

“Supporting Information for”

How the combination of PhIO and I₂ provides a species responsible for conducting organic reactions through radical mechanisms

Kaveh Farshadfar,^a Ali Gouranourim,^b and Alireza Ariafard^{*b}

^[a]*Department of Chemistry, Islamic Azad University, Central Tehran Branch, Poonak, Tehran 1469669191, Iran*

^[b]*School of Natural Sciences (Chemistry), University of Tasmania, Private Bag 75, Hobart, TAS 7001, Australia*

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Table S1. Total potential (E), enthalpy (H) and Gibbs free energies (G) of all structures optimized at the M06-2X-SMD/BS1 level of theory along with the total potential energies calculated by M06-2X-SMD/BS2//M06-2X-SMD/BS1 for all of the calculated structures, Cartesian coordinates and the spin expectation values of the doublet and triplet structures. (page S5)

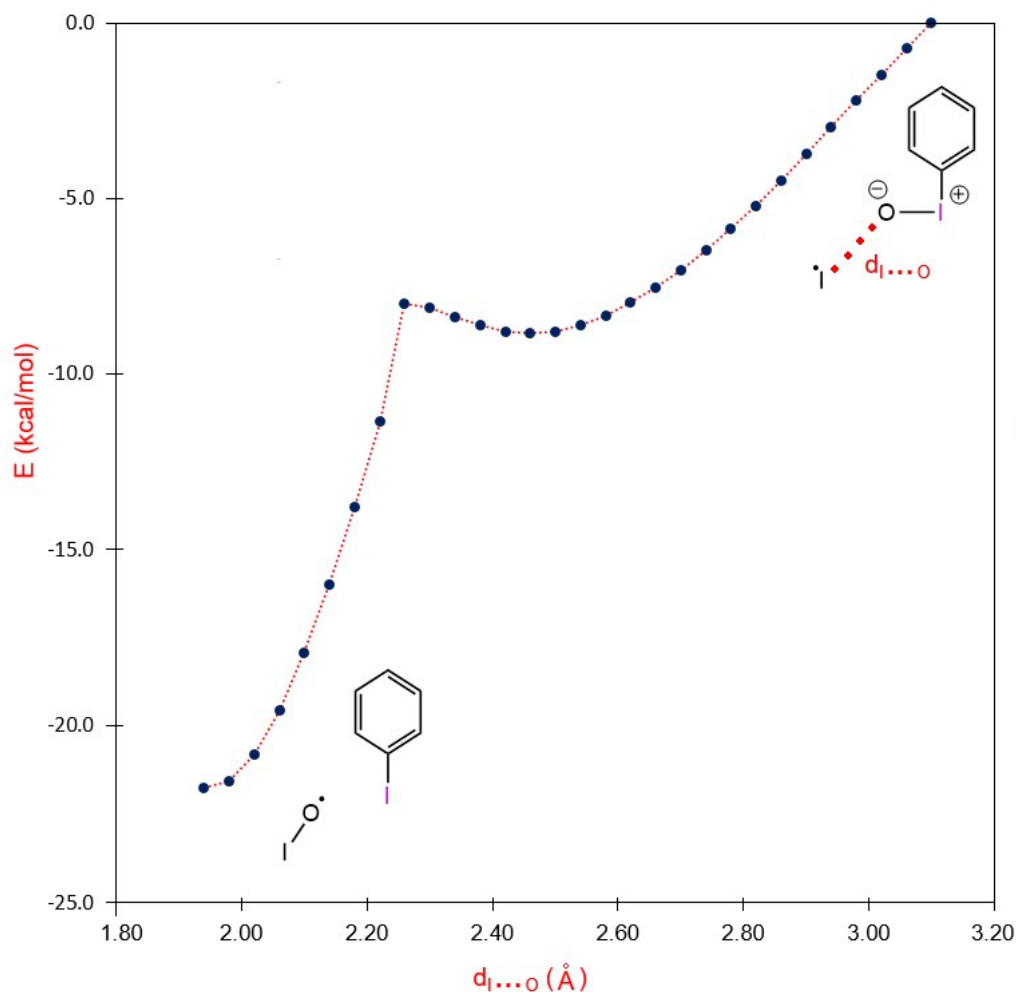
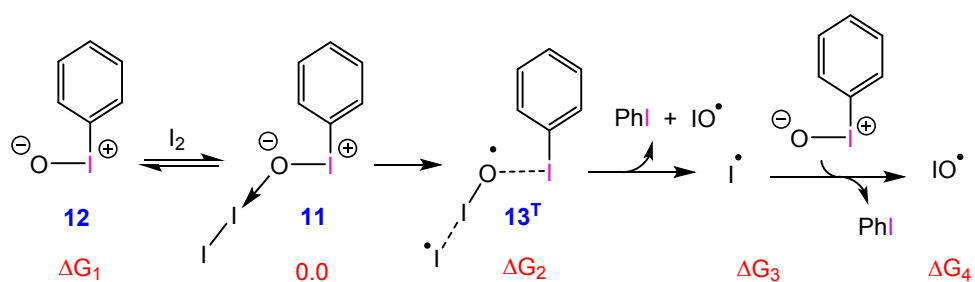


Fig. S1 Scan of potential energy surface associated with reaction between I^\bullet and PhIO

Basis set effect. Fig S2 shows our computational investigation related to the effect of the basis set size on the calculation results. It is obvious from this figure that the stability of the intermediates formed during transformation $2\text{PhIO} + \text{I}_2 \rightarrow \text{PhI} + 2\text{IO}^\bullet$ are overestimated when the double-zeta basis sets such as def2-SVP and SDD,6-31G(d) are utilized. For example, irrespective of calculation method [M06-2X or CCSD(T)], the use of double-zeta basis sets results in the reaction free energy for transformation $\text{PhIO} + 2\text{I}_2 \rightarrow 2\text{IO}^\bullet + \text{PhI}$ being < -15 kcal/mol. In contrast, the same reaction is calculated to be less exergonic using the triple- and *quadruple*-zeta basis sets and the computed relative free energies using these triple- and *quadruple*-zeta basis sets are very comparable (see entries 5-7 in Fig. S2). This finding is in agreement with the observations of Schaefer et al. who indicated that the computational results regarding the mechanistic investigation of an oxidative reaction mediated by a hypervalent iodine reagent show a better consistency with the experiment only if the basis set chosen for the calculations was large enough. For details see: H. Jiang, T.-Y. Sun, X. Wang, Y. Xie, X. Zhang, Y.-D. Wu and H. F. Schaefer III, *Org. Lett.*, 2017, **19**, 6502–6505.



entry	method	basis Set	ΔG ₁	ΔG ₂	ΔG ₃	ΔG ₄
1	CCSD(T)	def2-SVP	3.7	11.7	3.8	-24.7
2	CCSD(T)	def2-TZVP	1.4	17.1	14.1	-8.5
3	M06-2X	6-31g(d), SDD	14.6	10.0	10.1	-23.4
4	M06-2X	def2-SVP	8.5	11.0	8.7	-15.0
5	M06-2X	def2-TZVP	2.2	13.9	11.4	-5.1
6	M06-2X	def2-TZVPP	2.1	14.0	11.3	-5.1
7	M06-2X	def2-QZVPP	2.0	14.9	12.3	-3.6

Fig. S2 Relative free energies of possible intermediates formed during the reaction between PhIO and I₂ using the SMD/method/basis set//SMD/M06-2X/SDD,6-31G(d) calculations.

