Electronic supplementary information

POPULATION ANALYSIS OF TITANOCENE DICARBORANYL BY THE MULLIKEN AND NBO METHODS: A COMPARATIVE STUDY

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Table S1. Dipole moment and Mulliken charge characteristics of titanocene dicarboranyl obtained by HF and DFT methods at different levels of theory

Method	μ_g, **Debye**	***q*(Ti)**	***q*(Cp)**	***q*(Carb)**	***q*(>CMe$_2$)**
HF/QZVP	11.78	+1.43	–0.40	–0.19	–0.13
B3LYP/QZVP	10.52	+1.92	−0.74	−0.02	−0.19
CAM-B3LYP/QZVP	10.88	+1.54	−0.63	+0.10	−0.24
PBE0/QZVP	10.49	+1.41	−0.40	−0.09	−0.22
LC-ωPBE/QZVP	11.04	+0.88	–0.12	–0.10	–0.21
TPSSh/QZVP	10.19	+1.06	–0.10	–0.35	–0.09
M06/QZVP	10.61	**–0.12**	+0.34	–0.07	–0.22
M11/QZVP	10.64	+0.13	+0.98	−0.93	−0.12
HF/6-311G	11.41	+1.77	–0.17	–0.73	+0.02
B3LYP/6-311G	10.53	+1.42	–0.10	–0.65	+0.05
CAM-B3LYP/6-311G	10.74	+1.41	–0.10	–0.69	+0.08
M06/6-311G	10.39	+1.39	–0.07	–0.70	+0.08
HF/6-311+G	11.61	**+5.13**	–2.33	–1.44	+1.20
B3LYP/6-311+G	10.61	**+4.18**	–1.46	–1.36	+0.74
CAM-B3LYP/6-311+G	10.84	**+3.19**	–1.28	–0.80	+0.48
M06/6-311+G	10.57	+2.24	–0.85	–1.16	+0.89
HF/6-311++G(*d*,*p*)	11.84	+0.40	–0.09	–0.73	+0.61
B3LYP/6-311++G(*d*,*p*)	10.54	**–0.28**	+0.25	–0.48	+0.37
PBE0/6-311++G(*d*,*p*)	10.50	+0.49	+0.17	–0.80	+0.38
HF/6-311+G(*3df*,*3pd*)	11.81	+2.88	–0.85	–0.34	–0.25
HF/6-311G(*3df*,*3pd*)	11.86	+1.67	–0.04	+0.10	–0.90
HF/6-311G(*d*,*p*)	11.77	+1.64	–0.11	–0.76	+0.05
B3LYP/6-311G(*d*,*p*)	10.54	+1.32	−0.08	−0.66	+0.08
CAM-B3LYP/6-311G(*d*,*p*)	10.83	+1.32	–0.07	–0.70	+0.11
PBE0/6-311G(*d*,*p*)	10.46	+1.30	–0.03	–0.68	+0.05
TPSSh/6-311G(*d*,*p*)	10.18	+1.26	−0.04	−0.70	+0.10
M06/6-311G(*d*,*p*)	10.48	+1.28	−0.03	−0.68	+0.07
M06-L/6-311G(*d*,*p*)	10.00	+1.36	−0.06	−0.64	+0.02
M06-2X/6-311G(*d*,*p*)	10.48	+1.45	–0.10	–0.68	+0.06
M06-HF/6-311G(*d*,*p*)	9.98	+1.51	–0.18	–0.81	+0.24
M11/6-311G(*d*,*p*)	10.38	+1.47	–0.12	–0.73	+0.12
N12/6-311G(*d*,*p*)	9.90	+1.11	+0.01	–0.69	+0.06
HF/6-31++G(*d*,*p*)	11.89	**–2.23**	+0.55	+0.35	+0.22
B3LYP/6-31++G(*d*,*p*)	10.75	**–0.95**	+0.71	–0.17	–0.06

