Supporting Information

Influence of Supramolecular Interactions on Electron-Transfer Photochromism of the Crystalline Adducts of 4,4′-Bipyridine and Carboxylic Acids

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INDEX:

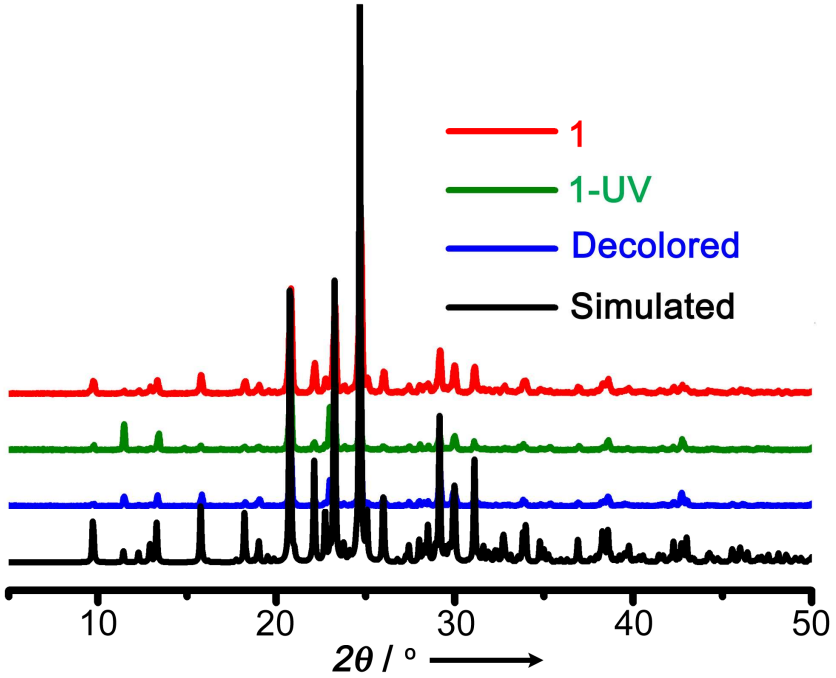


Figure S1. PXRD patterns for **1**, **1-UV**, and the decolored sample. The simulated data was obtained from the single-crystal X-ray diffraction data.

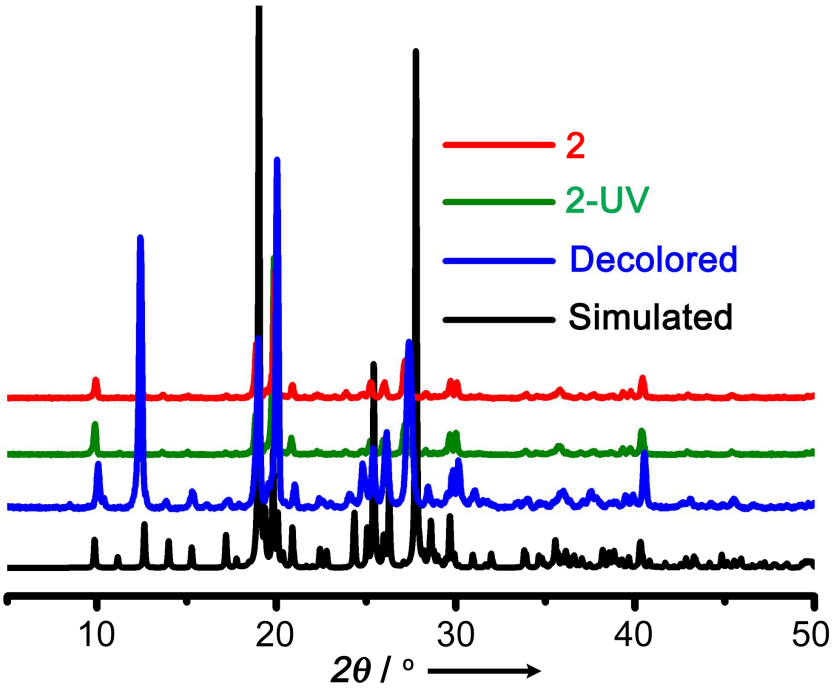


Figure S2. PXRD patterns for **2**, **2-UV**, and the decolored sample. The simulated data was obtained from the single-crystal X-ray diffraction data.

