Supplementary Information for ***Acta Phys. -Chim. Sin.*** **2015**, *31* (7), 1283-1301
doi: 10.3866/PKU.WHXB201504291

采用 12 种密度泛函理论方法表征三种三价铀复合物

丁万见 [1,*] 方维海 [1] 柴之芳 [2,3] 王东琪 [2,*]

([1] 北京师范大学化学学院，理论及计算光化学教育部重点实验室，北京 100875; [2] 中国科学院高能物理研究所，中国科学院核辐射与核能技术重点实验室，北京 100049; [3] 苏州大学核药物与交叉科学学院，江苏苏州 215123)

Performance of Twelve Density Functional Theory Methods in the Characterization of Three Trivalent Uranium Complexes

DING Wan-Jian[1,*] FANG Wei-Hai[1] CHAI Zhi-Fang[2,3] WANG Dong-Qi[2,*]

([1]*Key Laboratory of Theoretical and Computational Photochemistry, Ministry of Education, College of Chemistry, Beijing Normal University, Beijing 100875, P. R. China*; [2]*CAS Key Laboratory of Nuclear Radiation and Nuclear Energy Techniques, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100049, P. R. China*; [3]*School of Radiation Medicine and Interdisciplinary Sciences (RAD-X), Soochow University, Suzhou 215123, Jiangsu Province, P. R. China*)

[*]Corresponding authors. DINGWan-Jian, Email: dingwanjian@bnu.edu.cn; Tel: +86-10-58804232.
WANG Dong-Qi, Email: dwang@ihep.ac.cn; Tel: +86-10-88236606.

1 Full citation of Gaussian 09

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian 09, Gaussian, Inc., Wallingford CT, 2009.

2 Relative energies between the quartet and the doublet

Table S1 Relative energies between the quartet and the doublet[a]

Functional	Cpd2				Cpd3				Cpd4			
	$\Delta E^{d/q}$	$\Delta G^{d/q}$	$\Delta H^{d/q}$	$\Delta S^{d/q}$	$\Delta E^{d/q}$	$\Delta G^{d/q}$	$\Delta H^{d/q}$	$\Delta S^{d/q}$	$\Delta E^{d/q}$	$\Delta G^{d/q}$	$\Delta H^{d/q}$	$\Delta S^{d/q}$
BS1: SC-6-31G(*d*)												
BP86	-13.1	-12.7	-13.1	-1.3	-13.3	-14.0	-13.3	2.4	-10.6	-11.7	-10.7	3.3
PBE	-12.3	-12.5	-12.4	0.3	-13.6	-13.8	-13.5	0.9	-10.8	-11.1	-11.0	0.3
B3LYP	-16.4	-16.6	-16.4	0.7	-16.4	-17.2	-16.4	2.6	-16.2	-16.7	-16.2	1.8
B3PW91	-16.4	-16.5	-16.4	0.2	-16.6	-16.3	-16.7	-1.2	-16.0	-16.8	-16.0	2.9
BHandHLYP	-19.6	-19.6	-19.7	-0.6	-18.6	-19.3	-18.5	2.8	-19.4	-20.2	-19.4	3.0
PBE0	-17.6	-18.1	-17.5	1.7	-16.8	-17.1	-16.8	1.0	-16.5	-16.6	-16.5	0.3
X3LYP	-16.7	-18.0	-16.6	4.7	-16.3	-17.7	-16.1	5.5	-16.4	-17.1	-16.4	2.3
CAM-B3LYP	-17.6	-17.1	-17.7	-1.9	-17.0	-17.8	-16.9	2.9	-16.8	-17.0	-16.8	0.8
TPSS	-15.9	-15.6	-16.0	-1.2	-16.2	-15.4	-16.3	-3.1	-13.4	-14.3	-13.4	3.2
M06L	-20.9	-27.9	-20.9	0.8	-21.0	-21.0	-21.1	-0.5	-19.5	-21.0	-19.4	5.6
M06	-16.5	-16.8	-16.5	1.0	-17.0	-18.5	-16.8	5.5	-16.2	-16.2	-16.2	-0.3
M06-2X	-21.1	-21.4	-21.0	1.3	-19.1	-18.6	-19.1	-1.4	-18.3	-19.8	-18.2	5.3
BS2: SC-Def2-SVP												
BP86	-12.5	-12.3	-12.6	-1.0	-13.2	-13.7	-13.2	1.5	-10.6	-11.7	-10.5	4.0
PBE	-13.0	-13.7	-13.0	2.3	-13.7	-14.4	-13.6	2.6	-12.6	-12.1	-12.7	-2.0
B3LYP	-16.4	-16.1	-16.5	-1.5	-16.4	-16.9	-16.4	1.6	-16.1	-17.3	-15.9	4.9
B3PW91	-17.1	-16.5	-17.3	-2.7	-16.4	-16.9	-16.4	1.8	-16.1	-17.7	-15.9	6.1
BHandHLYP	-19.7	-20.1	-19.8	0.9	-21.4	-21.3	-21.5	-0.5	-19.4	-18.8	-19.5	-2.4
PBE0	-17.9	-18.7	-17.9	2.7	-17.0	-18.1	-16.9	4.1	-16.4	-16.7	-16.4	1.2
X3LYP	-17.4	-18.0	-17.3	2.2	-17.9	-17.7	-18.0	-1.0	-17.5	-19.0	-17.2	5.8
CAM-B3LYP	-16.8	-18.0	-16.7	4.4	-17.8	-18.7	-17.8	3.2	-15.5	-16.4	-15.3	3.7
TPSS	-15.9	-16.0	-16.0	0.2	-16.3	-16.4	-16.3	0.4	-12.7	-13.1	-12.8	1.0
M06L	-21.1	-22.4	-20.9	5.0	-22.4	-22.3	-22.4	-0.4	-19.4	-20.5	-19.3	4.2
M06	-16.7	-17.3	-16.6	2.3	-16.9	-16.8	-16.9	-0.5	-16.3	-17.1	-16.3	2.5

