 1.76 eV	8 H2C5.q1.m2-17 2-A1 (C2V) 1.79 eV	9 H2C5.q1.m4-1 4-PIG (D*H) 1.87 eV	10 H2C5.q1.m2-12 2-A' (CS) 2.22 eV
	*		Q	\$
11 H2C5.q1.m4-2 4-A (C1) 2.55 eV	12 H2C5.q1.m2-25 2-A (C1) 2.88 eV	13 H2C5.q1.m2-30 2-A' (CS) 2.95 eV	14 H2C5.q1.m4-29 4-A' (CS) 3.11 eV	15 H2C5.q1.m2-26 2-A' (CS) 3.18 eV
A	•	Ŕ	\$	
16 H2C5.q1.m2-27 2-A" (CS) 3.18 eV	17 H2C5.q1.m2-31 2-A' (CS) 3.24 eV	18 H2C5.q1.m4-28 4-A1 (C2V) 3.27 eV	19 H2C5.q1.m2-21 2-B1 (C2V) 3.38 eV	20 H2C5.q1.m4-14 4-A" (CS) 3.53 eV
•	Å	A STATE OF THE STA	*	7
21 H2C5.q1.m2-24 2-A" (CS) 3.56 eV	22 H2C5.q1.m4-4 4-A2 (C2V) 3.59 eV	23 H2C5.q1.m4-10 4-A (C1) 3.64 eV	24 H2C5.q1.m4-20 4-A (C1) 3.65 eV	25 H2C5.q1.m4-6 4-A (C1) 3.69 eV
7	D	*		*
26 H2C5.q1.m4-12 4-A' (CS) 3.82 eV	27 H2C5.q1.m4-27 4-A" (CS) 3.92 eV	28 H2C5.q1.m4-17 4-A" (CS) 3.93 eV	29 H2C5.q1.m4-19 4-A (C1) 3.94 eV	30 H2C5.q1.m4-21 4-A2 (C2V) 4.17 eV

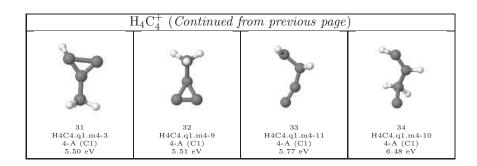
	$\mathrm{H_{2}C_{5}^{+}}$ (Co	ontinued from prev	ious page)	
4		*	7	
31 H2C5.q1.m4-26 4-A' (CS) 4.20 eV	32 H2C5.q1.m4-25 4-A' (CS) 4.33 eV	33 H2C5.q1.m2-5 2-A' (CS) 4.38 eV	34 H2C5.q1.m4-3 4-A" (CS) 4.39 eV	35 H2C5.q1.m4-8 4-A" (CS) 4.58 eV
		M	Ŷ	No.
36 H2C5.q1.m2-13 2-A2 (C2V) 4.62 eV	37 H2C5.q1.m4-18 4-A" (CS) 4.63 eV	38 H2C5.q1.m4-31 4-A" (CS) 4.72 eV	39 H2C5.q1.m4-22 4-A" (CS) 5.29 eV	40 H2C5.q1.m4-5 4-A (C1) 5.39 eV
	*	- 4	To	*
41 H2C5.q1.m2-9 2-A" (CS) 5.71 eV	42 H2C5.q1.m4-24 4-A' (CS) 5.81 eV	43 H2C5.q1.m4-13 4-A2 (C2V) 5.94 eV	44 H2C5.q1.m4-9 4-A (C1) 6.17 eV	45 H2C5.q1.m4-23 4-A (C1) 6.27 eV
46 H2C5.q1.m4-7 4-A" (CS) 6.72 eV				

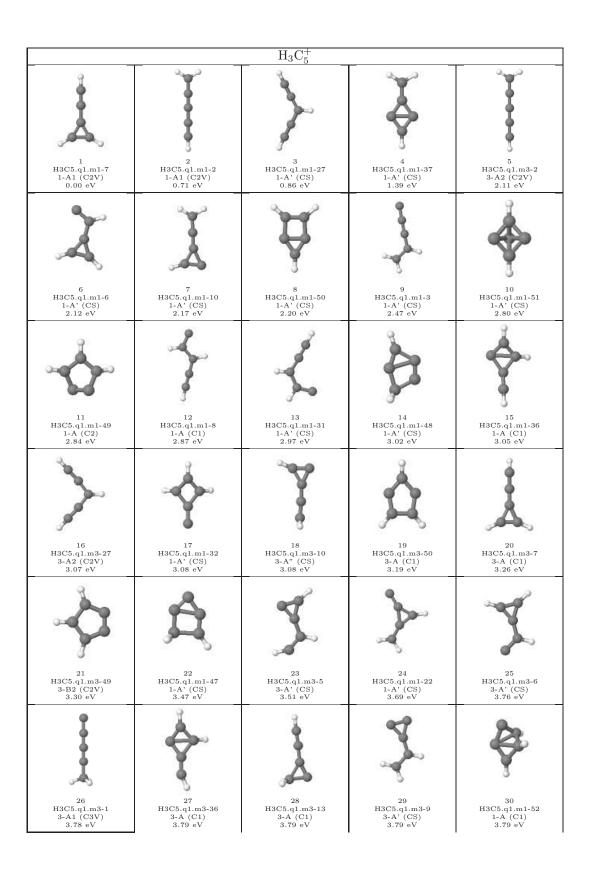
	C_7^+				
		\Diamond			
1	2	3	4	5	
C7.q1.m2-16	C7.q1.m2-8	C7.q1.m4-9	C7.q1.m4-4	C7.q1.m4-7	
2-A' (CS)	2-A (C1)	4-B2 (C2V)	?? (D*H)	4-B2 (C2V)	
0.00 eV	0.00 eV	0.75 eV	1.66 eV	2.09 eV	
6	7	8	9	10	
C7.q1.m2-12	C7.q1.m4-5	C7.q1.m2-11	C7.q1.m2-7	C7.q1.m2-15	
2-A" (CS)	4-A (C1)	2-A" (CS)	2-A (C2)	2-A (C1)	
2.31 eV	2.51 eV	2.61 eV	3.11 eV	3.53 eV	
*	S.	1			
11	12	13	14	15	
C7.q1.m4-11	C7.q1.m2-2	C7.q1.m4-15	C7.q1.m2-13	C7.q1.m4-2	
4-A2 (C1)	2-B2 (C2V)	4-A (C1)	2-A (C1)	4-A" (CS)	
3.59 eV	4.26 eV	4.27 eV	4.64 eV	5.08 eV	