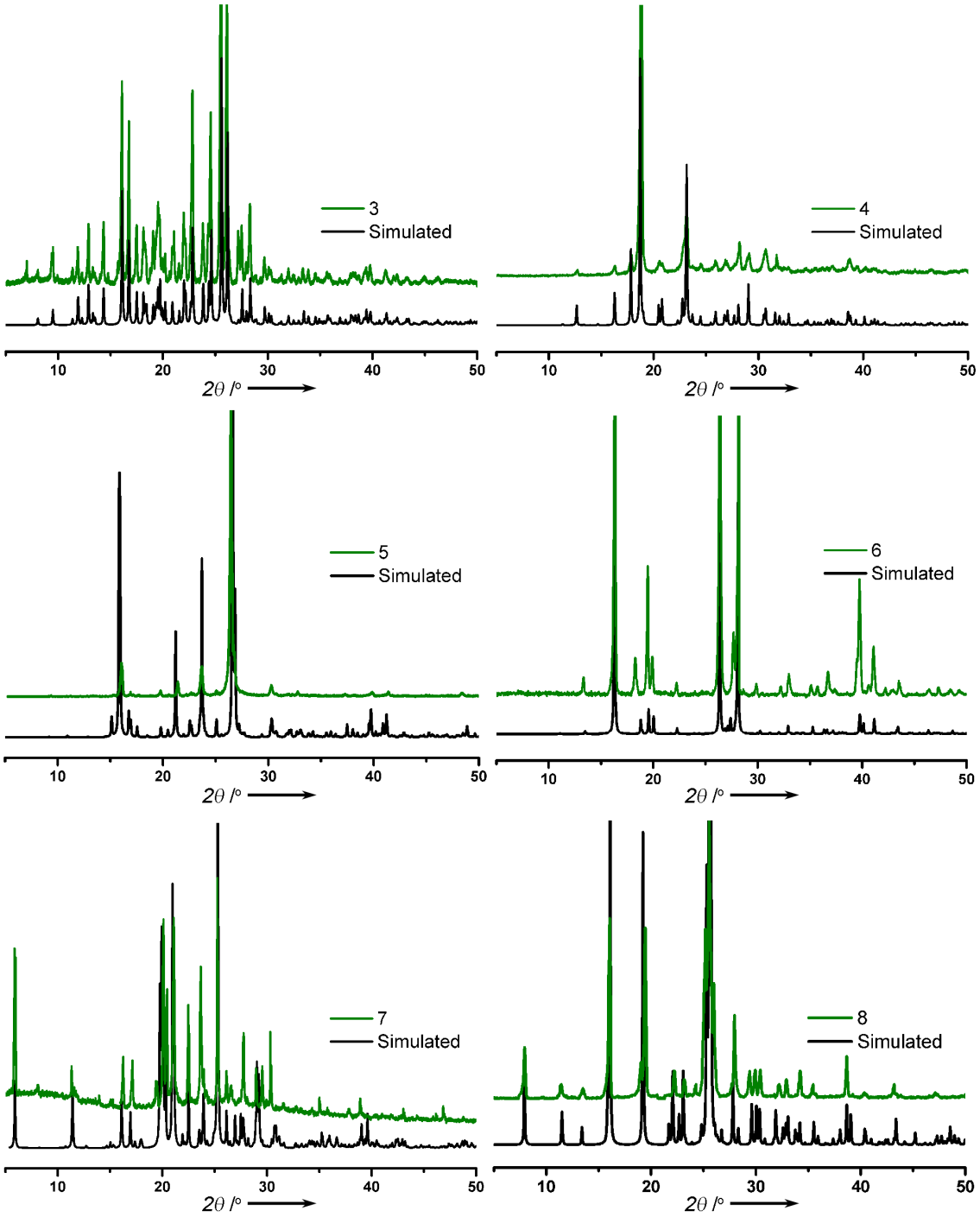


Figure S3. PXRD patterns of **3**−**8**. The simulated data was obtained from the single-crystal X-ray diffraction data.