M06-2X	-18.9	-18.4	-19.0	-1.9	-20.2	-23.4	-19.6	12.5	-18.9	-21.0	-18.5	8.4

[a] $\Delta A^{d\rightarrow q} = A^{q} - A^{d}$, where A is the total electronic energy E (kcal·mol^{-1}), Gibbs free energy G (kcal·mol^{-1}), enthalpy H (kcal·mol^{-1}), or entropy S (J·mol^{-1}·K^{-1}).

3 Deviation of key geometric parameters

Table S2 Deviation of key geometric parameters (distance d in _A, angle A in degree) in quartet state from calculations with small-core (BS1 & BS2) and large-core (BS3 & BS4) treatments of U[a]

Functional	BS1					BS2				
	Cpd2	Cpd3		Cpd4		Cpd2	Cpd3		Cpd4	
	d	*d*	*A*	*d*	*A*	*d*	*d*	*A*	*d*	*A*
BP86	0.03	0.03	1.54	0.05	2.18	0.03	0.03	1.11	0.05	1.87
PBE	0.03	0.03	1.67	0.05	1.88	0.03	0.03	1.24	0.05	1.86
B3LYP	0.08	0.05	1.02	0.05	0.72	0.08	0.05	0.67	0.05	0.64
B3PW91	0.05	0.04	1.24	0.03	0.57	0.05	0.04	0.79	0.03	0.30
BHandHLYP	0.07	0.05	0.95	0.06	1.13	0.07	0.05	0.75	0.06	1.34
PBE0	0.04	0.03	1.44	0.04	0.73	0.04	0.04	0.99	0.04	0.74
X3LYP	0.07	0.06	1.09	0.05	0.59	0.07	0.05	0.71	0.05	0.63
CAM-B3LYP	0.06	0.05	1.07	0.04	0.69	0.06	0.04	0.78	0.04	0.82
TPSS	0.03	0.03	1.65	0.05	1.65	0.03	0.03	1.21	0.04	1.62
M06L	0.06	0.03	1.93	0.04	2.14	0.05	0.03	1.47	0.03	1.57
M06	0.05	0.03	1.70	0.04	1.11	0.04	0.02	1.32	0.04	1.18
M06-2X	0.06	0.03	2.06	0.05	1.84	0.05	0.02	1.60	0.05	1.97
	BS3					BS4				
BP86	0.14	0.09	1.24	0.10	1.37	0.13	0.09	1.00	0.09	1.16
PBE	0.13	0.09	1.33	0.09	1.39	0.13	0.09	1.10	0.09	1.26
B3LYP	0.15	0.10	0.98	0.11	1.81	0.15	0.10	0.99	0.11	1.65
B3PW91	0.13	0.09	1.04	0.09	1.52	0.13	0.09	0.96	0.09	1.39
BHandHLYP	0.13	0.09	1.04	0.10	2.02	0.13	0.09	1.12	0.10	1.87
PBE0	0.12	0.08	1.24	0.08	1.55	0.12	0.08	1.06	0.08	1.45
TPSS	0.13	0.09	1.18	0.09	1.31	0.13	0.09	0.96	0.09	1.23
M06	0.12	0.08	1.57	0.08	1.69	0.11	0.07	1.44	0.08	1.81

[a] The standard deviation of the M geometrical parameters from their corresponding experimental value.

