

TABLE SI. $\text{H}_2\text{TiC}_4\text{H}_4$ structural results for various methods.

	RHF/TZV	MP2/ECP	MP2/TZV	BLYP/TZV	B3LYP/ECP	B3LYP/TZV
$r_{\text{Ti-C}}(\text{\AA})$	2.01	2.03	2.02	2.05	2.01	2.03
$r_{\text{CC}}(\text{\AA})$	1.34	1.38	1.37	1.37	1.37	1.36
	1.50	1.50	1.50	1.49	1.50	1.49
$r_{\text{Ti-H}}(\text{\AA})$	1.71	1.70	1.73	1.73	1.68	1.71
$r_{\text{C-H}}(\text{\AA})$	1.07	1.10	1.08	1.09	1.09	1.08
	1.08	1.10	1.09	1.10	1.09	1.09
$\alpha(\text{HCC})$	119.72	120.55	120.59	120.70	120.73	120.82
	115.36	114.81	113.23	115.01	114.34	114.55
$\alpha(\text{HTiH})$	108.83	109.88	112.87	111.20	109.05	110.46
$\alpha(\text{CTiC})$	91.56	102.48	99.15	93.77	97.91	94.94
$\alpha(\text{TiCC})$	101.64	93.15	95.06	99.80	96.94	98.77
$\alpha(\text{CCC})$	122.58	125.61	125.36	123.31	124.10	123.76

TABLE SII. HTiC_3H_3 results for various methods.

	RHF	MP2/ECP	MP2/TZV	LYP/TZV+2f	B3LYP/E	B3LYP/TZV
$r_{\text{Ti-C}}(\text{\AA})$	1.91	1.85	1.88	1.91	1.88	1.89
$r_{\text{CC}}(\text{\AA})$	1.43	1.44	1.44	1.45	1.44	1.44
$r_{\text{Ti-H}}(\text{\AA})$	1.81	1.73	1.78	1.78	1.74	1.77
$r_{\text{C-H}}(\text{\AA})$	1.07	1.08	1.08	1.09	1.09	1.08
	1.08	1.09	1.08	1.09	1.09	1.09
$\alpha(\text{HCC})$	117.26	121.18	121.72	119.90	119.66	119.88
	119.67	118.56	118.02	118.96	119.30	119.11
$\alpha(\text{HTiC})$	139.47	136.59	137.64	138.37	137.96	138.52
$\alpha(\text{CTiC})$	81.05	86.82	84.73	83.25	84.07	83.10
$\alpha(\text{TiCC})$	79.15	75.14	75.68	77.33	77.26	77.57
$\alpha(\text{CCC})$	120.66	122.88	123.91	122.08	121.41	121.78

TABLE SIII. HTiC₃H₃ triplet results for various methods.

	RHF/TZV	MP2/TZV	BLYP/TZV	B3LYP/TZV
$r_{\text{Ti-C}}(\text{\AA})$	2.05	2.01	2.02	2.01
	2.04	2.01	2.02	2.01
$r_{\text{C-C}}(\text{\AA})$	1.37	1.41	1.43	1.42
	1.46	1.41	1.43	1.42
$r_{\text{Ti-H}}(\text{\AA})$	1.81	1.79	1.78	1.77
$r_{\text{C-H}}(\text{\AA})$	1.07	1.08	1.09	1.08
	1.08	1.09	1.10	1.09
	1.07	1.08	1.09	1.08
$\alpha(\text{HCC})$	119.16	118.07	119.08	118.83
	118.83	118.57	119.45	119.49
$\alpha(\text{HTiC})$	142.83	141.92	142.06	142.01
$\alpha(\text{CTiC})$	73.62	76.16	75.95	75.90
$\alpha(\text{TiCC})$	83.86	80.49	81.51	81.51
$\alpha(\text{CCC})$	120.07	122.86	121.01	121.10

TABLE SIV. HTiC₅H₅ results for various methods.

	RHF/TZV	MP2/ECP	BLYP/TZV	B3LYP/ECP	B3LYP/TZV
$r_{\text{Ti-C}}(\text{\AA})$	1.93	1.95	1.95	1.92	1.93
$r_{\text{C-C}}(\text{\AA})$	1.38	1.43	1.40	1.40	1.39
	1.42	1.46	1.44	1.44	1.44
$r_{\text{Ti-H}}(\text{\AA})$	1.78	1.76	1.77	1.72	1.76
$r_{\text{C-H}}(\text{\AA})$	1.07	1.10	1.09	1.09	1.08
	1.08	1.10	1.10	1.09	1.09
	1.07	1.09	1.09	1.09	1.08
$\alpha(\text{HCC})$	119.95	122.65	121.21	121.40	121.40
	115.22	116.83	115.34	115.76	115.46
	116.00	117.77	116.83	117.09	116.82
$\alpha(\text{HTiC})$	124.86	119.41	123.32	122.19	123.37
$\alpha(\text{CTiC})$	101.62	93.60	99.55	99.48	99.40
$\alpha(\text{TiCC})$	86.38	87.31	86.03	85.50	86.06
$\alpha(\text{CCC})$	122.82	122.32	123.71	122.98	123.36
$\alpha(\text{CCC})$	127.51	121.69	126.04	125.23	125.98
d(652H)	110.50	84.87	103.39	98.66	101.09
d(653H)	175.55	169.39	176.65	175.04	175.73
d(654H)	162.94	172.17	165.13	165.57	165.11
d(261H)	148.71	143.84	141.01	138.01	140.95
d(354H)	171.54	160.76	173.52	170.92	172.71