CAM-B3LYP/6-31++G(*d*,*p*)	11.01	**–1.03**	+0.75	+0.02	–0.26
HF/6-31+G(*3df*,*3pd*)	11.81	+2.36	–1.31	–1.67	+1.81
B3LYP/6-31+G(*3df*,*3pd*)	10.64	+1.06	–0.48	–1.76	+1.71
HF/6-31+G(*d*)	11.92	**–2.29**	+0.43	+0.75	–0.03
B3LYP/6-31+G(*d*)	10.81	**–1.12**	+0.51	+0.04	+0.01
CAM-B3LYP/6-31+G(*d*)	11.07	**–1.34**	+0.63	+0.08	–0.04
HF/6-31G	11.23	+1.19	–0.09	–0.68	+0.18
B3LYP/6-31G	10.54	+0.65	+0.04	–0.49	+0.13
CAM-B3LYP/6-31G	10.73	+0.58	+0.06	–0.50	+0.15
M06/6-31G	10.51	+0.72	+0.03	–0.55	+0.16
TPSSh/6-31G	10.42	+0.74	+0.04	–0.55	+0.15
PBE0/6-31G	10.53	+0.75	+0.03	–0.54	+0.14
B3LYP/6-31+G	10.60	+1.70	–0.31	–0.78	+0.23
CAM-B3LYP/6-31+G	10.81	+1.54	–0.18	–0.76	+0.17
M06/6-31+G	10.56	+1.05	+0.15	–1.21	+0.54
TPSSh/6-31+G	10.44	+1.37	–0.10	–0.88	+0.29
PBE0/6-31+G	10.61	+1.46	–0.27	–0.83	+0.37
HF/6-31G(*3df*,*3pd*)	11.91	+1.29	–0.39	–1.22	+0.97
B3LYP/6-31G(*3df*,*3pd*)	10.75	+0.36	–0.26	–0.10	+1.08
HF/6-31G(*3df*,*p*)	11.95	+1.23	–0.32	–1.18	+0.88
B3LYP/6-31G(*3df*,*p*)	10.76	+0.33	–0.21	–0.92	+0.96
HF/6-31G(*d*,*p*)	11.86	+1.07	–0.03	–0.68	+0.17
B3LYP/6-31G(*d*,*p*)	10.74	+0.60	+0.08	–0.47	+0.10
CAM-B3LYP/6-31G(*d*,*p*)	10.98	+0.53	+0.10	–0.48	+0.11
TPSSh/6-31G(*d*,*p*)	10.53	+0.66	+0.08	–0.54	+0.13
PBE0/6-31G(*d*,*p*)	10.70	+0.66	+0.08	–0.52	+0.12
M06/6-31G(*d*,*p*)	10.81	+0.63	+0.08	–0.51	+0.12
M11/6-31G(*d*,*p*)	10.50	+0.70	+0.03	–0.51	+0.12
N12/6-31G(*d*,*p*)	9.95	+0.42	+0.14	–0.46	+0.11
HF/aug-cc-pVTZ	11.80	**–0.84**	+0.30	+0.46	–0.34
B3LYP/aug-cc-pVTZ	10.53	+1.35	–0.69	+0.39	–0.37
PBE0/aug-cc-pVTZ	10.49	+0.33	–0.30	+0.15	–0.02
TPSSh/aug-cc-pVTZ	10.2	**–0.42**	+0.05	+0.33	–0.17
BP86/aug-cc-pVTZ	9.93	+1.45	–0.70	+0.33	–0.36
HF/cc-pVTZ	11.82	+0.53	+0.15	–0.54	+0.12
B3LYP/cc-pVTZ	10.67	+0.58	+0.10	–0.44	+0.05
CAM-B3LYP/cc-pVTZ	10.92	+0.41	+0.17	–0.45	+0.07
PBE0/cc-pVTZ	10.66	+0.24	+0.22	–0.39	+0.06
TPSSh/cc-pVTZ	10.46	+0.02	+0.26	–0.40	+0.13
HF/cc-pVDZ	11.95	+0.60	+0.19	–0.52	+0.03
B3LYP/cc-pVDZ	10.77	**–0.24**	+0.32	–0.22	+0.02
CAM-B3LYP/cc-pVDZ	11.04	**–0.39**	+0.37	–0.22	+0.04
PBE0/cc-pVDZ	10.73	**–0.13**	+0.33	–0.29	+0.02
TPSSh/cc-pVDZ	10.51	**–0.18**	+0.34	–0.29	+0.04
HF/TZVP	11.89	**–0.06**	+0.00	–0.93	+0.95
B3LYP/TZVP	10.57	**–0.11**	+0.11	–0.78	+0.72
CAM-B3LYP/TZVP	10.90	**–0.14**	+0.21	–0.78	+0.64
PBE0/TZVP	10.55	**–0.24**	+0.19	–0.90	+0.83
LC-ωPBE/TZVP	11.08	**–0.24**	+0.35	–0.86	+0.63
TPSSh/TZVP	10.26	**–0.19**	+0.18	–0.96	+0.87
M06/TZVP	10.71	**–0.39**	+0.26	–0.77	+0.70
M06-L/TZVP	10.34	**–0.05**	–0.18	–1.10	+1.31
M06-2X/TZVP	10.62	+0.04	+0.20	–0.76	+0.55
M06-HF/TZVP	10.11	+0.60	+0.64	–0.65	–0.29