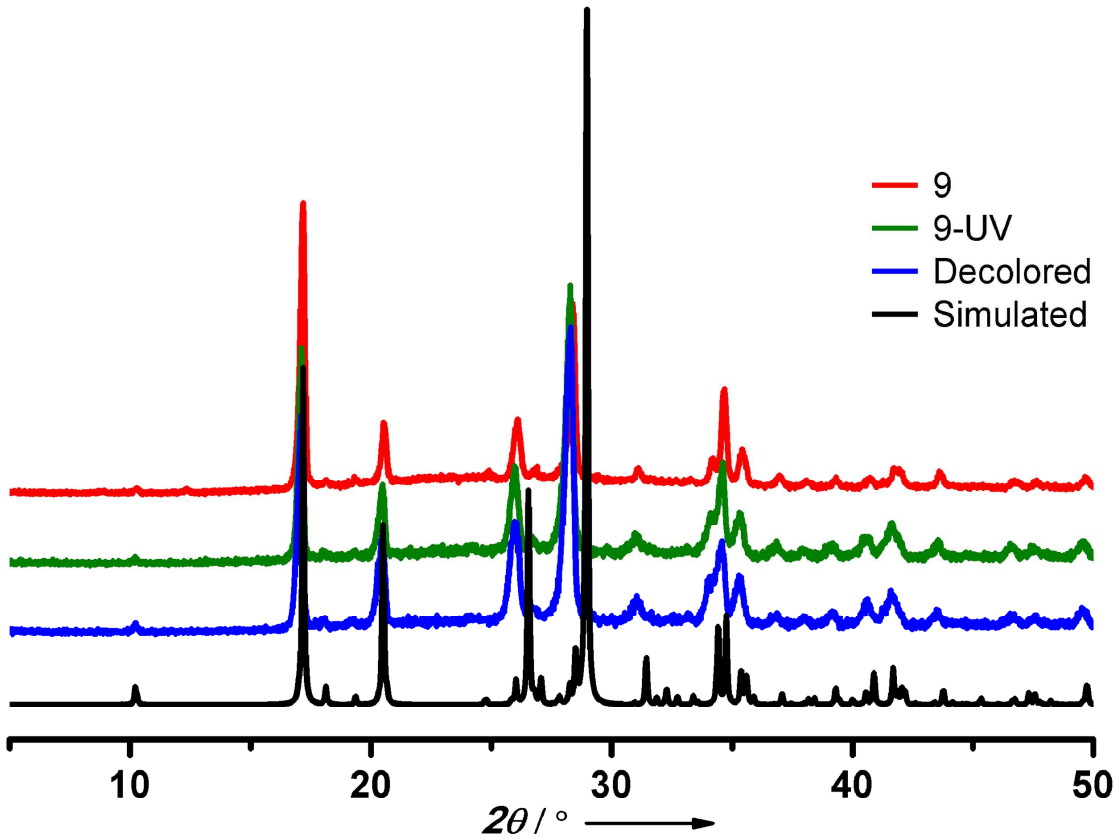


Figure S4. PXRD patterns for **9**, **9-UV**, and the decolored sample. **9-UV** represents the photoproduct of **9**.

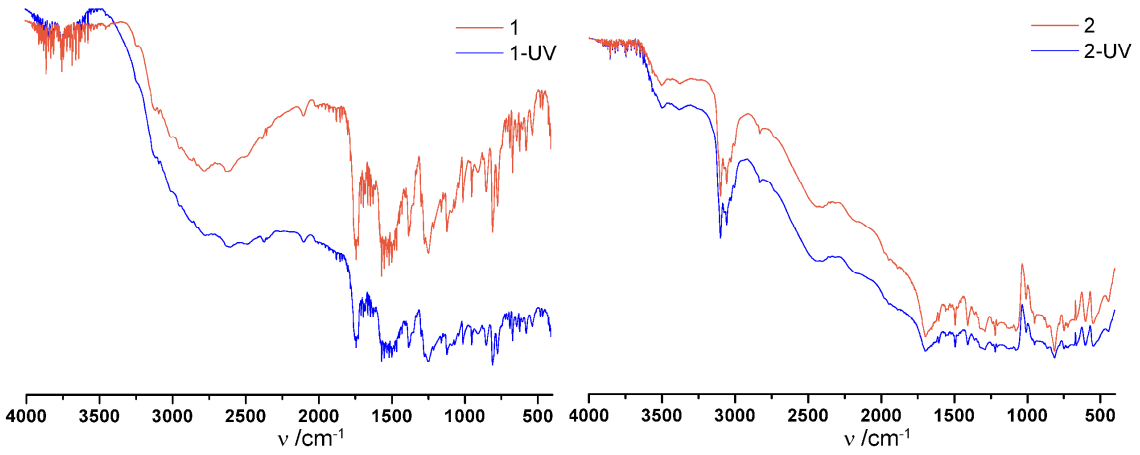


Figure S5. IR spectra of **1** and **2** before and after irradiation.

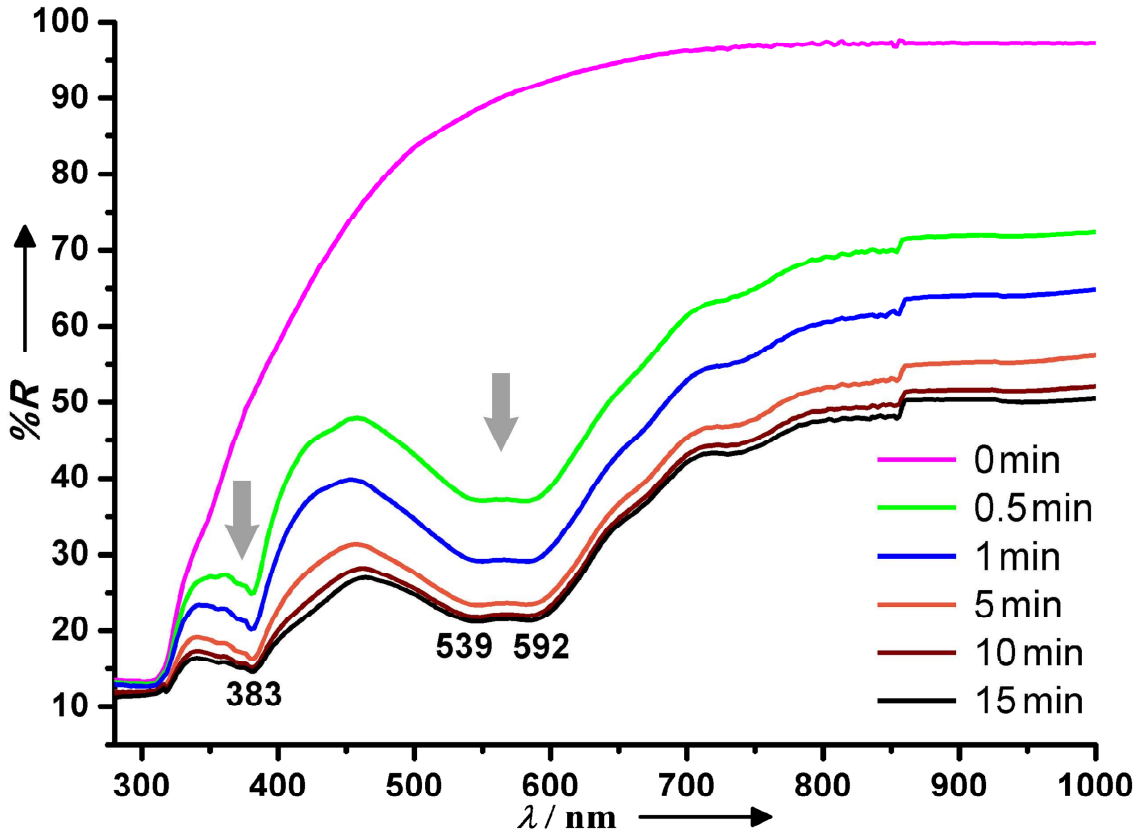
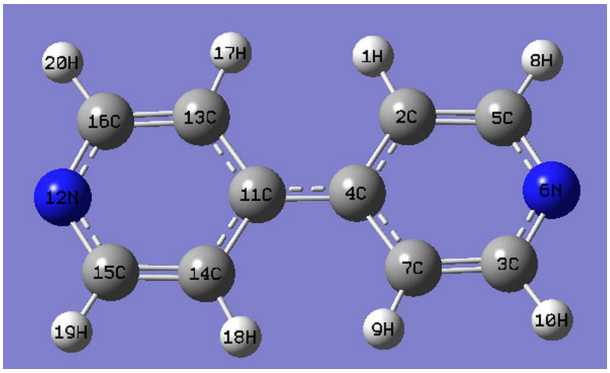