4 Reaction energies at quartet and doublet states

Table S3 Reaction energies (in kcal/mol) at the quartet state

Functional	Cpd2 + CO_2 → Cpd3			Cpd2 + CS_2 → Cpd4			Cpd2 + CO_2 → Cpd3			Cpd2 + CS_2 → Cpd4		
	ΔE	ΔG	ΔH	ΔE	ΔG	ΔH	ΔE	ΔG	ΔH	ΔE	ΔG	ΔH
	BS1						BS2					
BP86	-52.6	-42.2	-53.5	-45.4	-33.3	-46.1	-50.3	-40.8	-51.1	-46.8	-36.0	-47.2
PBE	-55.4	-46.0	-56.0	-49.6	-37.5	-50.3	-52.4	-43.1	-53.1	-50.4	-39.0	-50.9
B3LYP	-57.5	-48.7	-58.1	-44.6	-33.2	-45.0	-55.1	-45.9	-55.7	-45.4	-34.8	-45.7
B3PW91	-55.7	-47.1	-56.4	-48.2	-37.0	-48.7	-53.4	-43.8	-54.2	-49.8	-39.2	-50.2
BHandHLYP	-62.7	-53.4	-63.4	-52.1	-40.9	-52.6	-60.7	-51.4	-61.3	-53.7	-41.8	-54.2
PBE0	-59.0	-49.3	-59.7	-54.0	-42.7	-54.4	-56.9	-47.5	-57.6	-55.2	-43.1	-55.9
X3LYP	-58.7	-48.8	-59.4	-46.4	-34.8	-46.9	-56.6	-47.2	-57.2	-47.2	-36.8	-47.5
CAM-B3LYP	-64.4	-55.2	-65.0	-52.2	-41.8	-52.7	-61.9	-52.4	-62.6	-49.7	-38.2	-50.4
TPSS	-53.8	-44.1	-54.5	-46.9	-36.3	-47.1	-51.5	-42.0	-52.1	-48.9	-37.2	-49.4
M06L	-47.1	-35.5	-47.9	-48.3	-36.6	-48.8	-48.1	-36.9	-48.8	-50.2	-38.3	-50.6
M06	-55.1	-44.7	-55.5	-54.7	-43.5	-54.5	-52.1	-40.7	-52.9	-53.4	-42.6	-53.6
M06-2X	-56.0	-44.5	-57.0	-54.4	-43.9	-54.9	-56.3	-47.5	-57.0	-59.9	-48.7	-60.5
	BS3						BS4					
BP86	-52.8	-43.4	-53.6	-44.7	-32.2	-45.3	-50.8	-41.4	-51.5	-46.7	-37.1	-47.0
PBE	-55.0	-46.2	-55.5	-47.9	-36.3	-48.3	-52.9	-43.9	-53.5	-49.9	-38.3	-50.4
B3LYP	-57.3	-47.9	-57.9	-45.2	-33.7	-45.6	-55.3	-45.9	-56.0	-47.0	-35.8	-47.4
B3PW91	-55.5	-46.0	-56.2	-48.4	-36.1	-49.0	-53.8	-44.9	-54.4	-51.1	-40.0	-51.6
BHandHLYP	-62.9	-53.7	-63.5	-52.9	-41.5	-53.3	-61.0	-51.9	-61.7	-55.1	-43.5	-55.6
PBE0	-59.1	-49.5	-59.7	-53.9	-42.0	-54.4	-57.2	-48.2	-57.8	-56.4	-44.6	-57.0

TPSS	-53.7	-44.3	-54.3	-45.7	-33.3	-46.3	-51.6	-43.0	-52.2	-49.1	-38.7	-49.5
M06	-55.1	-46.0	-55.5	-54.3	-42.4	-54.7	-51.7	-39.8	-52.6	-54.1	-40.4	-54.9

Table S4 Reaction energies (in kcal mol^{-1}) at the doublet state[a]