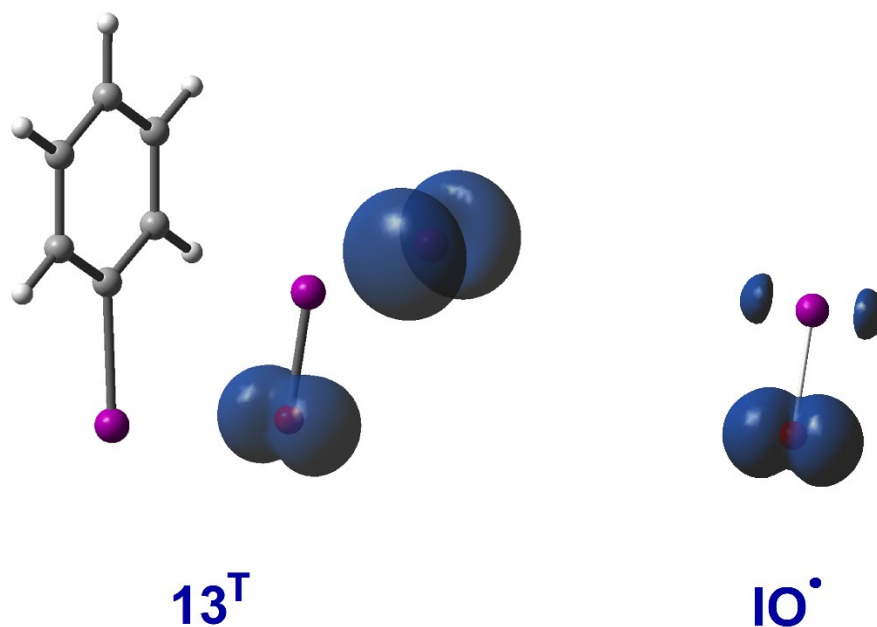
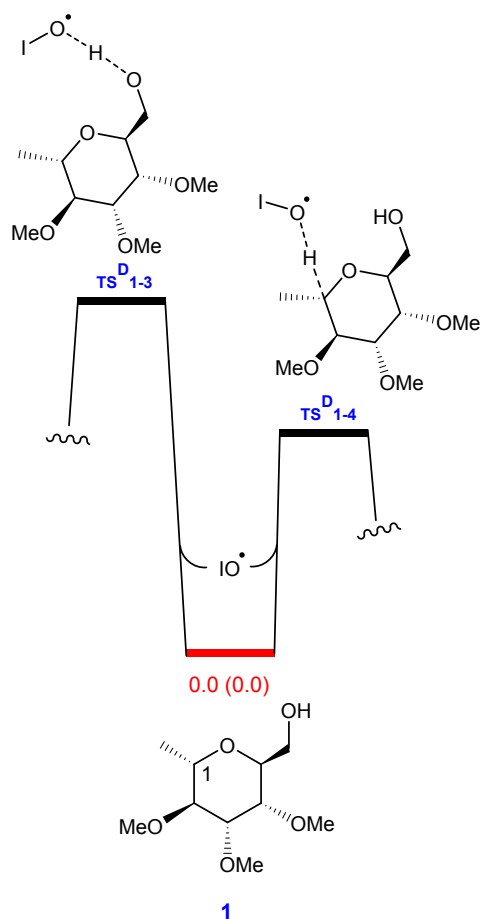


Fig. S3 Spin density plots for 13^T and IO[•].



method	M06-2X	M06-2X-D3	M06	M06-D3	B3LYP-D3
ΔG (TS ^D ₁₋₃)	16.6	16.3	16.3	15.5	13.2
ΔG (TS ^D ₁₋₄)	9.8	9.4	11.5	10.5	6.7

Fig. S4 Calculated free energies for TS^D₁₋₃ and TS^D₁₋₄ obtained by different levels of theory.

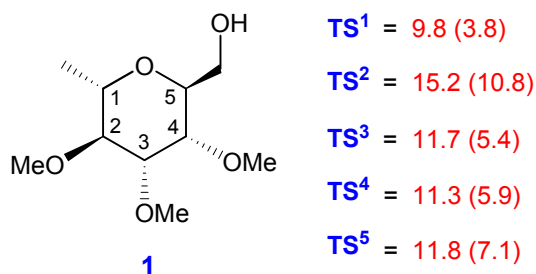


Fig. S5 Activation free energies for the IO[•]-mediated hydrogen abstraction of substrate **1** from different carbon sites on the ring.

Table S1. Total potential (E), enthalpy (H) and Gibbs free energies (G) of all structures optimized at the M06-2X-SMD/BS1 level of theory along with the total potential energies calculated by M06-2X-SMD/BS2//M06-2X-SMD/BS1 for all of the calculated structures, Cartesian coordinates and the spin expectation values of the doublet and triplet structures.