Figure S6. Time-dependent DR spectra of **9** when irradiated by a 300 W Xe lamp in air at room temperature.

Chart S1. The optimized geometries. The calculations were carried out using the Gaussian 09 suite of programs.[1]

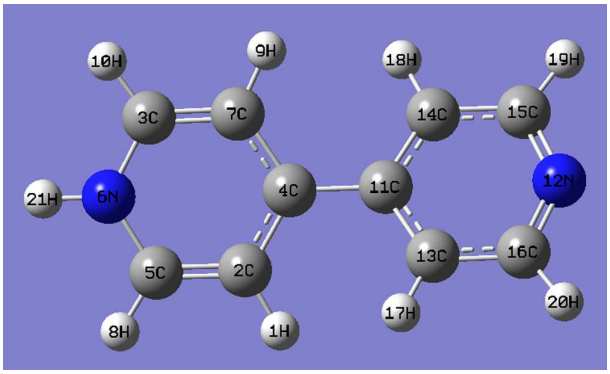
(1) The first singlet excited state of Bpy.



H	-0.10018000	2.18361500	-1.03024400
C	-0.04870100	1.20693900	-1.49431800
C	0.04731800	-1.16467400	-2.87849700

C	0.00000000	0.00000000	-0.72132900
C	-0.04731800	1.16467400	-2.87849700
N	0.00000000	0.00000000	-3.53383400
C	0.04870100	-1.20693900	-1.49431800
H	-0.08742100	2.07534900	-3.47071000
H	0.10018000	-2.18361500	-1.03024400
H	0.08742100	-2.07534900	-3.47071000
C	0.00000000	0.00000000	0.72132900
N	0.00000000	0.00000000	3.53383400
C	0.04870100	1.20693900	1.49431800
C	-0.04870100	-1.20693900	1.49431800
C	-0.04731800	-1.16467400	2.87849700
C	0.04731800	1.16467400	2.87849700
H	0.10018000	2.18361500	1.03024400
H	-0.10018000	-2.18361500	1.03024400
H	-0.08742100	-2.07534900	3.47071000
H	0.08742100	2.07534900	3.47071000

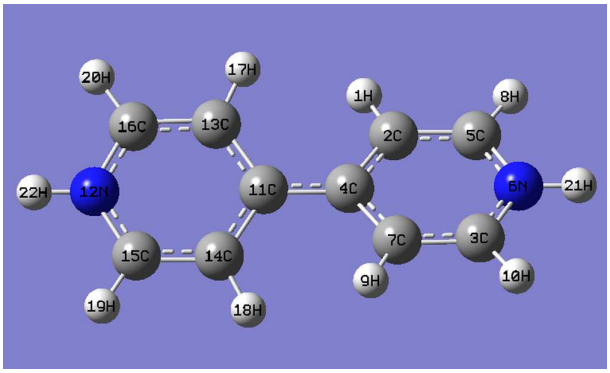
(2) The first singlet excited state of H(Bpy)$^{+}$.



H	-0.01901800	2.17688600	-0.92792000
C	0.00638600	1.21311900	-1.42301000
C	0.00000000	-1.20279300	-2.79194600
C	0.00000000	0.00000000	-0.67790900
C	0.00000000	1.20279300	-2.79194600
N	0.00000000	0.00000000	-3.47321800
C	-0.00638600	-1.21311900	-1.42301000
H	-0.01450700	2.10079200	-3.39434800
H	0.01901800	-2.17688600	-0.92792000
H	0.01450700	-2.10079200	-3.39434800
C	0.00000000	0.00000000	0.80550900
N	0.00000000	0.00000000	3.48619000
C	0.68278700	0.99297200	1.53414500
C	-0.68278700	-0.99297200	1.53414500
C	-0.66677300	-0.98366500	2.93429000
C	0.66677300	0.98366500	2.93429000