	Cpd2 + CO_2 → Cpd3			Cpd2 + CS_2 → Cpd4			Cpd2 + CO_2 → Cpd3			Cpd2 + CS_2 → Cpd4		
functional	ΔE	ΔG	ΔH	ΔE	ΔG	ΔH	ΔE	ΔG	ΔH	ΔE	ΔG	ΔH
	BS1						BS2					
BP86	-52.4	-40.9	-53.3	-47.8	-34.3	-48.5	-49.6	-39.4	-50.4	-48.7	-36.6	-49.3
PBE	-54.1	-44.7	-54.9	-51.1	-38.9	-51.7	-51.8	-42.4	-52.5	-50.9	-40.6	-51.3
B3LYP	-57.4	-48.2	-58.1	-44.7	-33.1	-45.2	-55.1	-45.1	-55.8	-45.6	-33.5	-46.3
B3PW91	-55.5	-47.3	-56.1	-48.6	-36.6	-49.2	-54.1	-43.3	-55.0	-50.8	-37.9	-51.6
BHandHLYP	-63.8	-53.7	-64.6	-52.3	-40.2	-52.9	-59.0	-50.1	-59.6	-54.0	-43.1	-54.5
PBE0	-59.7	-50.3	-60.4	-55.0	-44.1	-55.5	-57.8	-48.1	-58.6	-56.8	-45.0	-57.3
X3LYP	-59.1	-49.0	-59.9	-46.6	-35.7	-47.0	-56.0	-47.5	-56.6	-47.1	-35.8	-47.6
CAM-B3LYP	-65.0	-54.5	-65.8	-53.1	-41.9	-53.5	-60.9	-51.6	-61.5	-51.1	-39.8	-51.8
TPSS	-53.5	-44.4	-54.2	-49.4	-37.6	-49.8	-51.1	-41.6	-51.8	-52.2	-40.1	-52.6
M06L	-46.9	-35.7	-47.7	-49.6	-36.7	-50.4	-46.8	-37.0	-47.3	-51.8	-40.2	-52.2
M06	-54.5	-43.1	-55.2	-55.0	-44.1	-54.8	-51.9	-41.2	-52.6	-53.8	-42.5	-53.9
M06-2X	-58.0	-47.3	-59.0	-57.1	-45.5	-57.8	-55.1	-42.6	-56.3	-59.9	-46.2	-61.0

[a] $\Delta A^{d}_{Cpd3} = A^{d}_{Cpd3} - (A^{d}_{Cpd2} + A_{CO2})$, $\Delta A^{d}_{Cpd4} = A^{d}_{Cpd4} - (A^{d}_{Cpd2} + A_{CS2})$.

5 QTAIM topological analysis of selected bonds

Table S5 QTAIM topological analysis of U-X (X=C, O, S) and E-C^{9} (E=O, S) bonds in Cpd2, Cpd3 and Cpd4

	ρ_{BCP}	$\nabla^2\rho_{BCP}$	H_{BCP}	DI	ρ_{BCP}	$\nabla^2\rho_{BCP}$	H_{BCP}	DI
Cpd2	U-C^{8}				C^{8}-C^{12}			
BP86	0.070	0.075	-0.019	1.055	0.261	-0.596	-0.223	1.153
PBE	0.068	0.079	-0.018	1.050	0.262	-0.596	-0.224	1.151
B3LYP	0.065	0.075	-0.016	1.038	0.264	-0.630	-0.230	1.144
B3PW91	0.069	0.077	-0.018	1.052	0.265	-0.631	-0.232	1.146
BHandHLYP	0.064	0.079	-0.016	1.032	0.270	-0.684	-0.243	1.134
PBE0	0.068	0.077	-0.018	1.040	0.266	-0.640	-0.235	1.144
X3LYP	0.065	0.074	-0.016	1.033	0.265	-0.635	-0.231	1.143
CAM-B3LYP	0.065	0.079	-0.016	1.041	0.266	-0.643	-0.233	1.134
TPSS	0.067	0.077	-0.017	1.032	0.262	-0.609	-0.226	1.147
M06L	0.060	0.079	-0.013	0.985	0.270	-0.649	-0.241	1.154
M06	0.064	0.081	-0.016	1.025	0.268	-0.639	-0.236	1.145
M06-2X	0.061	0.085	-0.014	1.016	0.263	-0.620	-0.229	1.131
Cpd3	U-O^{10}				U-O^{11}			
BP86	0.054	0.180	-0.003	1.050	0.055	0.181	-0.003	1.049
PBE	0.055	0.184	-0.003	1.057	0.054	0.178	-0.003	1.045
B3LYP	0.051	0.179	-0.002	1.018	0.051	0.174	-0.002	1.005
B3PW91	0.053	0.187	-0.003	1.034	0.054	0.185	-0.003	1.026
BHandHLYP	0.050	0.190	-0.002	1.008	0.050	0.179	-0.002	0.983
PBE0	0.054	0.191	-0.003	1.032	0.053	0.185	-0.003	1.022
X3LYP	0.051	0.177	-0.002	1.011	0.050	0.175	-0.002	1.005
CAM-B3LYP	0.052	0.184	-0.003	1.018	0.051	0.184	-0.002	1.011
TPSS	0.055	0.191	-0.003	1.062	0.055	0.185	-0.003	1.046
M06L	0.049	0.177	-0.001	0.993	0.051	0.188	-0.001	1.026
M06	0.049	0.181	-0.001	0.999	0.050	0.185	-0.002	1.015
M06-2X	0.049	0.187	-0.002	0.990	0.056	0.204	-0.003	1.076

to be continued

The unit of ρ_{BCP} is e ƀohr^{-3}, and that of $\nabla^2\rho_{BCP}$ is e ƀohr^{-5}. H_{BCP} represents the total electron energy density at a bond critical point (BCP), and DI(A;B) the delocalization index between two atoms A and B.