I₂

E (M06-2X-SMD/BS1) = -22.7354557255 au
 H (M06-2X-SMD/BS1) = -22.731132 au
 G (M06-2X-SMD/BS1) = -22.760853 au
 E (M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -595.275781429 au
 I 0.00000000 0.00000000 1.40837200
 I 0.00000000 0.00000000 -1.40837200

12

E (M06-2X-SMD/BS1) = -317.966755286 au
 H (M06-2X-SMD/BS1) = -317.865289 au
 G (M06-2X-SMD/BS1) = -317.907548 au
 E (M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -604.386165870 au
 I -1.39788200 -0.27226700 -0.00004900
 C 0.73811500 -0.13439100 -0.00013300
 C 1.24191700 1.15389300 -0.00019700
 C 1.53805200 -1.26746800 0.00005900
 C 2.62737800 1.31486000 -0.00017400
 H 0.55160600 1.99517300 -0.00026200
 C 2.92137400 -1.08592700 0.00019500
 H 1.10620400 -2.26377400 0.00001500
 C 3.46320000 0.19916900 0.00008500
 H 3.05153400 2.31435900 -0.00035800
 H 3.57362500 -1.95383800 0.00042800
 H 4.54064300 0.33038700 0.00026500
 O -1.73950900 1.61588100 0.00043900

11

E (M06-2X-SMD/BS1) = -340.737768524 au
 H (M06-2X-SMD/BS1) = -340.630206 au
 G (M06-2X-SMD/BS1) = -340.688643 au
 E (M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -1199.67763930 au
 I -2.44070900 -1.28674200 -0.39223500
 C -2.61413300 0.80713900 -0.14635400
 C -3.28592800 1.29179900 0.97162400
 C -2.00243100 1.63446100 -1.08354400
 C -3.34850900 2.67205400 1.14729000
 H -3.74778900 0.61762800 1.68466800
 C -2.08299800 3.01185300 -0.88974200
 H -1.47714100 1.22171100 -1.93808700

C	-2.75128500	3.52529400	0.22023200
H	-3.86593200	3.07702800	2.01068500
H	-1.61544200	3.67925900	-1.60599800
H	-2.80603000	4.59935600	0.36545400
O	-0.98960200	-1.57606000	0.88323000
I	0.95592600	-0.68843600	0.40276300
I	3.71008100	0.49891200	-0.17844500

MECP1

E (M06-2X-SMD/BS1) = -340.703456135 au

I	-2.58211300	-1.31431450	-0.57703860
C	-2.67307360	0.76826960	-0.24175640
C	-3.31303980	1.23633000	0.90289810
C	-2.03362360	1.61806350	-1.14060950
C	-3.30480200	2.60688640	1.14914660
H	-3.80220190	0.55279760	1.58815300
C	-2.03977490	2.98646450	-0.87599330
H	-1.53691660	1.22770520	-2.02222400
C	-2.67090760	3.47827520	0.26420930
H	-3.79387340	2.99114990	2.03816140
H	-1.54257570	3.66248550	-1.56360540
H	-2.67034160	4.54416420	0.46666580
O	-0.83628350	-1.45074340	0.96116280
I	0.69737150	-0.18174520	0.75381770
I	3.74024160	0.35946000	-0.25144650

13^T

E (M06-2X-SMD/BS1) = -340.715937087 au

H (M06-2X-SMD/BS1) = -340.608902 au

G (M06-2X-SMD/BS1) = -340.672684 au

E (M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -1199.64954135 au

Spin expectation value = 2.0091

I	-2.51359300	-1.21206800	-0.54657800
C	-1.89754500	0.82789300	-0.53670200
C	-2.41151900	1.68769400	0.43043200
C	-0.95425200	1.25681900	-1.46570800
C	-1.96013900	3.00667700	0.46720800
H	-3.14617500	1.33829800	1.14837100
C	-0.51017300	2.57825500	-1.41314700
H	-0.56127800	0.57548900	-2.21316700
C	-1.00792800	3.45183200	-0.44829800
H	-2.35668200	3.68387500	1.21756700
H	0.22948900	2.91851400	-2.13160200
H	-0.65808700	4.47863500	-0.41232600

O	-0.03823300	-1.64397200	1.64219900
I	0.83630900	0.06250400	1.70827100
I	2.79516900	-0.29757000	-1.02865800

Phi

E (M06-2X-SMD/BS1) = -242.91124574 au

H (M06-2X-SMD/BS1) = -242.813301 au

G (M06-2X-SMD/BS1) = -242.851783 au

E (M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -529.265363864 au

I	1.55989300	0.00000400	-0.00008800
C	-0.57672100	0.00008200	0.00029500
C	-1.25635700	1.21406800	0.00036300
C	-1.25614900	-1.21395100	0.00037000
C	-2.65087800	1.20546500	-0.00002200
H	-0.71301800	2.15278200	0.00135500
C	-2.65072200	-1.20555300	-0.00003300
H	-0.71275100	-2.15259300	0.00144900
C	-3.34883300	-0.00012500	-0.00041200
H	-3.18838300	2.14874400	0.00003800
H	-3.18796200	-2.14898000	-0.00004200
H	-4.43425300	-0.00008800	-0.00150100

IO*

E (M06-2X-SMD/BS1) = -86.4455479281 au

H (M06-2X-SMD/BS1) = -86.440696 au

G (M06-2X-SMD/BS1) = -86.468004 au

E (M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -372.756426833 au

Spin expectation value = 0.7556

O	0.00000000	0.00000000	-1.68803700
I	0.00000000	0.00000000	0.25479800

I*

E (M06-2X-SMD/BS1) = -11.3413501498 au

H (M06-2X-SMD/BS1) = -11.33899 au

G (M06-2X-SMD/BS1) = -11.358853 au

E (M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -297.614151563 au

Spin expectation value = 0.7505

I	0.00000000	0.00000000	0.00000000
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1

E (M06-2X-SMD/BS1) = -768.838563862 au

H (M06-2X-SMD/BS1) = -768.510843 au

G (M06-2X-SMD/BS1) = -768.572317 au

E (M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -769.167510563 au

C	-0.92753900	0.65351700	-0.27454400
C	-0.63855600	-0.59227300	0.55458400
C	0.63958500	-1.25579200	0.04921900
C	1.79668100	-0.25112000	0.03213500
C	0.26957400	1.60603100	-0.21887100
H	0.89221200	-2.10147100	0.70819700
H	-0.48282200	-0.27888500	1.59810200
H	-1.09404000	0.35520100	-1.31931000
H	2.61904100	-0.67426500	-0.55530100
O	1.44637700	0.93893600	-0.67186500
C	2.35540700	0.10221900	1.40907700
H	2.81410400	-0.78635700	1.85440500
H	1.56219100	0.44293200	2.09056300
O	3.35790200	1.08823400	1.27676300
H	3.03395500	1.70109000	0.59415700
O	0.37942600	-1.72051500	-1.25989900
O	-1.70640200	-1.51457500	0.48695000
O	-2.05884000	1.33152000	0.23865000
C	0.07729900	2.81608700	-1.11006200
H	-0.02480700	2.49887800	-2.15317300
H	-0.82392800	3.35806600	-0.81307500
H	0.93593100	3.48936000	-1.03286200
H	0.39546200	1.93336600	0.82607900
C	1.17653100	-2.81999800	-1.63476300
H	0.90664000	-3.07863400	-2.66106800
H	2.25007200	-2.58815800	-1.60357400
H	0.98695000	-3.68604500	-0.98517900
C	-2.56440200	-1.46628600	1.60893100
H	-3.37287900	-2.17816900	1.42499100
H	-2.03532400	-1.76187600	2.52615200
H	-2.98955100	-0.46639800	1.75544700
C	-3.23076400	1.13353800	-0.52579100
H	-4.04276300	1.65266000	-0.01068500
H	-3.12154300	1.55551500	-1.53454800
H	-3.47949700	0.06885000	-0.61359500