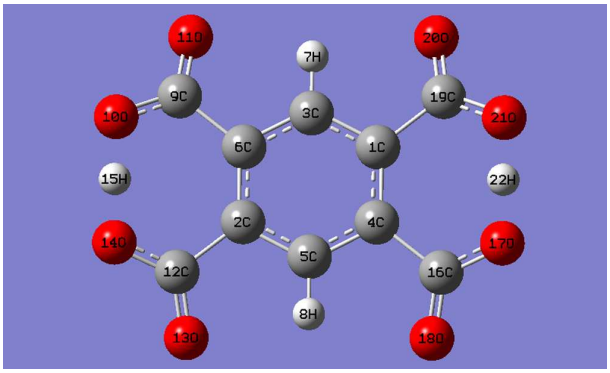
H	1.25988600	1.77038100	1.04962700
H	-1.25988600	-1.77038100	1.04962700
H	-1.17937900	-1.70317600	3.56500800
H	1.17937900	1.70317600	3.56500800
H	0.00000000	0.00000000	-4.48286800

(3) The first singlet excited state of $H_2(Bpy)^{2+}$.



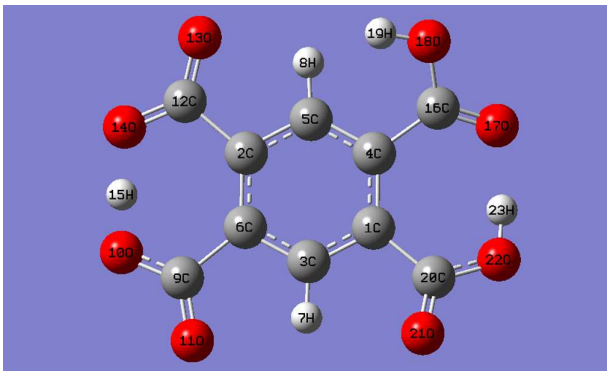
H	-0.42475800	2.14132400	-1.02551200
C	-0.21132000	1.18739200	-1.49349800
C	0.20585200	-1.16612800	-2.88865600
C	0.00000000	0.00000000	-0.72218200
C	-0.20585200	1.16612800	-2.88865600
N	0.00000000	0.00000000	-3.56527300
C	0.21132000	-1.18739200	-1.49349800
H	-0.37797800	2.05650200	-3.48384700
H	0.42475800	-2.14132400	-1.02551200
H	0.37797800	-2.05650200	-3.48384700
C	0.00000000	0.00000000	0.72218200
N	0.00000000	0.00000000	3.56527300
C	0.21132000	1.18739200	1.49349800
C	-0.21132000	-1.18739200	1.49349800
C	-0.20585200	-1.16612800	2.88865600
C	0.20585200	1.16612800	2.88865600
H	0.42475800	2.14132400	1.02551200
H	-0.42475800	-2.14132400	1.02551200
H	-0.37797800	-2.05650200	3.48384700
H	0.37797800	2.05650200	3.48384700
H	0.00000000	0.00000000	-4.58301500
H	0.00000000	0.00000000	4.58301500

(4) The ground state of $H_2(Pma)^{2-}$.



C	1.29047600	-0.62166400	-0.03788800
C	-1.29047600	0.62166400	-0.03788800
C	1.12129500	0.77026500	-0.06591000
C	0.11722600	-1.42764900	-0.03772000
C	-1.12129500	-0.77026500	-0.06591000
C	-0.11722600	1.42764900	-0.03772000
H	2.01263900	1.38272500	-0.10787200
H	-2.01263900	-1.38272500	-0.10787200
C	-0.01517400	2.96431900	-0.01295300
O	-1.05938200	3.64291400	0.36281000
O	1.05938200	3.49603300	-0.31628600
C	-2.76126600	1.07744300	-0.01471200
O	-3.64308500	0.26543200	-0.31831100
O	-3.02098800	2.29609300	0.36001700
H	-2.04398300	2.97267900	0.41713400
C	0.01517400	-2.96431900	-0.01295300
O	1.05938200	-3.64291400	0.36281000
O	-1.05938200	-3.49603300	-0.31628600
C	2.76126600	-1.07744300	-0.01471200
O	3.64308500	-0.26543200	-0.31831100
O	3.02098800	-2.29609300	0.36001700
H	2.04398300	-2.97267900	0.41713400

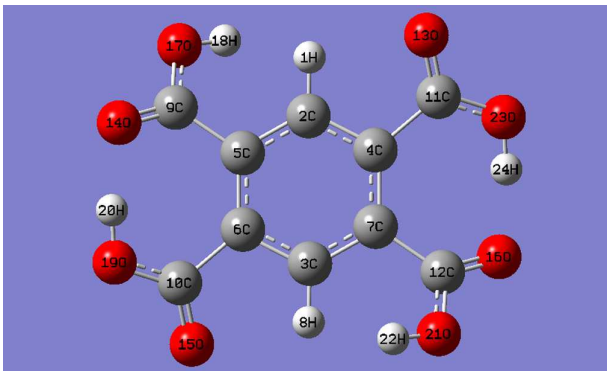
(5) The ground state of $H_3(Pma)^-$.