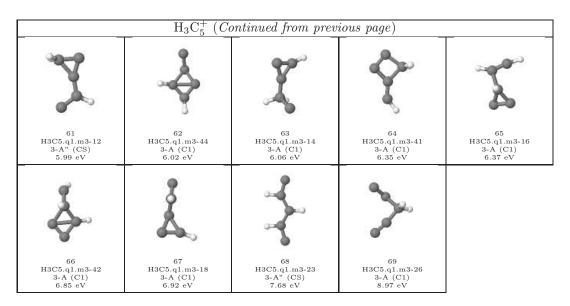


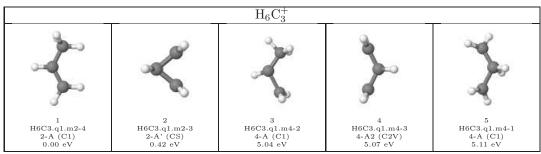


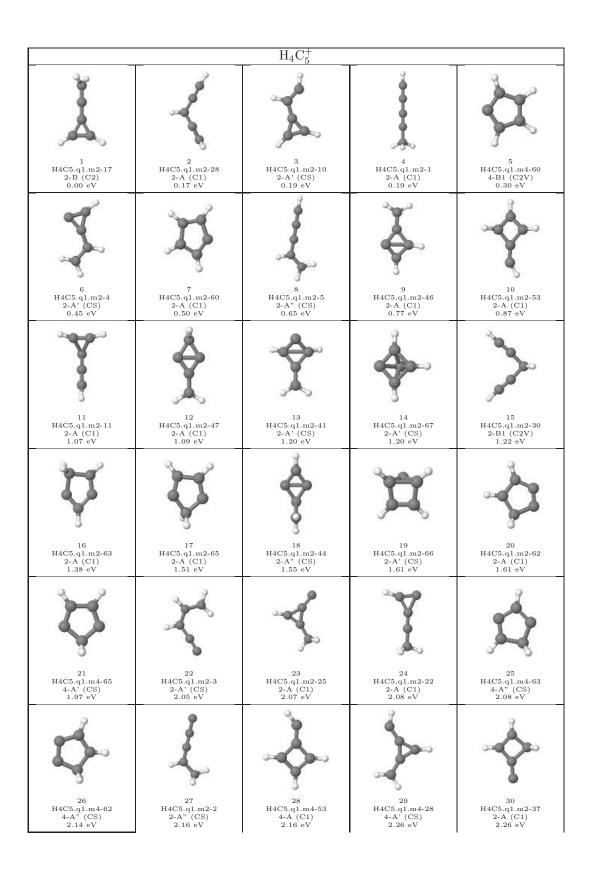




$\mathrm{H_{3}C_{5}^{+}}$ (Continued from previous page)				
	*	\$	\$	*
31 H3C5.q1.m1-34 1-A (C1) 3.86 eV	32 H3C5.q1.m3-37 3-A" (CS) 3.89 eV	33 H3C5.q1.m3-39 3-A (C1) 4.02 eV	34 H3C5.q1.m3-40 3-A (C1) 4.14 eV	35 H3C5.q1.m3-33 3-A (C1) 4.17 eV
*				*
36 H3C5.q1.m1-35 1-A' (CS) 4.17 eV	37 H3C5.q1.m1-1 1-A (C1) 4.20 eV	38 H3C5.q1.m1-43 1-A (C1) 4.22 eV	39 H3C5.q1.m3-32 3-A" (CS) 4.39 eV	40 H3C5.q1.m3-38 3-A" (CS) 4.42 eV
Þ		*	*	
41 H3C5.q1.m3-48 3-A" (CS) 4.48 eV	42 H3C5.q1.m3-3 3-A" (CS) 4.55 eV	43 H3C5.q1.m1-39 1-A (C1) 4.55 eV	44 H3C5.q1.m3-34 3-A (C1) 4.59 eV	45 H3C5.q1.m3-51 3-A (C1) 4.67 eV
à.	*			
46 H3C5.q1.m3-47 3-A" (CS) 4.70 eV	47 H3C5.q1.m1-4 1-A' (CS) 4.73 eV	48 H3C5.q1.m3-8 3-A (C1) 4.76 eV	49 H3C5.q1.m1-23 1-A1 (C2V) 4.93 eV	50 H3C5.q1.m3-4 3-A' (CS) 4.95 eV
*	*	\$	I	
51 H3C5.q1.m1-24 1-A (C1) 5.13 eV	52 H3C5.q1.m1-46 1-A (C1) 5.22 eV	53 H3C5.q1.m3-24 3-A" (CS) 5.22 eV	54 H3C5.q1.m1-15 1-A (C1) 5.27 eV	55 H3C5.q1.m3-28 3-A" (CS) 5.34 eV
1		\$		ф-
56 H3C5.q1.m1-9 1-A (C1) 5.38 eV	57 H3C5.q1.m3-53 3-A (C1) 5.41 eV	58 H3C5.q1.m3-35 3-A" (CS) 5.43 eV	59 H3C5.q1.m1-12 1-A' (CS) 5.46 eV	60 H3C5.q1.m3-46 3-A (C1) 5.54 eV



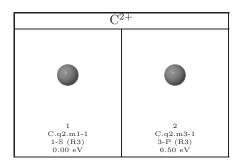




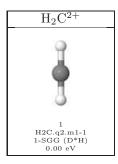
$\mathrm{H_4C_5^+}$ (Continued from previous page)				
\$			X	A
31 H4C5.q1.m4-59 4-B (C2) 2.28 eV	32 H4C5.q1.m4-41 4-B2 (C2V) 2.31 eV	33 H4C5.q1.m2-6 2-A (C1) 2.33 eV	34 H4C5.q1.m2-68 2-A (C1) 2.34 eV	35 H4C5.q1.m2-64 2-A' (CS) 2.37 eV
*			S	
36 H4C5.q1.m4-46 4-A' (CS) 2.40 eV	37 H4C5.q1.m2-40 2-A (C1) 2.50 eV	38 H4C5.q1.m4-17 4-A" (CS) 2.52 eV	39 H4C5.q1.m2-71 2-A (C1) 2.52 eV	40 H4C5.q1.m4-32 4-B2 (C2V) 2.54 eV
4		*	*	Y
41 H4C5.q1.m4-5 4-A' (CS) 2.57 eV	42 H4C5.q1.m2-45 2-A' (CS) 2.59 eV	43 H4C5.q1.m2-38 2-A (C1) 2.62 eV	44 H4C5.q1.m2-42 2-A (C1) 2.67 eV	45 H4C5.q1.m2-14 2-B1 (C2V) 2.73 eV
1	×		dona	X
46 H4C5.q1.m2-23 2-A (C1) 2.79 eV	47 H4C5.q1.m4-11 4-A' (CS) 2.93 eV	48 H4C5.q1.m2-8 2-A' (CS) 3.00 eV	49 H4C5.q1.m4-1 4-A (C1) 3.02 eV	50 H4C5.q1.m2-24 2-A (C1) 3.05 eV
	*	*	X	A
51 H4C5.q1.m4-52 4-A (C1) 3.11 eV	52 H4C5.q1.m4-4 4-A" (CS) 3.12 eV	53 H4C5.q1.m4-54 4-A (C1) 3.14 eV	54 H4C5.q1.m4-10 4-A (C1) 3.14 eV	55 H4C5.q1.m2-61 2-B2 (C2V) 3.19 eV
4	4	X	*	*
56 H4C5.q1.m2-29 2-A (C1) 3.27 eV	57 H4C5.q1.m4-50 4-A (C1) 3.31 eV	58 H4C5.q1.m4-25 4-A (C1) 3.33 eV	59 H4C5.q1.m4-22 4-A" (CS) 3.38 eV	60 H4C5.q1.m4-42 4-A" (CS) 3.46 eV

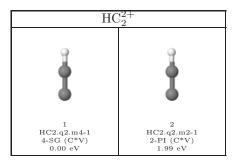
$\mathrm{H_4C_5^+}$ (Continued from previous page)				
61	62	63	64	65
H4C5.q1.m4-37	H4C5.q1.m4-6	H4C5.q1.m2-15	H4C5.q1.m4-2	H4C5.q1.m4-47
4-A" (CS)	4-A" (CS)	2-A' (CS)	4-A" (CS)	4-A" (CS)
3.51 eV	3.59 eV	3.60 eV	3.61 eV	3.62 eV
	*	*		\$
66	67	68	69	70
H4C5.q1.m4-27	H4C5.q1.m2-55	H4C5.q1.m4-38	H4C5.q1.m4-40	H4C5.q1.m4-55
4-A" (CS)	2-A (C1)	4-A" (CS)	4-A (C1)	4-A (C1)
3.65 eV	3.65 eV	3.67 eV	3.68 eV	3.68 eV
2	3		L	*
71	72	73	74	75
H4C5.q1.m4-18	H4C5.q1.m2-70	H4C5.q1.m2-49	H4C5.q1.m4-3	H4C5.q1.m4-14
4-A (C1)	2-A1 (C2V)	2-A' (CS)	4-A' (CS)	4-B2 (C2V)
3.74 eV	3.77 eV	3.80 eV	3.81 eV	3.83 eV
X	*	*		1
76	77	78	79	80
H4C5.q1.m2-7	H4C5.q1.m4-9	H4C5.q1.m4-23	H4C5.q1.m4-39	H4C5.q1.m4-7
2-A (C1)	4-A" (CS)	4-A" (CS)	4-A (C1)	4-A (C1)
3.89 eV	3.94 eV	3.98 eV	3.98 eV	3.99 eV
Q	*	0	\$	
81	82	83	84	85
H4C5.q1.m4-61	H4C5.q1.m4-56	H4C5.q1.m4-44	H4C5.q1.m4-43	H4C5.q1.m4-13
4-B1 (C2V)	4-A" (CS)	4-A' (CS)	4-A (C1)	4-A (C1)
4.08 eV	4.11 eV	4.22 eV	4.36 eV	4.38 eV
*	X	X		*
86	87	88	89	90
H4C5.q1.m4-15	H4C5.q1.m4-24	H4C5.q1.m4-8	H4C5.q1.m4-26	H4C5.q1.m4-29
4-A" (CS)	4-A (C1)	4-A (C1)	4-A (C1)	4-A (C1)
4.50 eV	4.53 eV	4.59 eV	4.61 eV	4.65 eV