M11/TZVP	10.56	+0.22	+0.28	–0.67	+0.28
M11-L/TZVP	10.01	+0.05	–0.20	–1.16	+1.33
HF/DGDZVP	11.76	+0.74	+0.22	–0.57	–0.01
B3LYP/DGDZVP	10.67	+0.06	+0.40	–0.42	–0.01
CAM-B3LYP/DGDZVP	10.98	**–0.04**	+0.43	–0.42	+0.02
TPSSh/DGDZVP	10.34	+0.20	+0.39	−0.49	–0.01
PBE0/DGDZVP	10.57	+0.21	+0.40	–0.47	–0.04
LC-ωPBE/DGDZVP	11.14	+0.00	+0.46	–0.48	+0.01
M06/DGDZVP	10.68	+0.20	+0.37	–0.42	–0.04
M06-HF/DGDZVP	10.39	**−0.03**	+0.25	−0.47	+0.24
M06-2X/DGDZVP	10.64	+0.27	+0.28	–0.46	+0.04
M06-L/DGDZVP	10.15	+0.71	+0.23	−0.45	−0.14
M11/DGDZVP	10.52	+0.24	+0.26	–0.42	+0.04
M11-L/DGDZVP	9.54	+1.04	+0.08	–0.51	+0.05
N12/DGDZVP	10.09	**–0.17**	+0.55	–0.48	+0.02
HF/3-21G	10.84	+2.07	–0.35	–0.75	+0.06
B3LYP/3-21G	10.18	+1.72	–0.26	–0.62	+0.01
B3LYP/3-21G(*d*)	10.22	+1.72	–0.26	–0.61	+0.02
CAM-B3LYP/3-21G	10.37	+1.68	–0.25	–0.62	+0.03
PBE0/3-21G	10.13	+1.85	–0.29	–0.66	+0.02
PBE0/3-21G(*d*)	10.17	+1.85	–0.29	–0.65	+0.02
LC-ωPBE/3-21G(*d*)	10.43	+1.71	–0.25	–0.66	+0.06
TPSSh/3-21G	9.92	+1.82	–0.28	–0.66	+0.03
M06/3-21G	10.58	+1.86	–0.30	–0.67	+0.04
M06-L/3-21G(*d*)	10.20	+2.19	–0.36	–0.75	+0.02
M06-2X/3-21G(*d*)	10.07	+1.71	–0.28	–0.63	+0.05
M06-HF/3-21G(*d*)	9.32	+1.24	–0.19	–0.54	+0.11
M11/3-21G	9.89	+1.71	–0.26	–0.67	+0.08
N12/3-21G	9.39	+1.71	–0.25	–0.62	+0.01
HF/CEP-121G	11.87	**–0.37**	+0.75	–0.87	+0.31
B3LYP/CEP-121G	10.82	**−1.00**	+0.79	–0.67	+0.38
CAM-B3LYP/CEP-121G	11.10	**–1.19**	+0.87	–0.68	+0.40
PBE0/CEP-121G	10.95	**–0.91**	+0.90	–0.79	+0.35
LC-ωPBE/CEP-121G	11.42	**–1.24**	+0.10	–0.78	+0.40
TPSSh/CEP-121G	10.81	**–1.05**	+0.90	–0.75	+0.38
M06/CEP-121G	11.000	**–0.98**	+0.91	–0.84	+0.42