C	1.22258100	-0.74531200	0.01917900

C	-1.26053100	0.69368500	-0.02101900
C	-0.01868300	-1.38390500	0.03303400
C	1.21841300	0.67803200	0.00005200
C	-0.01519300	1.33553700	-0.01311000
C	-1.25955900	-0.72210900	-0.00527200
H	-0.04069800	-2.46537400	0.08187400
H	-0.08462400	2.41912100	-0.05804200
C	-2.46666000	-1.68756400	-0.02262800
O	-3.66314000	-1.18641600	-0.12712500
O	-2.24544100	-2.89339900	0.05073800
C	-2.45698500	1.69052900	-0.03140000
O	-2.17065900	2.89330100	0.06865800
O	-3.63662000	1.21152400	-0.14514100
H	-3.67485000	-0.08034900	-0.15173200
C	2.43343700	1.54847600	-0.02598300
O	3.50207100	1.25862700	-0.55013300
O	2.33253300	2.76237000	0.55009300
H	1.45975400	2.87257100	0.95892900
C	2.41076100	-1.69792000	0.08213100
O	2.28041200	-2.81563600	0.54274900
O	3.58799300	-1.31219300	-0.42267800
H	3.59773100	-0.34810300	-0.65821500

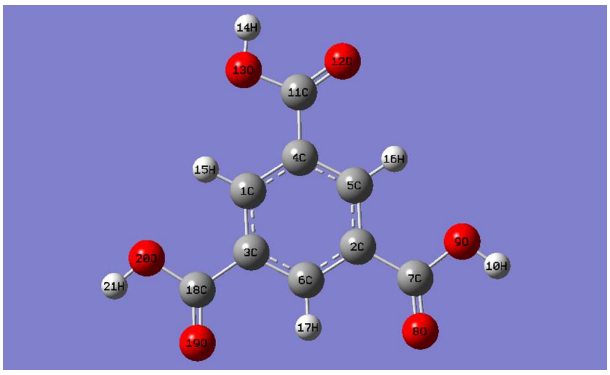
(6) The ground state of H_4(Pma).



H	0.03219400	2.43767400	0.24851500
C	-0.00194000	1.36247000	0.10219300
C	0.00194000	-1.36247000	-0.10219300
C	1.23756200	0.71470500	0.10411300
C	-1.22970800	0.69731500	-0.01083300
C	-1.23756200	-0.71470500	-0.10411300
C	1.22970800	-0.69731500	0.01083300
H	-0.03219400	-2.43767400	-0.24851500
C	-2.46866900	1.55301900	0.02514200
C	-2.41867100	-1.68186200	-0.26096100
C	2.41867100	1.68186200	0.26096100

C	2.46866900	-1.55301900	-0.02514200
O	2.21495900	2.77412200	0.75160900
O	-3.50563700	1.22082100	0.57261600
O	-2.21495900	-2.77412200	-0.75160900
O	3.50563700	-1.22082100	-0.57261600
O	-2.39986200	2.76270400	-0.54656600
H	-1.56511100	2.89836900	-1.01997100
O	-3.61647300	-1.33556400	0.18763300
H	-3.65147000	-0.40089100	0.51690700
O	2.39986200	-2.76270400	0.54656600
H	1.56511100	-2.89836900	1.01997100
O	3.61647300	1.33556400	-0.18763300
H	3.65147000	0.40089100	-0.51690700

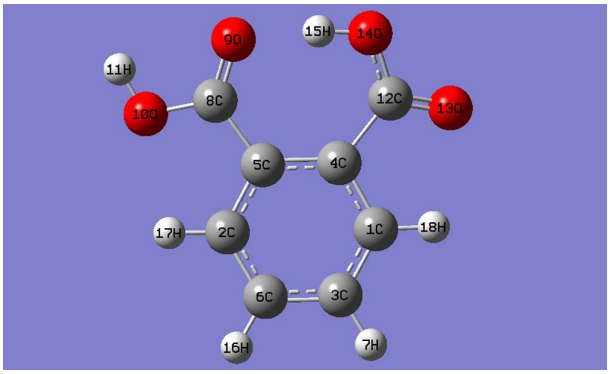
(7) The ground state of H_3(Tma).



C	-1.20656700	0.66301200	0.00000000
C	1.23379400	-0.71306600	0.00000000
C	-1.19014400	-0.73805800	0.00000000
C	0.00000000	1.37344800	0.00000000
C	1.21999200	0.68619600	0.00000000
C	0.02856700	-1.42449400	0.00000000
C	2.50761700	-1.48924600	0.00000000
O	2.57627700	-2.70194900	0.00000000
O	3.60747700	-0.69771000	0.00000000
H	4.38080500	-1.28596200	0.00000000
C	0.03798300	2.86349700	0.00000000
O	1.05519000	3.52815300	0.00000000
O	-1.19598600	3.42499000	0.00000000
H	-1.06880000	4.38826900	0.00000000
H	-2.14953500	1.19449600	0.00000000
H	2.14471900	1.25076600	0.00000000
H	0.03968600	-2.50884100	0.00000000
C	-2.44769300	-1.53937200	0.00000000
O	-2.49385300	-2.75297800	0.00000000
O	-3.56455300	-0.76988400	0.00000000

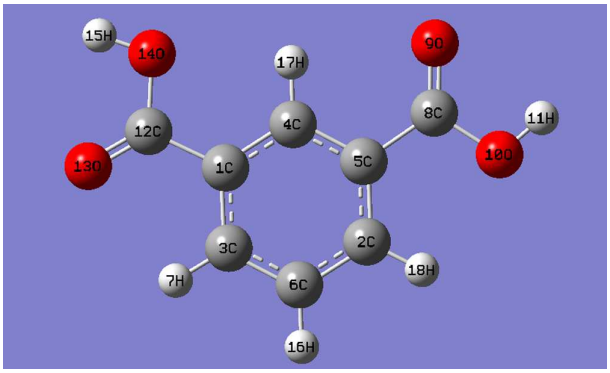
H	-4.32458100	-1.37521600	0.00000000

(8) The ground state of H_2(Opa).