TS^D₁₋₄

E (M06-2X-SMD/BS1) = -855.282407891 au

H (M06-2X-SMD/BS1) = -854.953723 au

G (M06-2X-SMD/BS1) = -855.026135 au

E (M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -1141.88874058 au

Spin expectation value = 0.7615

C	-1.53817300	-0.96099900	0.57917500
C	-2.03568500	-0.25897200	-0.67744400

C	-2.23115700	1.21910500	-0.36193400
C	-0.93049700	1.84134000	0.15474000
C	-0.24137400	-0.30288400	1.05822300
H	-2.54840400	1.74713700	-1.27396100
H	-1.26434200	-0.35788200	-1.45751400
H	-2.29512100	-0.85316700	1.37055600
H	-1.16908900	2.80288800	0.62111800
O	-0.34986000	1.07740800	1.22165200
C	0.12550900	2.11562300	-0.91056300
H	-0.31752700	2.71302900	-1.71311600
H	0.49940800	1.17722800	-1.34525200
O	1.18310800	2.87892300	-0.36439000
H	1.53912100	2.36186100	0.37767600
O	-3.23841000	1.30538500	0.62617000
O	-3.25363200	-0.81229000	-1.12518900
O	-1.27282400	-2.32236600	0.32441500
C	0.32476000	-0.90201700	2.32275400
H	-0.37346100	-0.74449900	3.15315000
H	0.48178900	-1.97398200	2.18438500
H	1.27792700	-0.42882600	2.57716800
H	0.52756700	-0.55576200	0.19503000
C	-3.94504300	2.52516000	0.60506100
H	-4.68209300	2.48355000	1.40984500
H	-3.28918800	3.38981500	0.77532300
H	-4.46574900	2.66299100	-0.35253400
C	-3.09574300	-1.73912500	-2.18215000
H	-4.08767500	-2.13787500	-2.40784000
H	-2.69723900	-1.24914500	-3.08158000
H	-2.42796400	-2.56308000	-1.90549100
C	-2.27003200	-3.19402500	0.82059300
H	-1.98787000	-4.20597300	0.52100400
H	-2.32489900	-3.14822700	1.91699400
H	-3.25646200	-2.95403200	0.40576300
O	1.51134400	-0.96479500	-0.78796800
I	3.23109600	-0.17968700	-0.18073500

IOH

E (M06-2X-SMD/BS1) = -87.1116296236 au

H (M06-2X-SMD/BS1) = -87.095062 au

G (M06-2X-SMD/BS1) = -87.124018 au

E (M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -373.42571897 au

H	-0.92608800	1.97975900	0.00000000
O	0.01518200	1.72725700	0.00000000
I	0.01518200	-0.29807200	0.00000000

4^D

E (M06-2X-SMD/BS1) = -768.179997427 au

H (M06-2X-SMD/BS1) = -767.866059 au

G (M06-2X-SMD/BS1) = -767.929889 au

E (M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -768.509647432 au

Spin expectation value = 0.7537

C	0.94796800	-0.62491700	-0.31268000
C	0.63692700	0.59671000	0.54678900
C	-0.65054100	1.24181200	0.04763500
C	-1.79471600	0.22521900	0.05551500
C	-0.24173700	-1.54646400	-0.38091200
H	-0.91074200	2.08948300	0.70016700
H	0.48528000	0.25644300	1.58105400
H	1.19677400	-0.26336700	-1.32683700
H	-2.64662200	0.64054400	-0.49228200
O	-1.45284700	-0.96241800	-0.67166500
C	-2.28469200	-0.18260200	1.43982200
H	-2.63152700	0.69826200	1.98849900
H	-1.46725800	-0.64614900	2.01130900
O	-3.37923400	-1.06735100	1.32594200
H	-3.09711100	-1.76398300	0.70942800
O	-0.40946200	1.69375500	-1.26912300
O	1.68966700	1.53526500	0.49611700
O	2.05119100	-1.33259300	0.22521800
C	-0.09230600	-2.89277800	-0.99830800
H	-0.03645100	-2.82638800	-2.09712600
H	0.82411200	-3.36724900	-0.64063800
H	-0.94519700	-3.53316200	-0.75051300
C	-1.23010500	2.77345100	-1.65414000
H	-0.96808200	3.02500700	-2.68407700
H	-2.29834200	2.52039000	-1.61665800
H	-1.05493000	3.64979900	-1.01483100
C	2.54740900	1.47916400	1.61847400
H	3.34960800	2.20056900	1.44497500
H	2.01494000	1.75698200	2.53911800
H	2.98111300	0.48104200	1.75127000
C	3.24553900	-1.15301200	-0.50804300
H	4.03252900	-1.69354900	0.02358600
H	3.15432900	-1.56415500	-1.52304300
H	3.52058000	-0.09327300	-0.58019600

TS^D₁₋₃

E (M06-2X-SMD/BS1) = -855.27138349 au

H (M06-2X-SMD/BS1) = -854.945319 au
G (M06-2X-SMD/BS1) = -855.017378 au
E (M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -1141.90475894 au
Spin expectation value = 0.7620