M06-2X/CEP-121G	10.88	**–0.84**	+0.80	–0.73	+0.36
M06-HF/CEP-121G	10.86	**–1.53**	+0.78	–0.41	+0.39
M06-L/CEP-121G	10.63	**–0.63**	+0.89	–0.95	+0.39
M06-2X/CEP-121G	10.88	**–0.84**	+0.80	–0,73	+0.36
M11/CEP-121G	10.80	**–0.82**	+0.79	–0.81	+0.43
M11-L/CEP-121G	10.40	**+0.11**	+0.64	–0.89	+0.20
N12/CEP-121G	10.63	**–1.43**	+1.00	–0.71	+0.43
HF/SDD	11.88	+0.50	+0.51	–0.83	+0.06
B3LYP/SDD	11.07	+0.10	+0.60	–0.79	+0.15
CAM-B3LYP/SDD	11.34	**–0.11**	+0.66	–0.78	+0.17
PBE0/SDD	11.15	+0.27	+0.64	–0.88	+0.11
TPSSh/SDD	11.00	+0.20	+0.63	–0.86	+0.13
M06/SDD	11.19	+0.31	+0.59	–0.89	+0.14
M06-2X/SDD	11.70	+0.21	+0.57	–0.84	+0.17
M06-HF/SDD	10.82	**–0.58**	+0.59	–0.56	+0.26
M06-L/SDD	10.81	+0.93	+0.48	–1.01	+0.06
M11/SDD	10.77	+0.14	+0.54	–0.81	+0.20
N12/SDD	10.70	+0.13	+0.72	–0.97	+0.18
HF/LANL2DZ	11.84	+0.32	+0.44	–0.70	+0.10
B3LYP/LANL2DZ	11.05	+0.28	+0.44	–0.71	+0.13
CAM-B3LYP/LANL2DZ	11.33	+0.11	+0.49	–0.70	+0.16

PBE0/LANL2DZ	11.10	+0.39	+0.49	–0.79	+0.11
LC-ωPBE/LANL2DZ	11.58	+0.11	+0.55	–0.77	+0.16
TPSSh/LANL2DZ	10.95	+0.37	+0.47	–0.76	+0.14
M06/LANL2DZ	11.13	+0.44	+0.45	–0.81	+0.13
M06-2X/LANL2DZ	11.00	+0.29	+0.43	–0.75	+0.18
M11/LANL2DZ	10.66	+0.32	+0.42	–0.77	+0.19

Notes. **Carb** stands for carboranyl $C_2B_{10}H_{10}$ and $>CMe_2$ is the bridging group; ***q*(Ti)** stands for the charge on Ti ion; ***q*(Cp)** is the charge on each Cp-ligand; ***q*(Carb)** is the charge on each carboranyl ligand; ***q*(>CMe$_2$)** is the charge on each $>CMe_2$ bridge; in a number of cases, the total charge of the complex differs from zero that is due to rounding of the Mulliken charges on the corresponding molecular fragments.