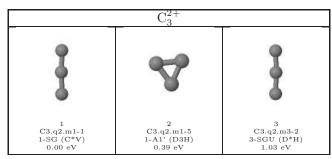
	${ m H_4C_5^+}$ (Co	ontinued from prev	ious page)	_
*	\$	3	7	>
91 H4C5.q1.m4-30 4-A (C1) 4.71 eV	92 H4C5.q1.m4-71 4-A (C1) 4.89 eV	93 H4C5.q1.m2-31 2-A" (CS) 4.91 eV	94 H4C5.q1.m4-19 4-A (C1) 4.97 eV	95 H4C5.q1.m4-33 4-A (C1) 5.01 eV
Þ	I	3	*	
96 H4C5.q1.m4-64 4-A" (CS) 5.17 eV	97 H4C5.q1.m4-16 4-A (C1) 5.37 eV	98 H4C5.q1.m2-34 2-A (C1) 5.42 eV	99 H4C5.q1.m4-51 4-A" (CS) 5.53 eV	100 H4C5.q1.m4-45 4-A" (CS) 5.59 eV
K	*	×	*	1
101 H4C5.q1.m4-57 4-A (C1) 6.08 eV	102 H4C5.q1.m4-58 4-A (C1) 6.27 eV	103 H4C5.q1.m4-34 4-A (C1) 6.74 eV	104 H4C5.q1.m4-20 4-A (C1) 6.86 eV	105 H4C5.q1.m4-21 4-A (C1) 7.31 eV

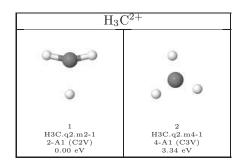


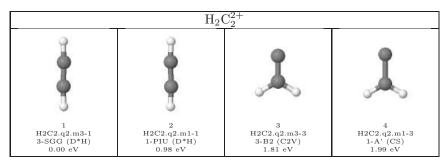
C_2^{2+}						
1	•	•	1			
1 C2.q2.m3-2 3-SGG (D*H) 0.00 eV	2 C2.q2.m1-3 1-SGG (D*H) 0.41 eV	3 C2.q2.m3-3 3-PIU (D*H) 0.65 eV	4 C2.q2.m1-2 1-DLTG (D*H) 0.92 eV			