C	1.71825400	1.04998900	-0.06408500
C	-0.95467400	1.75644600	-0.02180400
C	1.35934400	2.39471600	-0.11626300
C	0.76756000	0.01833500	-0.01753500
C	-0.60907300	0.38994900	-0.00041600
C	0.01246200	2.75325800	-0.09064000
H	2.13206400	3.15589100	-0.16638400
C	-1.75141100	-0.56412200	0.00563100
O	-1.72265800	-1.74642800	-0.32494300
O	-2.91715500	-0.01145200	0.39027700
H	-3.59570800	-0.70479400	0.32120800
C	1.42049100	-1.36921300	0.07520200
O	2.58368200	-1.45164900	0.41866300
O	0.73561400	-2.45844400	-0.25756400
H	-0.22299900	-2.26836300	-0.42585000
H	-0.28677100	3.79623000	-0.12064700
H	-2.00215500	2.02847000	0.00590100
H	2.76199500	0.76020400	-0.04623000

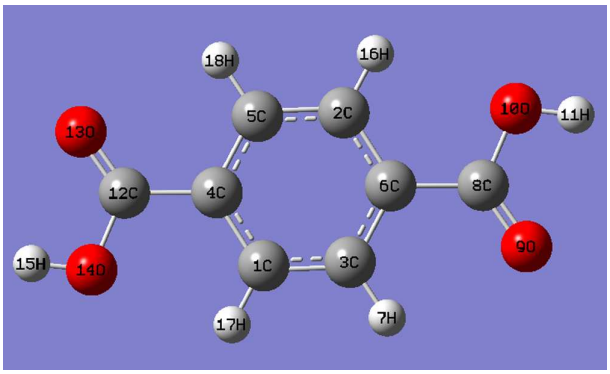
(9) The ground state of H_2(Mpa).



C	-1.23427400	-0.13060800	0.00000000
C	1.13512700	-1.61960300	0.00000000

C	-1.28106500	-1.53352700	0.00000000
C	0.00000000	0.52725100	0.00000000
C	1.18597100	-0.21722700	0.00000000
C	-0.09915900	-2.27229900	0.00000000
H	-2.24930600	-2.02280100	0.00000000
C	2.47622900	0.52573400	0.00000000
O	2.58145700	1.73686700	0.00000000
O	3.56087200	-0.29138100	0.00000000
H	4.34411800	0.28334800	0.00000000
C	-2.52459500	0.61309300	0.00000000
O	-3.62353900	0.09158600	0.00000000
O	-2.36429100	1.95915500	0.00000000
H	-3.25399200	2.34925100	0.00000000
H	-0.13790100	-3.35701500	0.00000000
H	0.05403700	1.60924600	0.00000000
H	2.05766100	-2.18871800	0.00000000

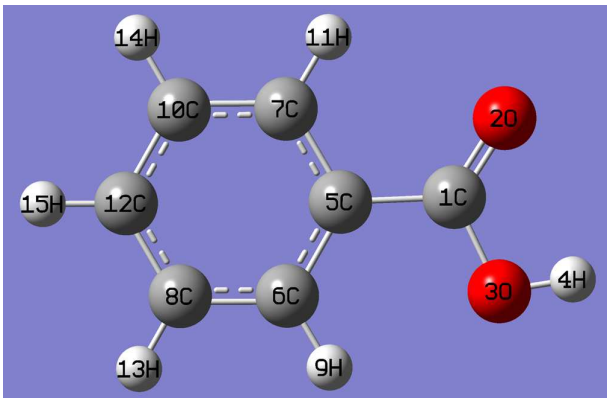
(10) The ground state of H_2(Ppa).



C	-1.19254400	0.73642300	0.00000000
C	1.19254400	-0.73642300	0.00000000
C	-1.23653700	-0.65478500	0.00000000
C	0.04636000	1.39634800	0.00000000
C	1.23653700	0.65478500	0.00000000
C	-0.04636000	-1.39634800	0.00000000
H	-2.18335700	-1.18361700	0.00000000
C	-0.14857500	-2.88327000	0.00000000
O	-1.19254400	-3.50640700	0.00000000
O	1.05972000	-3.50050900	0.00000000
H	0.88727400	-4.45661900	0.00000000
C	0.14857500	2.88327000	0.00000000
O	1.19254400	3.50640700	0.00000000
O	-1.05972000	3.50050900	0.00000000
H	-0.88727400	4.45661900	0.00000000
H	2.11001200	-1.31315400	0.00000000
H	-2.11001200	1.31315400	0.00000000