C	-2.04685200	0.98520200	-0.25310700
C	-2.64109700	-0.22252400	0.46226400
C	-1.95912700	-1.49367400	-0.03368400
C	-0.43561500	-1.37243500	0.13101200
C	-0.52944500	1.02294400	-0.04469800
H	-2.33194600	-2.35505200	0.54283700
H	-2.43922300	-0.11447400	1.53946400
H	-2.25666200	0.89845700	-1.32855100
H	0.04384400	-2.19433500	-0.41267100
O	0.05317800	-0.19744800	-0.48866800
C	0.01864400	-1.49533700	1.59091200
H	-0.37108200	-2.45203900	1.98022300
H	-0.38217100	-0.70484000	2.24059000
O	1.39871400	-1.58769800	1.70513200
H	1.91577400	-0.52516100	1.61846600
O	-2.29134300	-1.64405500	-1.39778000
O	-4.03416800	-0.31755600	0.24555300
O	-2.59945200	2.18035300	0.26775500
C	0.12288200	2.14351800	-0.82735300
H	0.00431900	1.96946200	-1.90236800
H	-0.34415700	3.09726100	-0.56752300
H	1.18931400	2.19588400	-0.59316600
C	-2.25052400	-2.98008300	-1.84301500
H	-2.50827300	-2.97374900	-2.90435800
H	-1.25455100	-3.42910100	-1.72774500
H	-2.97852600	-3.60014900	-1.30124800
C	-4.80642000	0.18854800	1.31525000
H	-5.85528500	0.11168200	1.01809400
H	-4.65411000	-0.40269200	2.22958700
H	-4.56793800	1.23650500	1.53150300
C	-3.57176000	2.76602300	-0.57310200
H	-3.96233700	3.64376000	-0.05213700
H	-3.13007700	3.08596000	-1.52719900
H	-4.39564900	2.07224600	-0.78134600
O	2.28153500	0.49759300	1.24266900
I	3.56112100	0.19936400	-0.24103200
H	-0.33251200	1.17145700	1.02810200

3^D

E (M06-2X-SMD/BS1) = -768.166739428 au

H (M06-2X-SMD/BS1) = -767.854296 au
G (M06-2X-SMD/BS1) = -767.916679 au
E (M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -768.489086568 au
Spin expectation value = 0.7532

C	0.95403200	-0.61591700	-0.26384000
C	0.56433900	0.61469300	0.54575800
C	-0.75309500	1.17466600	0.01712100
C	-1.83012800	0.07966000	0.00781200
C	-0.17278100	-1.65178400	-0.21019900
H	-1.07164300	2.01211600	0.65740000
H	0.42007700	0.30209400	1.59242200
H	1.11123100	-0.31743800	-1.30989700
H	-2.67880600	0.44166800	-0.58375500
O	-1.38854800	-1.07906400	-0.67469500
C	-2.36816200	-0.24263500	1.40653600
H	-2.68489000	0.67355900	1.93408800
H	-1.58508900	-0.68417400	2.05462900
O	-3.37113900	-1.17170000	1.39925300
O	-0.51684000	1.63395200	-1.29789600
O	1.56040000	1.61423900	0.48097600
O	2.12622100	-1.20279100	0.27005000
C	0.11690900	-2.85048100	-1.09093800
H	0.20431000	-2.53309900	-2.13541600
H	1.05328300	-3.32260000	-0.78320400
H	-0.69139700	-3.58308200	-1.01566900
C	-1.37859500	2.67678800	-1.69134000
H	-1.12519900	2.93271600	-2.72246800
H	-2.43624900	2.38144000	-1.65431300
H	-1.24109200	3.56404400	-1.05746800
C	2.40972800	1.63884100	1.61020600
H	3.16587400	2.40598400	1.42589300
H	1.85260000	1.90388200	2.52021100
H	2.90500400	0.67395300	1.77007500
C	3.28873900	-0.92827300	-0.48474300
H	4.13098700	-1.38145700	0.04392200
H	3.22133800	-1.36763400	-1.48974700
H	3.46049400	0.15074800	-0.58245200
H	-0.27750500	-1.98317400	0.83600100

14^T

E (M06-2X-SMD/BS1) = -854.635312164 au
H (M06-2X-SMD/BS1) = -854.314547 au
G (M06-2X-SMD/BS1) = -854.389884 au
E (M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -1141.27144568 au

Spin expectation value = 2.0090

C	1.57869800	1.23874400	0.36024000
C	1.04762700	0.27970500	-0.69654000
C	1.96721700	-0.92997200	-0.79746900
C	2.15527400	-1.60757400	0.56605000
C	1.82672300	0.51322300	1.65478500
H	1.53779800	-1.65411300	-1.50788100
H	0.05789600	-0.05468700	-0.36713700
H	2.52279600	1.67245100	-0.01889400
H	3.02570900	-2.26943600	0.48056700
O	2.52021300	-0.66843400	1.57748900
C	1.00071300	-2.48873400	1.04223800
H	1.31787800	-2.94901200	1.98398300
H	0.85809900	-3.29652900	0.30961000
O	-0.20354000	-1.80508400	1.30593300
H	-0.72558300	-1.75255200	0.48421400
O	3.21516000	-0.46090500	-1.27386900
O	0.95457400	0.91366800	-1.95678000
O	0.63852500	2.27827000	0.58459500
C	2.18417100	1.29827000	2.86928900
H	3.23064700	1.64441800	2.83322400
H	1.53985400	2.17685900	2.94836600
H	2.07022400	0.69131200	3.77335500
C	3.92780700	-1.41804100	-2.02209100
H	4.87798600	-0.96190500	-2.30882700
H	4.13784100	-2.32880200	-1.44401400
H	3.37703200	-1.70032300	-2.93022300
C	-0.36577900	1.26820100	-2.30759500
H	-0.31414100	1.79501400	-3.26394400
H	-0.99899800	0.37655600	-2.42584500
H	-0.82338200	1.92737800	-1.55802900
C	0.99405400	3.50013200	-0.02805400
H	0.17886700	4.20318600	0.16111900
H	1.92007200	3.90636500	0.40269200
H	1.12966400	3.38709000	-1.11084800
O	-1.95081100	-1.28463800	-0.85029600
I	-3.17381600	-0.12301900	0.08711000

MECP2

E (M06-2X-SMD/BS1) = -340.710970074 au

C	0.87988490	0.48101090	0.98373200
C	1.44068160	0.79306990	-0.40069220
C	2.64401540	-0.09954710	-0.65514940
C	2.25079550	-1.57869650	-0.51797160