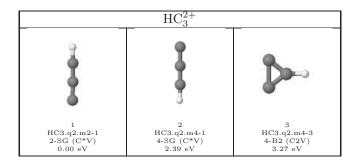


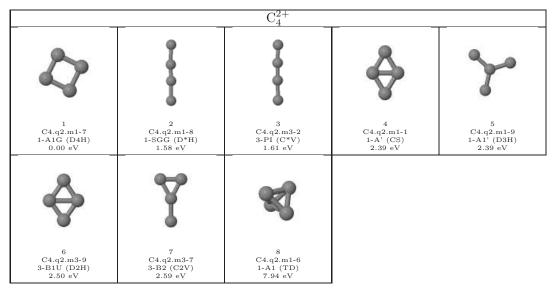


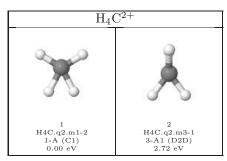


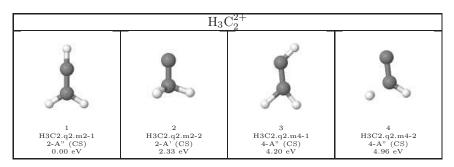


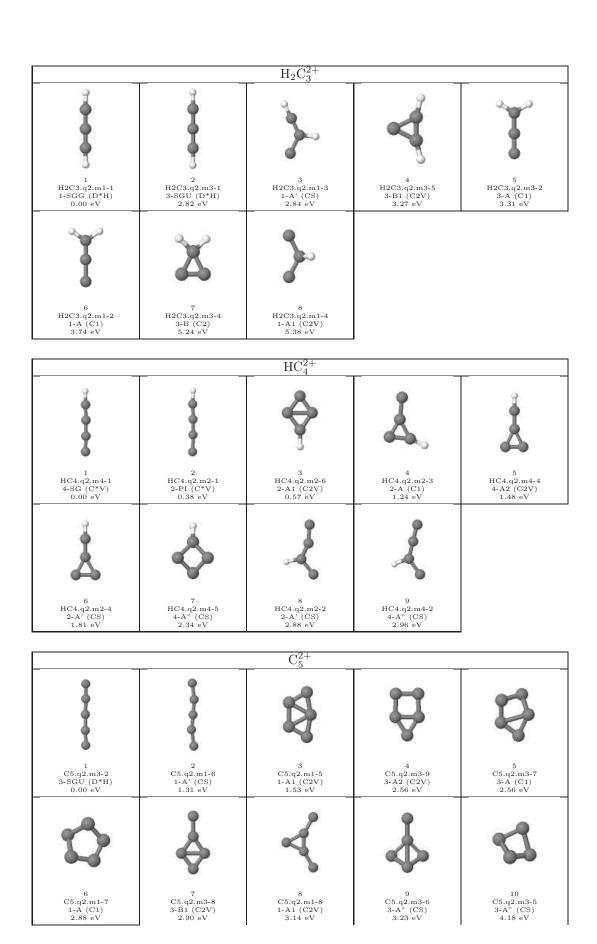


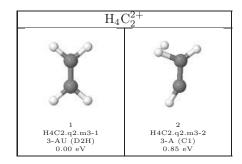


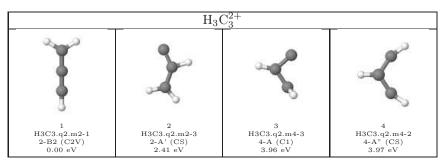


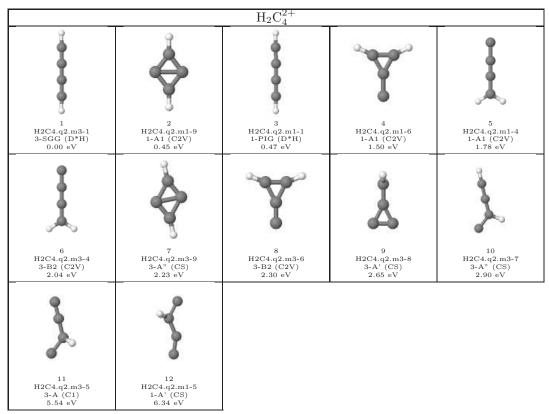




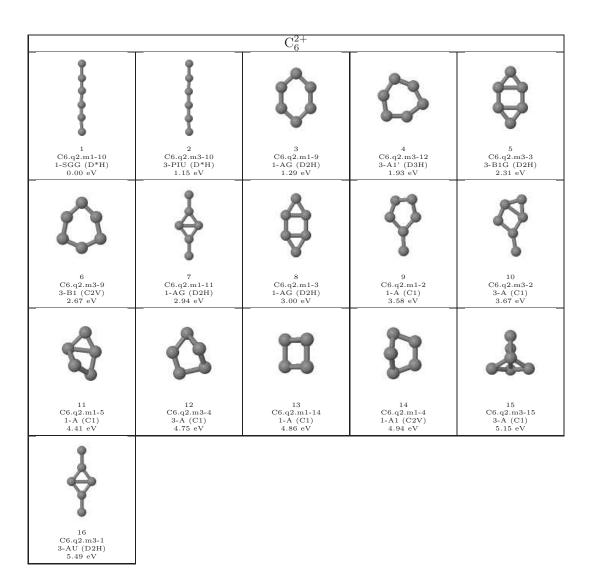


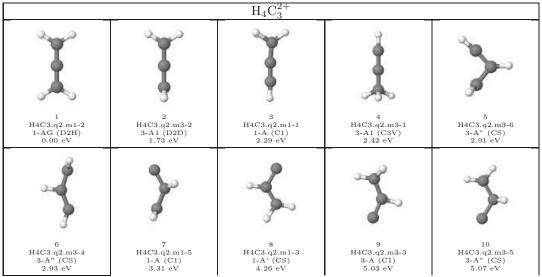






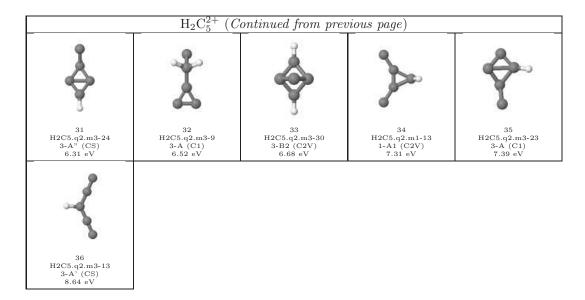
		HC_5^{2+}		
		Å	♦	B
1 HC5.q2.m2-1 2-SG (C*V) 0.00 eV	2 HC5.q2.m4-1 4-SG (C*V) 1.86 eV	3 HC5.q2.m4-2 4-A2 (C2V) 2.08 eV	4 HC5.q2.m2-12 2-B1 (C2V) 2.30 eV	5 HC5.q2.m2-8 2-A' (CS) 2.39 eV
į,	\triangle	♦	N	\$
6 HC5.q2.m4-3 4-A" (CS) 2.45 eV	7 HC5.q2.m2-13 2-A (C2) 3.00 eV	8 HC5.q2.m4-12 4-A2 (C2V) 3.12 eV	9 HC5.q2.m4-8 4-A (C1) 3.20 eV	10 HC5.q2.m4-11 4-A" (CS) 3.25 eV
	1	į		1
11 HC5.q2.m2-4 2-A" (CS) 3.53 eV	12 HC5.q2.m2-2 2-B2 (C2V) 3.98 eV	13 HC5.q2.m4-6 4-A" (CS) 4.08 eV	14 HC5.q2.m4-4 4-B2 (C2V) 4.30 eV	15 HC5.q2.m2-3 2-A' (CS) 4.38 eV
~	\$	7		
16 HC5.q2.m4-9 4-A (C1) 4.42 eV	17 HC5.q2.m4-10 4-A" (CS) 5.73 eV	18 HC5.q2.m2-6 2-A (C1) 6.03 eV		

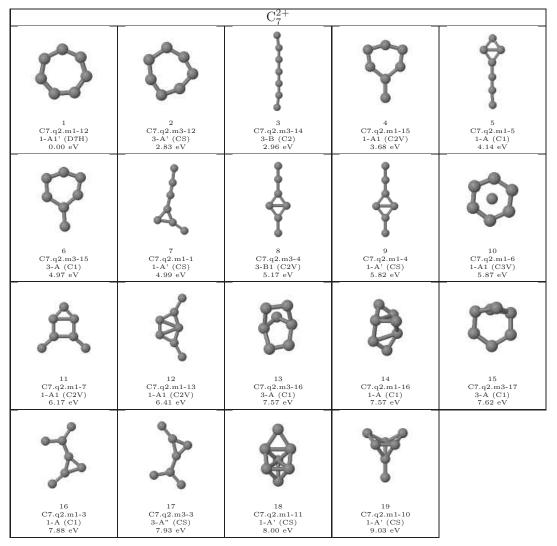


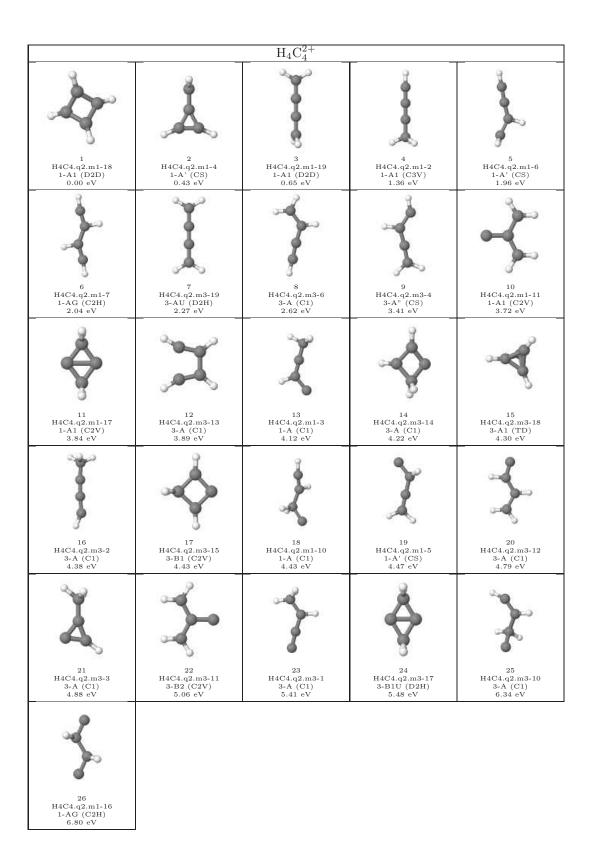


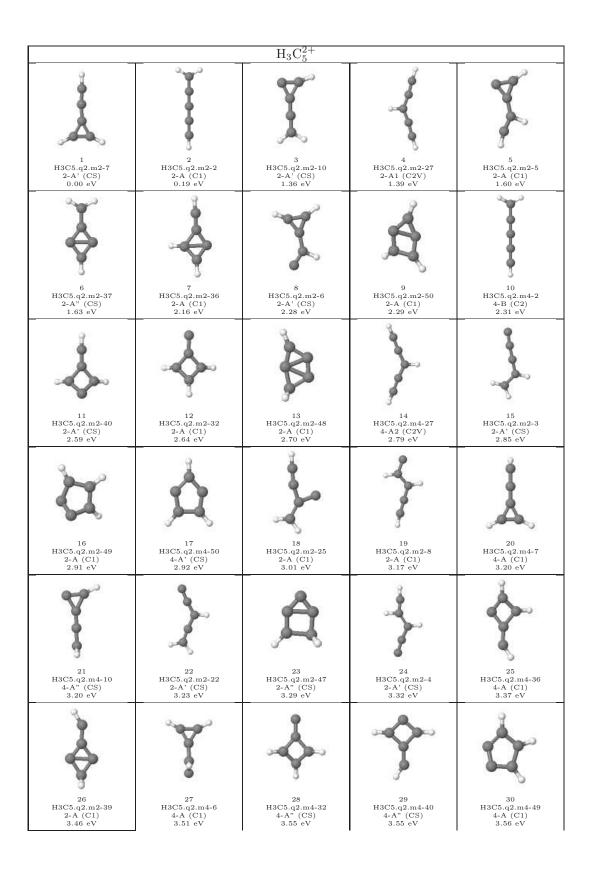
		$H_3C_4^{2+}$		
1 H3C4.q2.m2-2 2-B1 (C2V) 0.00 eV	2 H3C4.q2.m2-5 2-A" (CS) 0.38 eV	3 H3C4.q2.m2-12 2-A' (CS) 0.62 eV	4 H3C4.q2.m2-7 2-A (C1) 1.04 eV	5 H3C4.q2.m2-13 2-A' (CS) 1.78 eV
6 H3C4.q2.m4-5 4-A" (CS) 2.67 eV	7 H3C4.q2.m2-11 2-A (C1) 2.82 eV	8 H3C4.q2.m2-1 2-A1 (C3V) 2.84 eV	9 H3C4.q2.m4-2 4-A" (CS) 2.86 eV	10 H3C4.q2.m2-6 2-A (C1)
11 H3C4.q2.m2-3 2-A' (CS)	12 H3C4.q2.m4-3 4-A" (CS)	13 H3C4.q2.m2-8 2-A' (CS)	14 H3C4.q2.m2-4 2-A (C1)	3.25 eV 15 H3C4.q2.m4-7 4-A (C1)
3.25 eV 16 H3C4.q2.m4-6 4-A" (CS) 4.31 eV	3.52 eV 17 H3C4.q2.m4-12 4-A (C1) 4.77 eV	3.56 eV 18 H3C4.q2.m4-15 4-A1 (C3V) 4.81 eV	3.74 eV 19 H3C4.q2.m4-14 4-A (C1) 4-91 eV	20 H3C4.q2.m4-13 4-A" (CS) 4.93 eV
21 H3C4.q2.m4-8 4-A" (CS) 4.95 eV	22 H3C4.q2.m4-9 4-A" (CS) 5.24 eV	23 H3C4.q2.m4-10 4-A" (CS) 5.28 eV	24 H3C4.q2.m4-1 4-A' (CS) 5.33 eV	4.00 69