continued

	ρ_{BCP}	$\nabla^2\rho_{BCP}$	H_{BCP}	DI	ρ_{BCP}	$\nabla^2\rho_{BCP}$	H_{BCP}	DI
Cpd3	$O^{10}-C^9$				$O^{11}-C^9$			
BP86	0.350	-0.268	-0.580	1.488	0.353	-0.251	-0.587	1.508
PBE	0.350	-0.263	-0.580	1.484	0.355	-0.232	-0.590	1.515
B3LYP	0.361	-0.207	-0.604	1.502	0.365	-0.184	-0.612	1.528
B3PW91	0.362	-0.157	-0.604	1.500	0.366	-0.135	-0.612	1.524
BHandHLYP	0.373	-0.078	-0.627	1.504	0.379	-0.051	-0.638	1.539
PBE0	0.364	-0.126	-0.607	1.502	0.368	-0.114	-0.616	1.524
X3LYP	0.362	-0.204	-0.606	1.506	0.365	-0.183	-0.612	1.526
CAM-B3LYP	0.366	-0.196	-0.615	1.507	0.369	-0.164	-0.620	1.527
TPSS	0.349	-0.210	-0.575	1.482	0.353	-0.184	-0.584	1.509
M06L	0.359	-0.046	-0.591	1.524	0.358	-0.052	-0.589	1.501
M06	0.364	-0.178	-0.608	1.521	0.365	-0.174	-0.611	1.513
M06-2X	0.366	-0.031	-0.606	1.538	0.359	-0.079	-0.593	1.477
Cpd4	U-S^{10}				U-S^{11}			
BP86	0.046	0.084	-0.008	1.199	0.046	0.083	-0.008	1.197
PBE	0.046	0.084	-0.008	1.190	0.045	0.082	-0.007	1.182
B3LYP	0.033	0.071	-0.003	0.982	0.033	0.067	-0.003	0.974
B3PW91	0.037	0.079	-0.005	1.029	0.037	0.076	-0.005	1.021
BHandHLYP	0.032	0.072	-0.003	0.951	0.032	0.067	-0.003	0.945
PBE0	0.037	0.076	-0.005	1.005	0.037	0.079	-0.004	1.021
X3LYP	0.034	0.072	-0.003	0.985	0.033	0.067	-0.003	0.973
CAM-B3LYP	0.034	0.075	-0.003	0.976	0.034	0.071	-0.004	0.969
TPSS	0.043	0.086	-0.006	1.153	0.043	0.084	-0.006	1.147
M06L	0.036	0.082	-0.004	1.032	0.038	0.087	-0.004	1.062
M06	0.035	0.075	-0.004	0.997	0.035	0.074	-0.004	0.997
M06-2X	0.034	0.073	-0.004	0.969	0.035	0.076	-0.004	0.991
Cpd4	$S^{10}-C^9$				$S^{11}-C^9$			
BP86	0.206	-0.387	-0.184	1.336	0.208	-0.399	-0.192	1.357
PBE	0.209	-0.402	-0.193	1.359	0.208	-0.397	-0.190	1.352
B3LYP	0.215	-0.395	-0.241	1.427	0.215	-0.380	-0.244	1.429
B3PW91	0.216	-0.376	-0.248	1.417	0.216	-0.356	-0.251	1.417
BHandHLYP	0.219	-0.180	-0.267	1.437	0.219	-0.184	-0.266	1.429
PBE0	0.217	-0.316	-0.257	1.425	0.216	-0.331	-0.255	1.416
X3LYP	0.215	-0.374	-0.247	1.433	0.214	-0.377	-0.244	1.424
CAM-B3LYP	0.218	-0.282	-0.261	1.429	0.218	-0.269	-0.261	1.432
TPSS	0.208	-0.407	-0.199	1.360	0.209	-0.411	-0.207	1.372
M06L	0.210	-0.335	-0.235	1.404	0.210	-0.346	-0.231	1.388
M06	0.212	-0.374	-0.228	1.429	0.210	-0.378	-0.222	1.411
M06-2X	0.216	-0.263	-0.258	1.442	0.213	-0.305	-0.250	1.405