C	0.62103620	-0.99722150	1.13152470
H	3.02605490	0.07974950	-1.67174130
H	0.67168230	0.55977050	-1.14958670
H	1.62903570	0.81134800	1.72541380
H	3.18417640	-2.15166290	-0.49710690
O	1.63780660	-1.83917610	0.73857650
C	1.39992650	-2.14897770	-1.67535820
H	1.62474270	-3.21606140	-1.76159640
H	1.72209620	-1.67023700	-2.61397760
O	0.00622550	-2.08225210	-1.50316300
H	-0.29222570	-1.16254770	-1.39523110
O	3.63068000	0.23827250	0.29957450
O	1.80399380	2.15290260	-0.51471310
O	-0.33363130	1.18329060	1.20044110
C	-0.05253930	-1.49061740	2.36682880
H	0.65938130	-1.56813920	3.20386780
H	-0.84987970	-0.80380260	2.66095490
H	-0.48370070	-2.48514360	2.20767820
C	4.94697670	-0.01281650	-0.13550350
H	5.61537750	0.27945210	0.67738660
H	5.11671870	-1.07403450	-0.36331900
H	5.18842230	0.58048600	-1.02904290
C	0.82832350	2.92906530	-1.18247700
H	1.16693100	3.96796730	-1.15031070
H	0.72993420	2.62137330	-2.23351380
H	-0.15378090	2.85090970	-0.70177150
C	-0.18657290	2.31708610	2.03040470
H	-1.16279290	2.80583660	2.08099380
H	0.11919400	2.02790130	3.04582930
H	0.55094760	3.02183040	1.62674240
O	-1.61424940	0.23648930	-1.17383220
I	-2.94412840	-0.61145080	-0.06125470

16

E (M06-2X-SMD/BS1) = -854.777209526 au

H (M06-2X-SMD/BS1) = -854.453760 au

G (M06-2X-SMD/BS1) = -854.524360 au

E (M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -1141.40493760 au

C	1.05518400	-0.03211400	1.00832700
C	1.25380100	0.92491200	-0.16988100
C	2.61422800	0.69395700	-0.82749600
C	2.78924400	-0.81849900	-1.05141600
C	1.46322000	-1.46074900	0.60968200
H	2.65785100	1.21829300	-1.79651500

H	0.47417200	0.69676300	-0.90746800
H	1.67709800	0.28837100	1.85367300
H	3.72016000	-1.04889200	-1.57122300
O	2.81439900	-1.45991200	0.22180000
C	1.57039400	-1.49028700	-1.69906300
H	1.85313800	-2.41720800	-2.20533000
H	1.02897200	-0.84479700	-2.39761400
O	0.73550500	-1.80964000	-0.57804300
H	-0.98696400	-0.84373200	-0.66590800
O	3.59095200	1.20405100	0.04759700
O	1.11642100	2.26657500	0.24586600
O	-0.31724900	-0.04820000	1.35906200
C	1.21825900	-2.48873800	1.68341500
H	1.79191100	-2.23497900	2.57919200
H	0.15594200	-2.51245600	1.93498300
H	1.52956400	-3.47114800	1.32039800
C	4.91358200	1.07716300	-0.42324400
H	5.53719600	1.72594600	0.19613200
H	5.28607300	0.04835800	-0.33514400
H	4.99936300	1.39771700	-1.47154800
C	-0.14869600	2.81641300	-0.06688700
H	-0.15960300	3.83696400	0.32383000
H	-0.31060800	2.84995600	-1.15366800
H	-0.96712500	2.24520600	0.38834600
C	-0.60819100	0.58071400	2.59135900
H	-1.69375300	0.55952800	2.71425900
H	-0.14158200	0.04567000	3.42921800
H	-0.26277500	1.62209100	2.59757200
O	-1.59380900	-0.41697700	-1.30692100
I	-3.27707400	0.00253900	-0.27692100

2

E (M06-2X-SMD/BS1) = -854.777209526 au

H (M06-2X-SMD/BS1) = -854.453760 au

G (M06-2X-SMD/BS1) = -854.524360 au

E (M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -1141.40493760 au

C	0.83446200	-0.25821500	-0.38949000
C	0.25975300	0.84784900	0.49455600
C	-1.26376700	0.90433500	0.34123200
C	-1.82340600	-0.52295100	0.47040000
C	0.03802100	-1.55747100	-0.16071700
H	-1.69778400	1.54222900	1.12943100
H	0.49405600	0.58703500	1.53540600
H	0.71363400	0.02291700	-1.44402700

H	-2.91221300	-0.54162500	0.40101300
O	-1.28945700	-1.31995500	-0.58321600
C	-1.28976200	-1.26458700	1.70021700
H	-1.96534200	-2.07287100	1.99742900
H	-1.11195600	-0.60861100	2.55886500
O	-0.05816300	-1.82139800	1.23983000
O	-1.52842900	1.45379400	-0.92759000
O	0.83128800	2.09956300	0.17908200
O	2.19790900	-0.46108000	-0.07864300
C	0.61578800	-2.75296400	-0.87344500
H	0.66808600	-2.55912700	-1.94862500
H	1.62215100	-2.94958600	-0.49877200
H	-0.01924100	-3.62375000	-0.69296800
C	-2.89876800	1.61519900	-1.21375800
H	-2.96873500	2.27385200	-2.08256000
H	-3.38597900	0.66256500	-1.45889600
H	-3.43265000	2.08006700	-0.37226200
C	1.85220000	2.49250000	1.07379100
H	2.25396500	3.43973100	0.70555700
H	1.45505400	2.64691800	2.08713000
H	2.65971900	1.75228200	1.12320300
C	3.07972100	0.03775400	-1.06359000
H	4.09651800	-0.11721700	-0.69466500
H	2.96037200	-0.49971100	-2.01460200
H	2.91971200	1.10882300	-1.24153500

6

E (M06-2X-SMD/BS1) = -1890.63993265 au

H (M06-2X-SMD/BS1) = -1890.108491 au

G (M06-2X-SMD/BS1) = -1890.209082 au

E (M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -1891.33995373 au

C	1.75061600	-0.70794000	-1.94679600
C	1.76966900	-1.27891200	-0.53172900
C	2.81202700	0.91384800	-0.71382100
C	4.29317100	2.22320600	0.80212000
O	5.49121800	2.68969900	1.18495700
O	3.33994100	2.41976500	1.52009500
C	6.64722900	2.45872500	0.37894300
H	7.45863200	2.99484000	0.87058200
H	6.89044800	1.39366800	0.33681900
H	6.51400800	2.85291300	-0.63177800
O	2.79518000	0.25279900	-1.97777800
H	1.98521900	-1.48323900	-2.68298000
C	0.41211200	-0.05097100	-2.29335200