		${ m H}_{2}{ m C}_{5}^{2+}$		
				Å.
1 H2C5.q2.m1-1 1-SGG (D*H) 0.00 eV	2 H2C5.q2.m1-29 1-A1 (C2V) 2.68 eV	3 H2C5.q2.m1-6 1-A (C1) 2.78 eV	4 H2C5.q2.m1-20 1-A' (CS) 2.78 eV	5 H2C5.q2.m3-6 3-A" (CS) 2.85 eV
j		4		*
6 H2C5.q2.m3-4 3-B1 (C2V) 3.02 eV	7 H2C5.q2.m1-2 1-A (C1) 3.03 eV	8 H2C5.q2.m1-4 1-A (C1) 3.15 eV	9 H2C5.q2.m3-2 3-B (C2) 3.19 eV	10 H2C5.q2.m3-20 3-A" (CS) 3.75 eV
A	B	A	1	4
11 H2C5.q2.m1-28 1-A1 (C2V) 3.82 eV	12 H2C5.q2.m3-29 3-B2 (C2V) 3.87 eV	13 H2C5.q2.m1-15 1-A1 (C2V) 4.10 eV	14 H2C5.q2.m3-10 3-A (C1) 4.15 eV	15 H2C5.q2.m1-14 1-A' (CS) 4.21 eV
*	~	A	•	*
16 H2C5.q2.m3-17 3-B1 (C2V) 4.41 eV	17 H2C5.q2.m3-14 3-A' (CS) 4.44 eV	18 H2C5.q2.m3-28 3-B (C2) 4.54 eV	19 H2C5.q2.m3-19 3-A (C1) 4.94 eV	20 H2C5.q2.m3-25 3-A (C1) 5.00 eV
*	\$	*		A
21 H2C5.q2.m1-24 1-A' (CS) 5.02 eV	22 H2C5.q2.m1-17 1-A' (CS) 5.02 eV	23 H2C5.q2.m1-21 1-A1 (C2V) 5.07 eV	24 H2C5.q2.m3-26 3-B2 (C2V) 5.20 eV	25 H2C5.q2.m1-27 1-A' (CS) 5.28 eV
Z)	3			\$
26 H2C5.q2.m3-27 3-A" (CS) 5.35 eV	27 H2C5.q2.m1-3 1-A' (CS) 5.53 eV	28 H2C5.q2.m1-16 1-A (C1) 5.56 eV	29 H2C5.q2.m3-16 3-A (C1) 5.80 eV	30 H2C5.q2.m3-18 3-A (C1) 6.28 eV



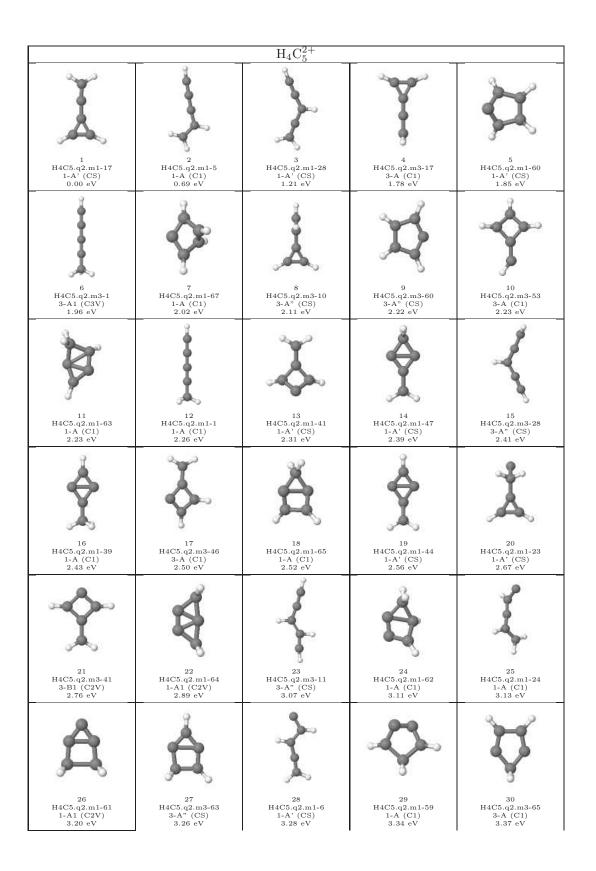






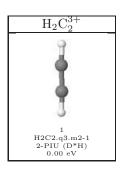
$\mathrm{H_{3}C_{5}^{2+}}$ (Continued from previous page)				
31	32	33	34	35
H3C5.q2.m2-38	H3C5.q2.m4-1	H3C5.q2.m4-5	H3C5.q2.m2-33	H3C5.q2.m2-1
2-A (C1)	4-A1 (C3V)	4-A (C1)	2-A (C1)	2-A (CI)
3.56 eV	3.59 eV	3.60 eV	3.65 eV	3.72 eV
36	37	38	39	40
H3C5.q2.m2-14	H3C5.q2.m4-37	H3C5.q2.m4-33	H3C5.q2.m4-9	H3C5.q2.m2-34
2-A (C1)	4-A" (CS)	4-A (C1)	4-A (C1)	2-A' (CS)
3.96 eV	3.97 eV	3.98 eV	4.05 eV	4.12 eV
			D	
41	42	43	44	45
H3C5.q2.m4-3	H3C5.q2.m2-28	H3C5.q2.m2-44	H3C5.q2.m4-48	H3C5.q2.m4-28
4-A (C1)	2-A' (CS)	2-A (C1)	4-A" (CS)	4-A" (CS)
4.33 eV	4.65 eV	4.66 eV	4.71 eV	4.87 eV
	*		*	X
46	47	48	49	50
H3C5.q2.m4-15	H3C5.q2.m4-31	H3C5.q2.m4-4	H3C5.q2.m4-39	H3C5.q2.m2-15
4-A (C1)	4-A" (CS)	4-A" (CS)	4-A (C1)	2-A" (CS)
4.89 eV	4.91 eV	5.02 eV	5.03 eV	5.17 eV
		7	a	X
51	52	53	54	55
H3C5.q2.m4-8	H3C5.q2.m4-38	H3C5.q2.m4-11	H3C5.q2.m4-47	H3C5.q2.m4-14
4-A' (CS)	4-A (C1)	4-A (C1)	4-A" (CS)	4-A (C1)
5.20 eV	5.25 eV	5.36 eV	5.46 eV	5.52 eV
		No.		>
56	57	58	59	60
H3C5.q2.m4-13	H3C5.q2.m2-29	H3C5.q2.m4-19	H3C5.q2.m4-16	H3C5.q2.m2-20
4-A (C1)	2-A (C1)	4-A (C1)	4-A" (CS)	2-A (C1)
5.53 eV	5.71 eV	5.73 eV	5.80 eV	5.85 eV

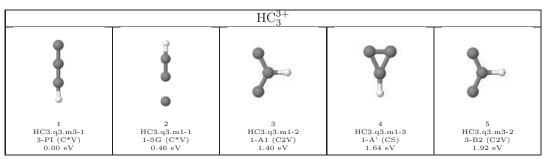
	$\mathrm{H_{3}C_{5}^{2+}}$ (Continued from previous page)				
*	4	\$			
61 H3C5.q2.m4-44 4-A (C1) 5.99 eV	62 H3C5.q2.m4-42 4-A (C1) 6.03 eV	63 H3C5.q2.m4-34 4-A (C1) 6.31 eV	64 H3C5.q2.m2-23 2-A' (CS) 6.37 eV	65 H3C5.q2.m4-18 4-A (C1) 6.73 eV	
4		3	土	1	
66 H3C5.q2.m4-26 4-A (C1) 6.88 eV	67 H3C5.q2.m4-20 4-A (C1) 7.07 eV	68 H3C5.q2.m4-23 4-A' (CS) 7.25 eV	69 H3C5.q2.m2-11 2-A' (CS) 7.32 eV	70 H3C5.q2.m4-29 4-A" (CS) 7.92 eV	
4	1				
71 H3C5.q2.m4-12 4-A (C1) 8.12 eV	72 H3C5.q2.m4-21 4-A (C1) 8.22 eV				