6 Electrostatic potential and electron density

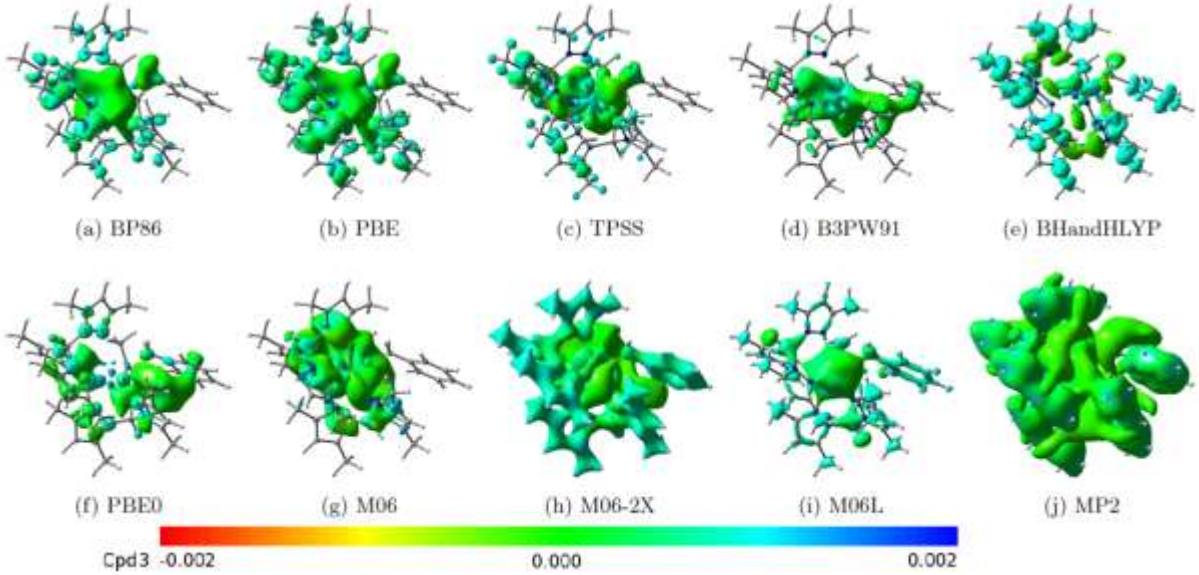

Fig.S1 The ESP difference between CAM-B3LYP and other methods on the CAM-B3LYP optimized geometries of Cpd2

The isovalue for the surfaces is 0.006.

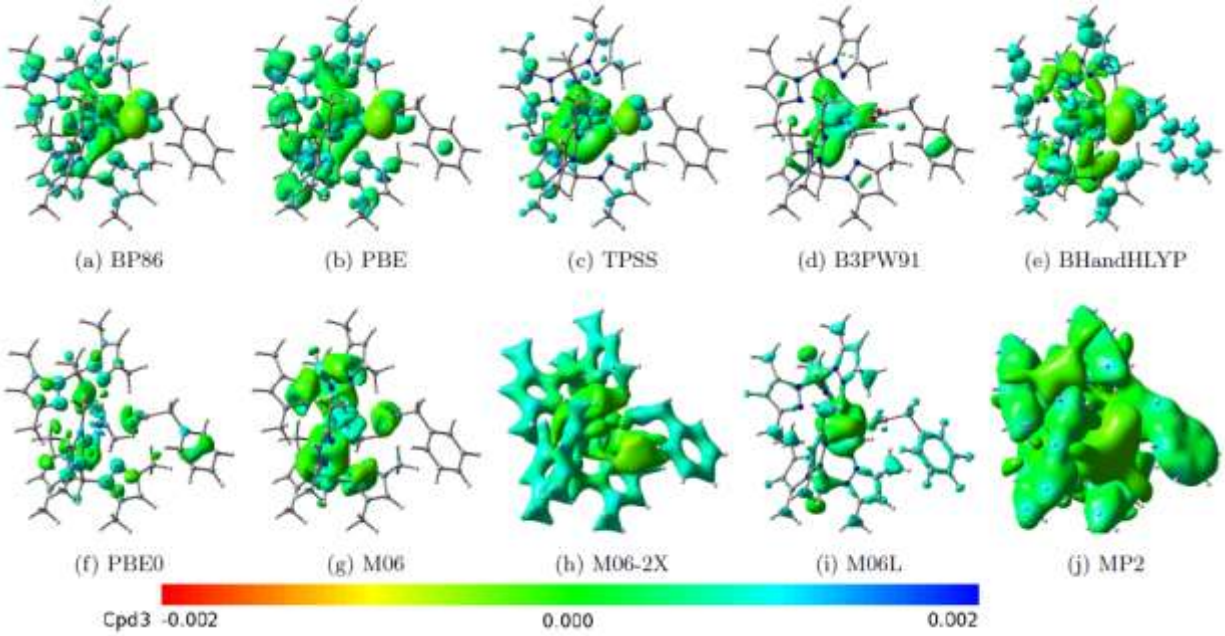

Fig.2 ESP difference between CAM-B3LYP and other methods on the CAM-B3LYP optimized geometries of Cpd3

The isovalue for the surfaces is 0.006.