H	0.14081900	0.67752700	-1.52158700
H	0.51156300	0.49218500	-3.23855300
N	-0.64703000	-1.05043600	-2.37293700
H	-0.61657500	-1.69778100	-3.15441700
P	-2.08213700	-0.92981800	-1.60857600
O	-3.05129300	-2.00621100	-1.89030600
O	-1.62903500	-0.77385900	-0.05987100
O	-2.58719200	0.56831900	-1.98169000
C	-2.52554600	-0.80635600	1.00729300
C	-3.35979100	-1.90157700	1.20504100
C	-2.52057700	0.27582400	1.88047700
C	-4.23046100	-1.88887700	2.29355700
H	-3.33385500	-2.73223000	0.50896600
C	-3.39519700	0.27266000	2.96320800
H	-1.85108600	1.10879900	1.69221800
C	-4.25525500	-0.80595400	3.17005500
H	-4.89132200	-2.73507400	2.45410700
H	-3.40515400	1.11886300	3.64323300
H	-4.93855700	-0.80327800	4.01323900
C	-3.50271700	1.23446400	-1.17304800
C	-4.72710400	0.65532700	-0.85177800
C	-3.14637400	2.49431400	-0.70729700
C	-5.59164200	1.34506500	-0.00549300
H	-4.97987000	-0.32564200	-1.24195700
C	-4.02818200	3.17905900	0.12580500
H	-2.18485400	2.91312200	-0.98723900
C	-5.24522200	2.60282200	0.48671000
H	-6.54074500	0.89437900	0.26742200
H	-3.75664100	4.16132000	0.49982600
H	-5.92418900	3.13423500	1.14584600
C	2.41573900	-0.15749600	0.32028600
H	0.77947200	-1.58997200	-0.18462300
H	1.76115700	0.24550900	1.09638200
O	2.70377500	-2.34228100	-0.45629400
O	3.56197000	-0.76130700	0.89350800
C	3.44973800	-2.17035800	0.73423000
C	4.83183300	-2.74959900	0.52888100
H	5.45228900	-2.55764000	1.40816400
H	4.76666900	-3.82968000	0.37303900
H	5.29171900	-2.28690200	-0.34824900
C	2.71595000	-2.77439200	1.92507000
H	2.59040100	-3.85138500	1.78266500
H	3.28394500	-2.60059600	2.84316500
H	1.72655100	-2.31886000	2.03805000

H	2.06294900	1.71624500	-0.69553000
C	4.19818500	1.49566900	-0.51784800
H	4.93504900	0.68911300	-0.55956000
H	4.42750900	2.19316000	-1.33209100

TS^D₆₋₉

E (M06-2X-SMD/BS1) = -1977.0935547 au

H (M06-2X-SMD/BS1) = -1976.561195 au

G (M06-2X-SMD/BS1) = -1976.66847 au

E (M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -2264.09373543 au

Spin expectation value = 0.7623

C	1.75083000	1.71665400	-0.80647700
C	2.83309800	1.07256100	-1.68683900
C	2.64973800	0.11311200	0.52378300
H	1.71433000	-0.65183500	0.44499000
O	0.65286300	-1.50175700	0.71448700
I	0.74878700	-3.03508000	-0.54718300
C	2.28506200	-0.61494600	2.89333300
O	1.21547000	0.19066700	2.86102300
O	2.41314400	-1.52282000	3.67869200
C	0.12813300	-0.19769300	3.70805300
H	-0.66438900	0.52637900	3.52668900
H	-0.21140300	-1.20023500	3.43651800
H	0.43724900	-0.18196600	4.75535100
O	2.14568100	1.40830400	0.53460600
H	1.73403000	2.80460700	-0.89130200
C	0.37039900	1.10338900	-1.07213900
H	-0.09784900	1.61821400	-1.91629900
H	0.47570900	0.04280100	-1.34163300
N	-0.45110300	1.25870700	0.12902200
H	0.08577800	1.06635800	0.97819200
P	-1.95018200	0.58490800	0.20647700
O	-2.48672800	0.44017100	1.57354400
O	-2.87004900	1.46047900	-0.80144400
O	-1.85784200	-0.75441600	-0.68552800
C	-3.32755500	2.70070600	-0.36495100
C	-2.58402700	3.83816500	-0.65803600
C	-4.53579200	2.77340700	0.31903500
C	-3.07138100	5.08130000	-0.25984200
H	-1.64348900	3.74034900	-1.19099900
C	-5.01145500	4.02203400	0.71179500
H	-5.08301300	1.86094300	0.53217900
C	-4.28272800	5.17556400	0.42354400
H	-2.50075200	5.97682900	-0.48515700

H	-5.95400300	4.09156400	1.24569400
H	-4.65810700	6.14613900	0.73179300
C	-2.94219600	-1.62606800	-0.71923500
C	-3.09755500	-2.54918100	0.30941800
C	-3.81218000	-1.58096600	-1.80172400
C	-4.15429500	-3.45371600	0.24482300
H	-2.39411200	-2.54528600	1.13631700
C	-4.86406600	-2.49382300	-1.85479500
H	-3.65762000	-0.84234500	-2.58147600
C	-5.03645600	-3.42896800	-0.83551500
H	-4.28696000	-4.17924200	1.04127400
H	-5.54978900	-2.47100100	-2.69601900
H	-5.85753300	-4.13724500	-0.88196400
C	3.43478200	-0.03740800	-0.78280700
H	2.42359900	0.70505000	-2.63142300
H	3.36364400	-1.04874700	-1.18948800
O	3.91648500	1.92893100	-1.96586200
O	4.79626700	0.30201700	-0.64828300
C	5.02115500	1.62933600	-1.11956600
C	5.09610000	2.61142800	0.04002300
H	5.92528700	2.34182000	0.70073700
H	5.26593100	3.62188500	-0.34272300
H	4.16498400	2.60171500	0.61187500
C	6.28177500	1.62514700	-1.96095200
H	6.45156000	2.61928500	-2.38299200
H	7.14286200	1.35274500	-1.34489600
H	6.17515700	0.90175700	-2.77310500
C	3.30875200	-0.24621700	1.83604600
H	3.97291900	-1.10273200	1.70501700
H	3.90756100	0.60136600	2.19149200

TS^D₆₋₈

E (M06-2X-SMD/BS1) = -1977.06727127 au

H (M06-2X-SMD/BS1) = -1976.536171 au

G (M06-2X-SMD/BS1) = -1976.645781 au

E (M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -2264.07229479 au

Spin expectation value = 0.7629

C	1.44305900	-1.83559300	-0.48333900
C	1.88408200	-1.10941800	0.78224400
C	3.16260700	-0.47914400	-1.19168600
C	5.34270400	0.69988100	-1.38793500
O	6.68149500	0.71212000	-1.46587100
O	4.76397600	1.74607300	-1.20568000
C	7.40596200	-0.50690000	-1.63454100