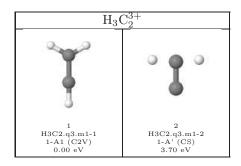


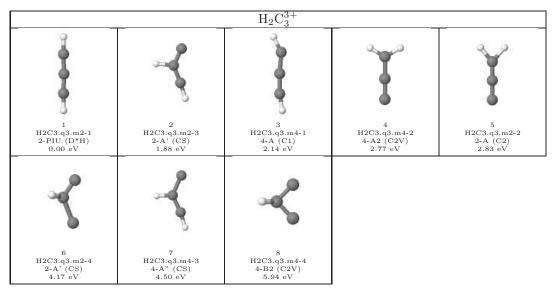
$\mathrm{H_4C_5^{2+}}$ (Continued from previous page)				
31	32	33	34	35
H4C5.q2.m1-14 1-A' (CS) 3.38 eV	H4C5.q2.m1-30 1-A' (CS) 3.50 eV	H4C5.q2.m3-22 3-A (C1) 3.58 eV	H4C5.q2.m1-16 1-A' (CS) 3.68 eV	H4C5.q2.m1-56 1-A' (CS) 3.69 eV
I	*	*	-	D.
36 H4C5.q2.m1-22 1-A (C1) 3.74 eV	37 H4C5.q2.m1-2 1-A' (CS) 3.83 eV	38 H4C5.q2.m1-13 1-A (C1) 3.84 eV	39 H4C5.q2.m1-38 1-A' (CS) 3.85 eV	40 H4C5.q2.m3-59 3-A" (CS) 3.98 eV
Z			d	
41 H4C5.q2.m3-7 3-A (C1) 3.98 eV	42 H4C5.q2.m1-25 1-A (C1) 4.00 eV	43 H4C5.q2.m3-66 3-B2 (C2V) 4.02 eV	44 H4C5.q2.m3-62 3-A" (CS) 4.02 eV	45 H4C5.q2.m1-37 1-A (C1) 4.05 eV
*	\$. L.	Z	\$
46 H4C5.q2.m3-14 3-B1 (C2V) 4.07 eV	47 H4C5.q2.m1-54 1-A (C1) 4.20 eV	48 H4C5.q2.m3-3 3-A (C1) 4.22 eV	49 H4C5.q2.m3-23 3-A (C1) 4.24 eV	50 H4C5.q2.m3-47 3-A (C1) 4.32 eV
*	7		\$	>
51 H4C5.q2.m3-37 3-A (C1) 4.38 eV	52 H4C5.q2.m3-15 3-A (C1) 4.41 eV	53 H4C5.q2.m3-44 3-A" (CS) 4.50 eV	54 H4C5.q2.m3-39 3-A (C1) 4.61 eV	55 H4C5.q2.m3-25 3-A" (CS) 4.63 eV
2	1	\$	*	X
56 H4C5.q2.m3-2 3-A (C1) 4.64 eV	57 H4C5.q2.m1-29 1-A (C1) 4.66 eV	58 H4C5.q2.m3-40 3-A (C1) 4.67 eV	59 H4C5.q2.m3-6 3-A" (CS) 4.71 eV	60 H4C5.q2.m3-18 3-A (C1) 4.74 eV

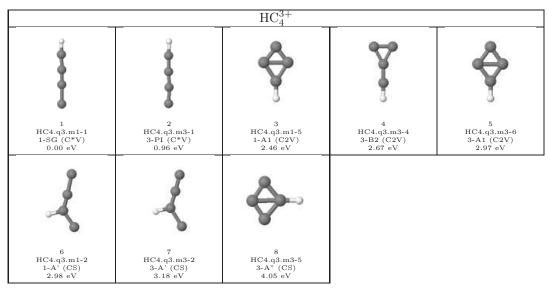
	$H_4C_5^{2+}$ (C	ontinued from preu	vious page)	
>	į.	*		
61 H4C5.q2.m3-26 3-A (C1) 4.77 eV	62 H4C5.q2.m3-8 3-A (C1) 4.82 eV	63 H4C5.q2.m3-56 3-A" (CS) 5.02 eV	64 H4C5.q2.m1-3 1-A (C1) 5.08 eV	65 H4C5.q2.m3-27 3-A (C1) 5.09 eV
*	*		X	x
66 H4C5.q2.m3-38 3-A" (CS) 5.13 eV	67 H4C5.q2.m3-29 3-A (C1) 5.18 eV	68 H4C5.q2.m3-43 3-A (C1) 5.22 eV	69 H4C5.q2.m3-24 3-A (C1) 5.67 eV	70 H4C5.q2.m1-20 1-A (C1) 6.04 eV
Q	¥	*		
71 H4C5.q2.m3-64 3-A2 (C2V) 6.31 eV	72 H4C5.q2.m1-15 1-A (C1) 6.41 eV	73 H4C5.q2.m1-18 1-A (C1) 6.61 eV	74 H4C5.q2.m3-49 3-A' (CS) 6.76 eV	75 H4C5.q2.m1-34 1-A (C2) 6.78 eV
	*	X	*	
76 H4C5.q2.m1-36 1-A (C1) 6.83 eV	77 H4C5.q2.m3-45 3-A' (CS) 6.93 eV	78 H4C5.q2.m3-21 3-A (C1) 7.21 eV	79 H4C5.q2.m3-20 3-A (C1) 7.24 eV	80 H4C5.q2.m3-34 3-A (C1) 7.52 eV