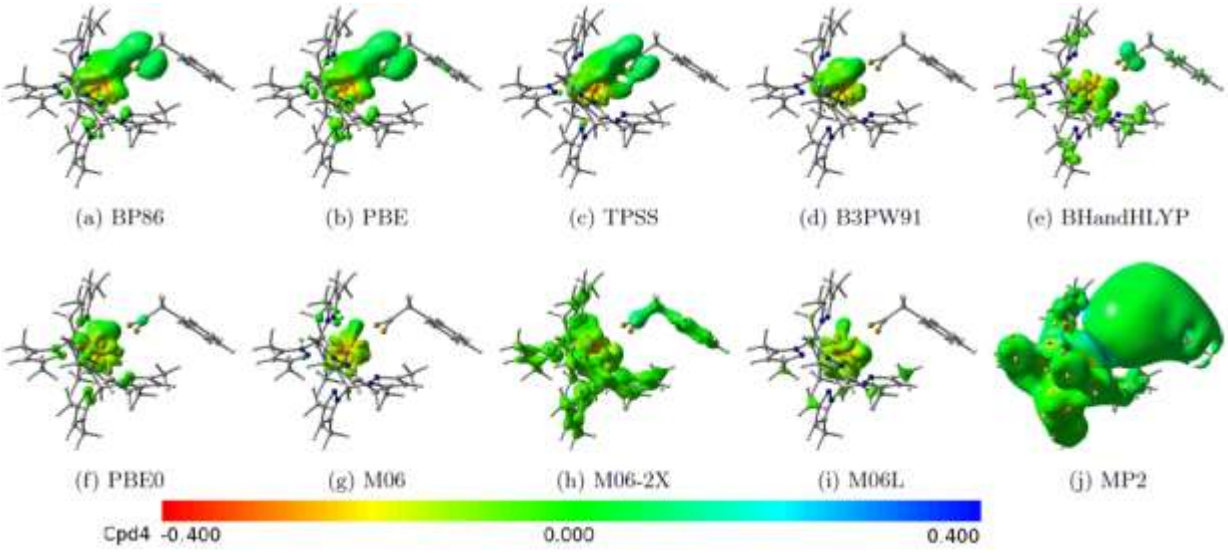

Fig.S3 ESP difference between CAM-B3LYP and other methods on the CAM-B3LYP optimized geometries of Cpd4

The isovalue for the surfaces is 0.01.

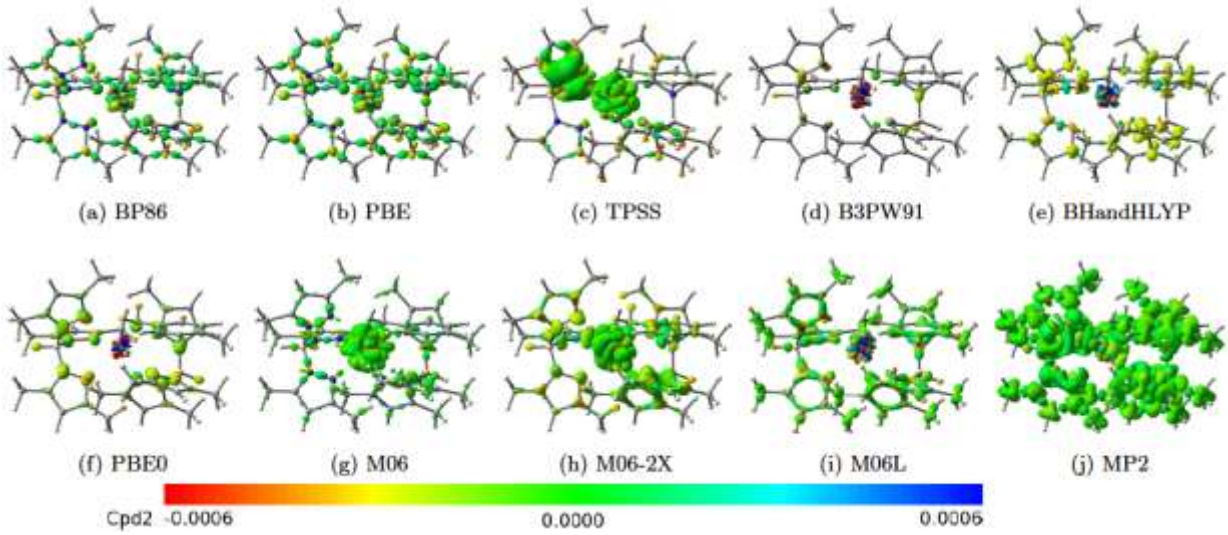

Fig.S4 The electron density di_erence between CAM-B3LYP and other methods on the CAM-B3LYP optimized geometries of Cpd2

The isovalue for the surfaces is 0.003.