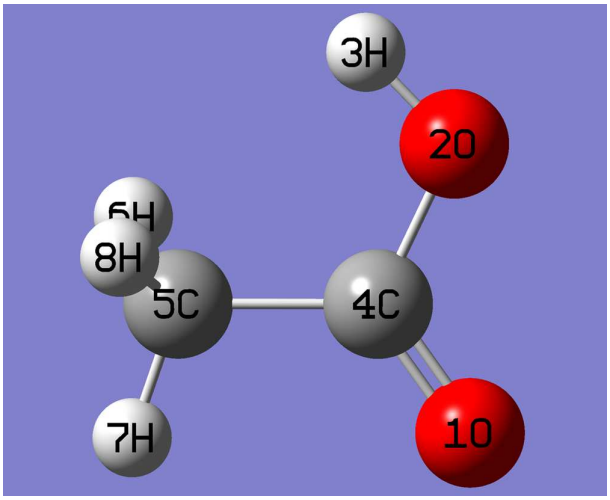
H	2.18335700	1.18361700	0.00000000

(11) The ground state of H(Bza).



C	-1.70402900	0.12232600	0.00000100
O	-2.33984500	1.15991000	-0.00016500
O	-2.31740400	-1.09120300	0.00012400
H	-3.27335900	-0.91786200	-0.00001200
C	-0.22020100	0.03031200	-0.00000100
C	0.44831400	-1.20364300	-0.00004900
C	0.51486900	1.22540200	0.00013300
C	1.84321200	-1.23685100	-0.00002200
H	-0.12388000	-2.12430700	-0.00002200
C	1.90804400	1.18638800	0.00003900
H	-0.02127600	2.16847000	0.00020300
C	2.57342500	-0.04437800	-0.00007200
H	2.36019400	-2.19177000	-0.00003800
H	2.47520600	2.11234000	0.00011300
H	3.65930300	-0.07387000	-0.00010000

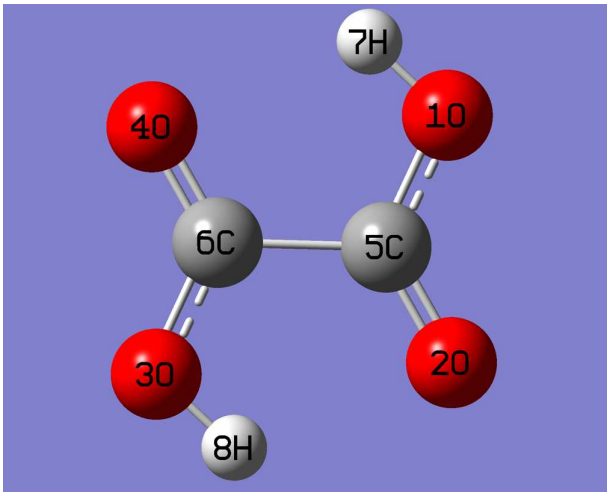
(12) The ground state of H(Ac).



O	0.68056500	1.21016000	-0.00000200

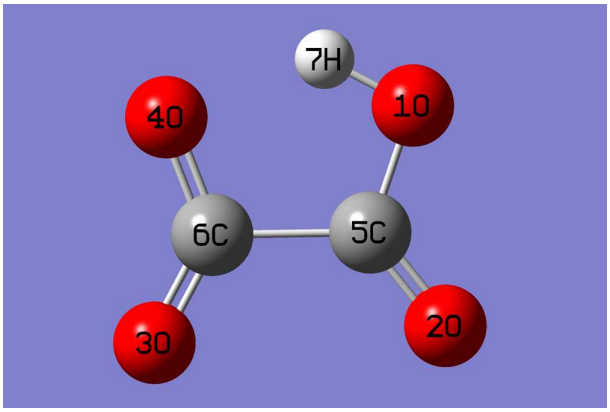
O	0.87342300	-1.00559800	0.00002600
H	0.30655200	-1.79032800	-0.00012400
C	0.12789100	0.13902500	-0.00003200
C	-1.37613100	-0.05902700	-0.00000300
H	-1.69165700	-0.61959500	0.88726600
H	-1.86573300	0.91436400	-0.00068600
H	-1.69162800	-0.62091700	-0.88644100

(13) The ground state of $H_2(Oa)$.



O	1.53861700	0.90419200	0.00086500
O	1.14218900	-1.31397900	-0.00079600
O	-1.53813200	-0.90460500	0.00085500
O	-1.14291400	1.31404000	-0.00076200
C	0.75508500	-0.16699000	-0.00008500
C	-0.75509000	0.16745200	-0.00016700
H	0.96613400	1.69689400	0.00000500
H	-0.96418200	-1.69685600	0.00020900

(14) The ground state of $H(Oa)^-$.



O	1.27958300	1.07960500	0.00002800
O	1.43266200	-1.16880400	-0.00004500

O	-1.49984700	-1.10468400	0.00000200
O	-1.20308100	1.16096500	-0.00005000
C	0.75151000	-0.16432800	0.00003100
C	-0.83561600	-0.06150700	0.00006800
H	0.43010200	1.61834900	-0.00007000

(1) Gaussian 09, Revision A.01, 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, Inc., Wallingford CT, **2009**.