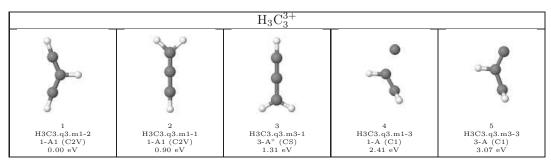


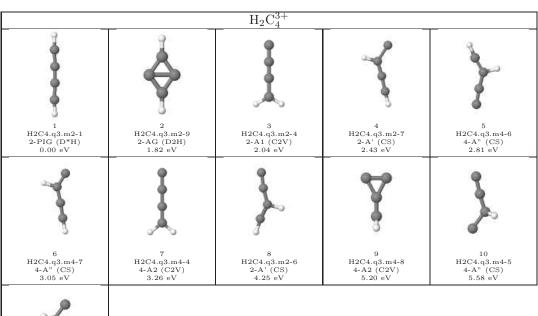






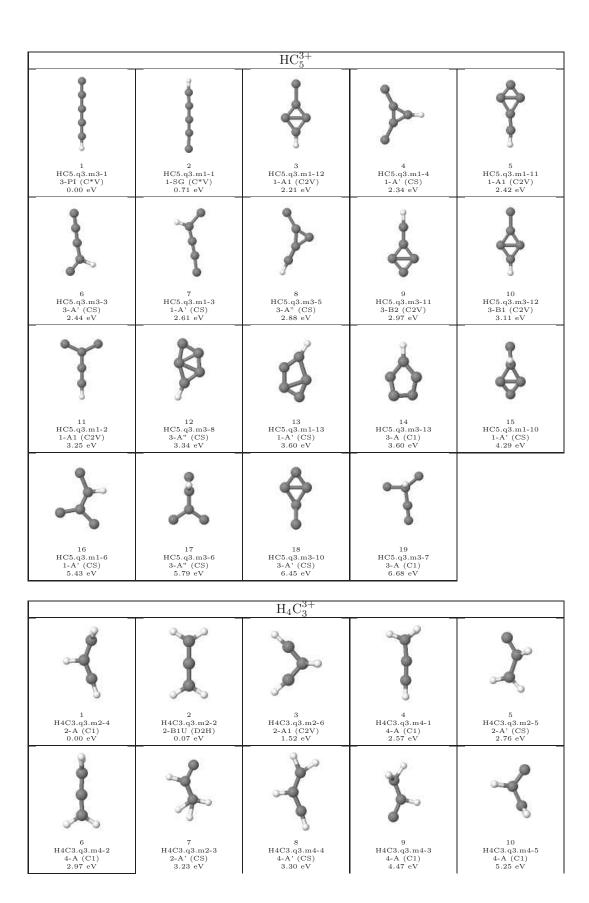


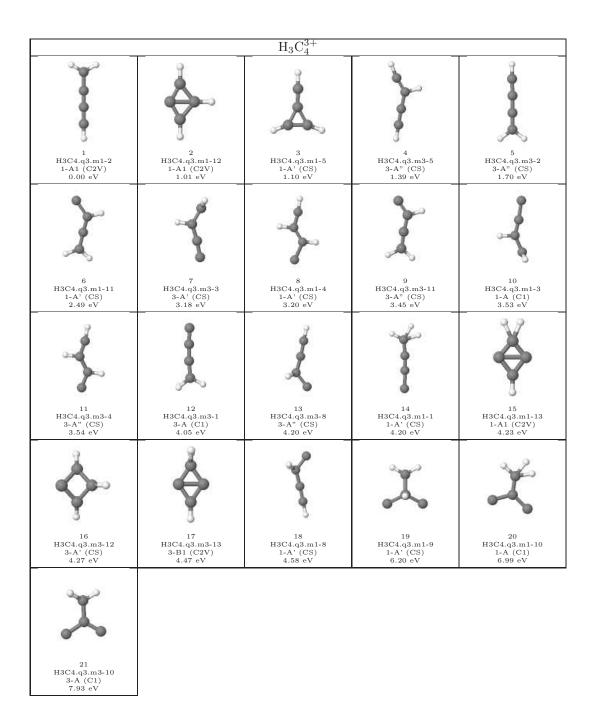


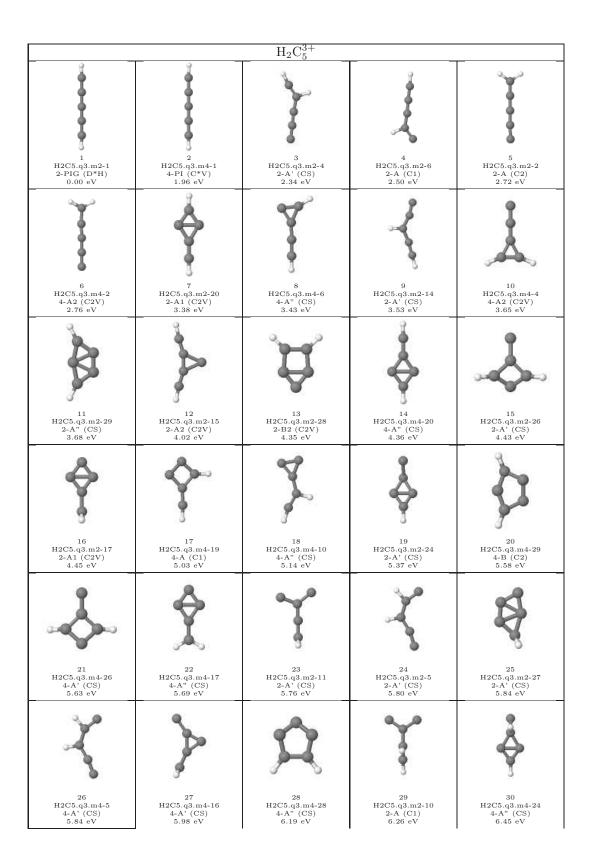


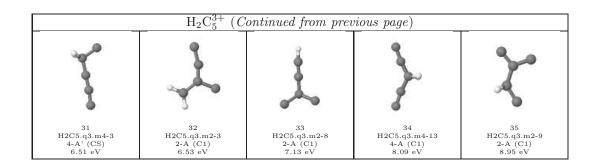


11 H2C4.q3.m2-5 2-A" (CS) 6.24 eV

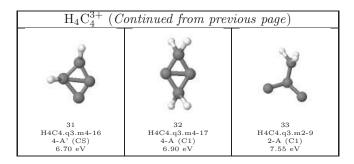


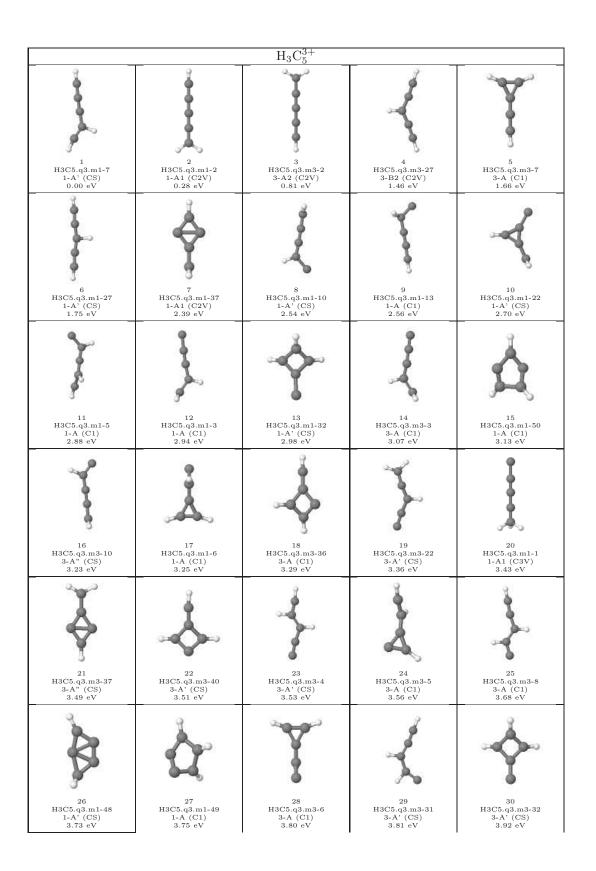




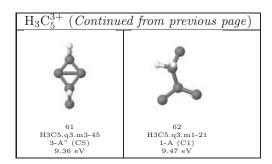


		${ m H_4C_4^{3+}}$		_
	X		*	
1 H4C4.q3.m2-6 2-A (C1) 0.00 eV	2 H4C4.q3.m2-19 2-B2 (D2) 0.01 eV	3 H4C4.q3.m2-7 2-BG (C2H) 0.38 eV	4 H4C4.q3.m2-13 2-A2 (C2V) 0.49 eV	5 H4C4.q3.m2-2 2-A (C1) 0.78 eV
A	I			\rightarrow
6 H4C4.q3.m2-4 2-A' (CS) 0.85 eV	7 H4C4.q3.m4-19 4-B3G (D2H) 2.11 eV	8 H4C4.q3.m2-14 2-A" (CS) 2.16 eV	9 H4C4.q3.m2-12 2-A' (CS) 2.33 eV	10 H4C4.q3.m2-15 2-A (C1) 2.50 eV
11 H4C4.q3.m4-6 4-A (C1) 2.59 eV	12 H4C4.q3.m4-4 4-A (C1) 2.79 eV	13 H4C4.q3.m4-7 4-A (C1) 2.84 eV	14 H4C4.q3.m2-5 2-A' (CS) 3.00 eV	15 H4C4.q3.m2-3 2-A (C1) 3.13 eV
	*		\$	1
16 H4C4.q3.m4-2 4-A" (CS) 3.31 eV	17 H4C4.q3.m2-10 2-A (C1) 3.45 eV	18 H4C4.q3.m4-11 4-A" (CS) 3.78 eV	19 H4C4.q3.m2-17 2-A1 (C2V) 3.84 eV	20 H4C4.q3.m4-1 4-A (C1) 4.06 eV
1	*	-	*	X
21 H4C4.q3.m4-8 4-A (C1) 4.18 eV	22 H4C4.q3.m2-1 2-A (C1) 4.20 eV	23 H4C4.q3.m2-11 2-A' (CS) 4.29 eV	24 H4C4.q3.m4-5 4-A (C1) 4.52 eV	25 H4C4.q3.m4-3 4-A (C1) 4.74 eV
1	-	\$		3
26 H4C4.q3.m4-10 4-A (C1) 4.84 eV	27 H4C4.q3.m4-18 4-A1 (C3V) 5.59 eV	28 H4C4.q3.m4-14 4-A (C1) 5.65 eV	29 H4C4.q3.m4-15 4-A2 (C2V) 5.76 eV	30 H4C4.q3.m2-16 2-AG (C2H) 6.18 eV