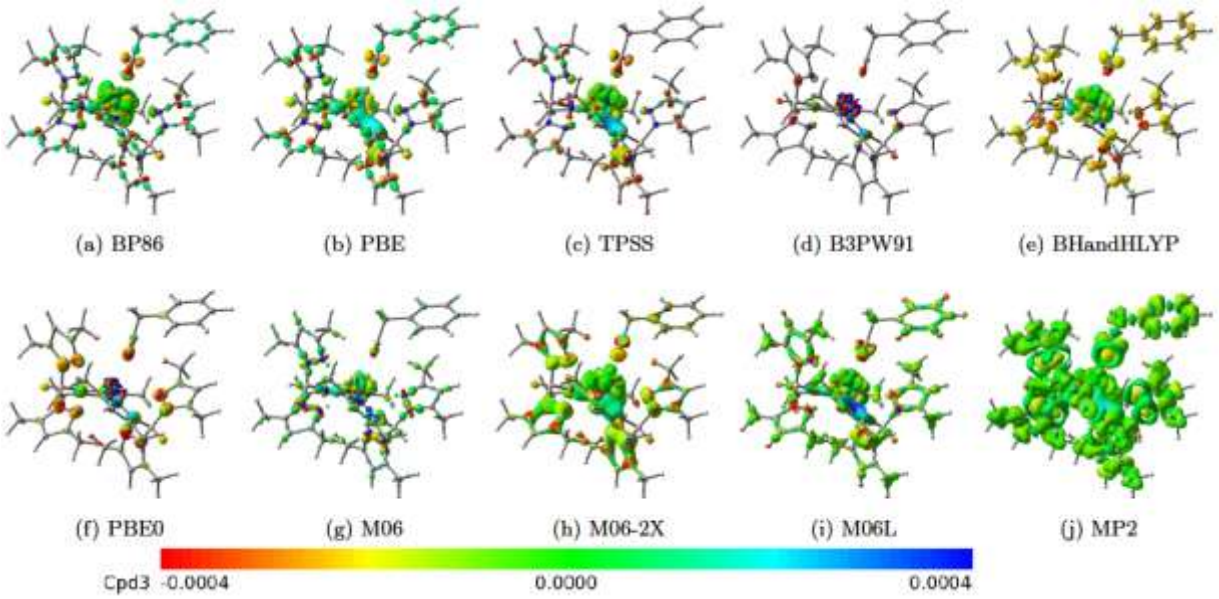

Fig.S5 The electron density di_erence between CAM-B3LYP and other methods on the CAM-B3LYP optimized geometries of Cpd3

The isovalue for the surfaces is 0.003.

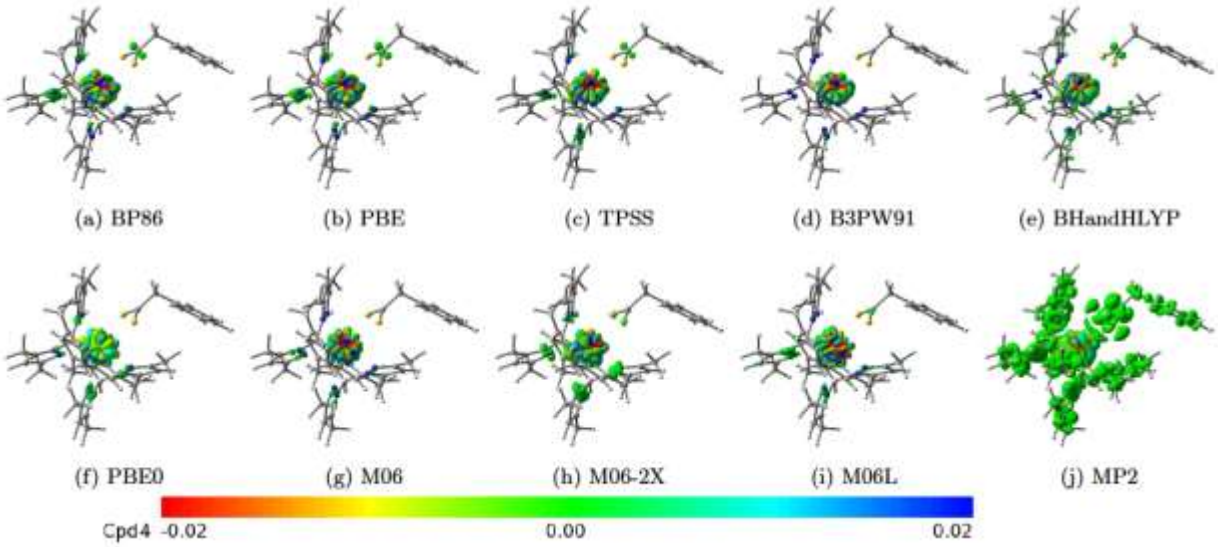

Fig.S6 The electron density di_erence between CAM-B3LYP and other methods on the CAM-B3LYP optimized geometries of Cpd4

The isovalue for the surfaces is 0.006.