$\mathrm{H_3C_5^{3+}}$ (Continued from previous page)				
A	♦		X	A. Company
31	32	33	34	35
H3C5.q3.m3-50	H3C5.q3.m1-39	H3C5.q3.m3-1	H3C5.q3.m3-9	H3C5.q3.m1-31
3-B (C2)	1-A' (CS)	3-A (C1)	3-A (C1)	1-A (C1)
3.96 eV	4.13 eV	4.17 eV	4.17 eV	4.46 eV
36	37	38	39	40
H3C5.q3.m3-13	H3C5.q3.m1-47	H3C5.q3.m3-49	H3C5.q3.m3-38	H3C5.q3.m3-39
3-A (C1)	1-A' (CS)	3-A" (CS)	3-A" (CS)	3-A (C1)
4.47 eV	4.53 eV	4.59 eV	4.63 eV	5.11 eV
X.	7		*	
41	42	43	44	45
H3C5.q3.m3-15	H3C5.q3.m1-11	H3C5.q3.m1-14	H3C5.q3.m1-8	H3C5.q3.m3-28
3-A' (CS)	1-A (C1)	1-A (C1)	1-A' (CS)	3-A (C1)
5.13 eV	5.33 eV	5.59 eV	5.67 eV	5.76 eV
\$	7	32	>	
46	47	48	49	50
H3C5.q3.m1-34	H3C5.q3.m1-9	H3C5.q3.m3-23	H3C5.q3.m3-24	H3C5.q3.m1-23
1-A' (CS)	1-A' (CS)	3-B2 (C2V)	3-A (C1)	1-A' (CS)
5.76 eV	5.83 eV	5.91 eV	6.18 eV	6.25 eV
	*		*	\$
51	52	53	54	55
H3C5.q3.m1-29	H3C5.q3.m3-20	H3C5.q3.m3-34	H3C5.q3.m3-44	H3C5.q3.m1-45
1-A' (CS)	3-A (C1)	3-A (C1)	3-A (C1)	1-A' (CS)
6.28 eV	6.33 eV	6.37 eV	6.61 eV	6.65 eV
*	1		مال	
56	57	58	59	60
H3C5.q3.m3-29	H3C5.q3.m1-16	H3C5.q3.m3-43	H3C5.q3.m1-19	H3C5.q3.m3-26
3-A (C1)	1-A (C1)	3-A (C1)	1-A (C1)	3-A" (CS)
6.81 eV	6.86 eV	7.03 eV	7.04 eV	7.82 eV



		$H_4C_5^{3+}$		
	2	3	4	5
H4C5.q3.m2-28 2-A' (CS) 0.00 eV	H4C5.q3.m2-17 2-B1 (C2V) 0.02 eV	H4C5.q3.m2-11 2-A' (CS) 0.13 eV	H4C5.q3.m2-10 2-A (C1) 0.39 eV	H4C5.q3.m2-53 2-A' (CS) 0.54 eV
6	7	8	9	10
H4C5.q3.m2-1 2-A (C1) 0.67 eV	H4C5.q3.m2-46 2-A (C1) 1.14 eV	H4C5.q3.m2-32 2-A1 (C2V) 1.17 eV	H4C5.q3.m4-28 4-A" (CS) 1.21 eV	H4C5.q3.m2-41 2-A' (CS) 1.22 eV
A			3	*
11 H4C5.q3.m2-60 2-A' (CS) 1.58 eV	12 H4C5.q3.m4-17 4-A" (CS) 2.04 eV	13 H4C5.q3.m4-1 4-A (C1) 2.07 eV	14 H4C5.q3.m2-6 2-A (C1) 2.13 eV	15 H4C5.q3.m2-44 2-A (C1) 2.26 eV
. and he		a free		
16 H4C5.q3.m4-5 4-A" (CS) 2.28 eV	17 H4C5.q3.m4-11 4-A' (CS) 2.40 eV	18 H4C5.q3.m2-8 2-A' (CS) 2.42 eV	19 H4C5.q3.m2-14 2-A (C1) 2.48 eV	20 H4C5.q3.m4-30 4-A2 (C2V) 2.54 eV
	1	*	A	7
21 H4C5.q3.m2-30 2-A (C1) 2.55 eV	22 H4C5.q3.m2-16 2-A' (CS) 2.59 eV	23 H4C5.q3.m2-24 2-A (C1) 2.64 eV	24 H4C5.q3.m2-65 2-A (C1) 2.92 eV	25 H4C5.q3.m4-10 4-A (C1) 2.97 eV
	*	*		7
26 H4C5.q3.m4-3 4-A (C1) 2.99 eV	27 H4C5.q3.m2-54 2-A (C1) 3.02 eV	28 H4C5.q3.m2-39 2-A (C1) 3.06 eV	29 H4C5.q3.m2-3 2-A (C1) 3.07 eV	30 H4C5.q3.m2-23 2-A' (CS) 3.34 eV

$\mathrm{H_4C_5^{3+}}$ (Continued from previous page)				
		*	1	*
31 H4C5.q3.m4-6 4-A" (CS) 3.35 eV	32 H4C5.q3.m2-2 2-A (C1) 3.51 eV	33 H4C5.q3.m4-14 4-A2 (C2V) 3.56 eV	34 H4C5.q3.m4-25 4-A (C1) 3.68 eV	35 H4C5.q3.m2-25 2-A (C1) 3.68 eV
Ø-	1	\$	-	*
36 H4C5.q3.m2-62 2-A (C1) 3.71 eV	37 H4C5.q3.m4-4 4-A (C1) 3.82 eV	38 H4C5.q3.m2-59 2-A (C1) 3.88 eV	39 H4C5.q3.m2-56 2-A' (CS) 3.98 eV	40 H4C5.q3.m2-38 2-A' (CS) 3.98 eV
4	*		7	*
41 H4C5.q3.m2-27 2-A (C1) 4.02 eV	42 H4C5.q3.m4-46 4-A (C1) 4.03 eV	43 H4C5.q3.m4-24 4-A" (CS) 4.11 eV	44 H4C5.q3.m4-32 4-A" (CS) 4.15 eV	45 H4C5.q3.m4-22 4-A (C1) 4.18 eV
Å	*	\$	4	
46 H4C5.q3.m4-60 4-A (C1) 4.18 eV	47 H4C5.q3.m4-26 4-A" (CS) 4.21 eV	48 H4C5.q3.m4-41 4-A" (CS) 4.23 eV	49 H4C5.q3.m4-13 4-A' (CS) 4.24 eV	50 H4C5.q3.m4-2 4-A (C1) 4.30 eV
\(\frac{1}{2} \)	B		*	
51 H4C5.q3.m4-50 4-A' (CS) 4.39 eV	52 H4C5.q3.m2-64 2-B1 (C2V) 4.39 eV	53 H4C5.q3.m4-33 4-A (C1) 4.45 eV	54 H4C5.q3.m4-9 4-A" (CS) 4.45 eV	55 H4C5.q3.m4-8 4-A' (CS) 4.52 eV
	Å	Å		*
56 H4C5.q3.m2-33 2-A' (CS) 4.54 eV	57 H4C5.q3.m4-65 4-A" (CS) 4.57 eV	58 H4C5.q3.m4-63 4-A (C1) 4.62 eV	59 H4C5.q3.m4-29 4-A" (CS) 4.63 eV	60 H4C5.q3.m4-23 4-A (C1) 4.72 eV

	$\mathrm{H_4C_5^{3+}}$ (Continued from previous page)				
61 H4C5.q3.m2-29 2-A' (CS) 4.73 eV	62 H4C5.q3.m2-51 2-A (C1) 4.75 eV	63 H4C5.q3.m4-55 4-A (C1) 4.78 eV	64 H4C5.q3.m4-7 4-A (C1) 4.79 eV	65 H4C5.q3.m4-54 4-A (C1) 4.94 eV	
66 H4C5.q3.m4-39 4-A (C1)	67 H4C5.q3.m4-40 4-A (C1)	68 H4C5.q3.m4-38 4-A2 (C2V)	69 H4C5.q3.m4-62 4-A (C1)	70 H4C5.q3.m4-44 4-A" (CS)	
71 H4C5.q3.m4-59 4-A' (CS)	5.10 eV 5.10 eV 72 H4C5.q3.m4-18 4-A (C1)	73 H4C5-q3.m4-43 4-A (CI)	5.20 eV 5.20 eV H4C5.q3.m4-47 4-A" (CS)	5.26 eV 5.26 eV 75 H4C5.q3.m4-56 4-A" (CS)	
5.31 eV 76 H4C5.q3.m4-42 4-A (C1)	5.32 eV 77 H4C5.q3.m4-37 4-A (C1)	5.35 eV 78 H4C5.q3.m4-15 4-A" (CS)	79 H4C5-q3.m2-57 2-A (C1)	5.40 eV 80 H4C5.q3.m2-45 2-A (C1)	
81 H4C5.q3.m4-64 4-A (C1) 6.14 eV	5.44 eV 82 H4C5.q3.m4-12 4-A (C1) 6.69 eV	83 H4C5.q3.m2-19 2-A (C1) 6.82 eV	5.75 eV 84 H4C5.q3.m4-34 4-A" (CS) 6.86 eV	5.76 eV 85 H4C5.q3.m4-57 4-A (C1) 6.95 eV	