H	8.44741000	-0.21300900	-1.76373200
H	7.31633500	-1.14037600	-0.74749800
H	7.07223500	-1.05253800	-2.52091600
O	2.55022100	-1.75923800	-1.36070900
H	1.22930700	-2.88938900	-0.28458200
C	0.21580900	-1.16780600	-1.12565900
H	0.43411400	-0.12571300	-1.38853600
H	-0.01112300	-1.69887000	-2.06171100
N	-0.92391200	-1.27827300	-0.23215300
P	-1.85477500	0.08391900	0.04041500
O	-3.08770600	-0.14690000	0.81342700
O	-0.74755700	1.04566700	0.71383500
O	-2.07437400	0.71377600	-1.43310300
C	-1.05897700	2.24323000	1.36518100
C	-1.95072800	2.26501400	2.43107900
C	-0.41029500	3.39041700	0.92401100
C	-2.21291100	3.48528100	3.05183500
H	-2.43356200	1.34958200	2.75336400
C	-0.68150800	4.59994400	1.55726700
H	0.28000900	3.32587400	0.08917900
C	-1.58604100	4.65138600	2.61772000
H	-2.91151300	3.51826500	3.88203800
H	-0.18595700	5.50337000	1.21588800
H	-1.79793600	5.59697400	3.10629300
C	-2.31307700	2.08245100	-1.57232500
C	-3.38216000	2.68689800	-0.91882900
C	-1.44432800	2.80313300	-2.38171500
C	-3.55641300	4.06189900	-1.05741400
H	-4.04840900	2.09074600	-0.30297800
C	-1.64023400	4.17527100	-2.52157800
H	-0.62683400	2.29008900	-2.87839400
C	-2.68786500	4.80752200	-1.85337500
H	-4.37738100	4.54879500	-0.54070500
H	-0.96570900	4.75038200	-3.14809400
H	-2.83035700	5.87839700	-1.95669600
C	2.92657000	-0.08198200	0.28382600
H	1.04922500	-0.67189800	1.33958400
H	2.60605400	0.95787800	0.37848800
O	2.64784100	-1.98626200	1.58901600
O	4.07541500	-0.31962300	1.07715500
C	3.73496000	-1.24294300	2.10799500
C	4.90153600	-2.17970500	2.33132000
H	5.78188000	-1.61052400	2.64135600
H	4.65813300	-2.90464300	3.11259600

H	5.12282900	-2.71352600	1.40322100
C	3.32417300	-0.48451100	3.36329000
H	3.01924700	-1.18612500	4.14473900
H	4.16279400	0.11389700	3.72973400
H	2.48730200	0.18793300	3.14772100
H	2.67689000	0.25782700	-1.84276700
C	4.62566600	-0.61795800	-1.56390200
H	5.08227800	-1.39012700	-0.94041500
H	4.71844700	-0.93831000	-2.60879000
H	-1.65087400	-2.24929400	-0.59832700
O	-2.42977300	-2.77348000	-1.26403000
I	-3.87373000	-3.45720400	-0.09045900

g^D

E (M06-2X-SMD/BS1) = -1889.96180953 au

H (M06-2X-SMD/BS1) = -1889.444176 au

G (M06-2X-SMD/BS1) = -1889.543876 au

E (M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -1890.65640933 au

Spin expectation value = 0.7532

C	1.71762800	-0.72532900	-1.93977900
C	1.85493800	-1.36002900	-0.55703300
C	2.68934900	0.92537800	-0.66491800
C	4.14401000	2.25096900	0.85805400
O	5.32509000	2.77130700	1.22233000
O	3.20915700	2.34730300	1.61933300
C	6.46054700	2.65469300	0.36391700
H	7.25543600	3.21811200	0.85199400
H	6.76811800	1.61067900	0.26006300
H	6.26301700	3.08723500	-0.62023000
O	2.65902900	0.32996700	-1.96315100
H	1.97201200	-1.43792000	-2.72830500
C	0.29917500	-0.18435700	-2.17496600
H	0.03597100	0.58497500	-1.43575400
H	0.28191600	0.29727000	-3.16654200
N	-0.62714700	-1.28143600	-2.23465100
P	-2.13924400	-1.05390200	-1.52473600
O	-3.12159100	-2.12171000	-1.77022800
O	-1.69224400	-0.82466600	0.00811400
O	-2.57011400	0.41210300	-2.05011500
C	-2.59306500	-0.83802400	1.08004000
C	-3.39490400	-1.94612100	1.32490800
C	-2.61874100	0.28649500	1.89625300
C	-4.26682300	-1.90574100	2.41197400
H	-3.34380000	-2.80952300	0.67149800

C	-3.49284800	0.30826700	2.97926000
H	-1.97286400	1.12790900	1.66747000
C	-4.32135800	-0.78399300	3.23647700
H	-4.90377400	-2.76149700	2.61255100
H	-3.52684200	1.18429000	3.61935300
H	-5.00442800	-0.76162900	4.07948800
C	-3.44812400	1.18401500	-1.28386000
C	-4.70306200	0.69546100	-0.93583300
C	-3.01176300	2.44193200	-0.88909400
C	-5.52662100	1.48645600	-0.13791700
H	-5.01518900	-0.28904600	-1.27046900
C	-3.85284500	3.22629600	-0.10295000
H	-2.02642200	2.78443900	-1.18908200
C	-5.10477100	2.74754200	0.28102200
H	-6.50258700	1.11201000	0.15414600
H	-3.52298600	4.21020600	0.21539100
H	-5.75220500	3.35799500	0.90220700
C	2.41641100	-0.22104200	0.32996100
H	0.91698300	-1.79315200	-0.18938800
H	1.74566700	0.08847700	1.13433900
O	2.89534800	-2.31683900	-0.57591700
O	3.62401400	-0.74141200	0.85585100
C	3.65759600	-2.14166700	0.60556400
C	5.08554800	-2.55432000	0.32675900
H	5.71032900	-2.34823200	1.19974700
H	5.13107700	-3.62395400	0.10576100
H	5.46407600	-1.99335000	-0.53168700
C	3.02853600	-2.89459500	1.77033900
H	3.01248000	-3.96772100	1.56069300
H	3.60299000	-2.71856900	2.68393100
H	2.00115500	-2.55375800	1.93546500
H	1.89019300	1.67169000	-0.57403800
C	4.04064000	1.59153400	-0.49673800
H	4.82858900	0.84320200	-0.61511000
H	4.18355200	2.34709300	-1.27826800

g^D

E (M06-2X-SMD/BS1) = -1889.98419608 au

H (M06-2X-SMD/BS1) = -1889.466698 au

G (M06-2X-SMD/BS1) = -1889.562736 au

E (M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -1890.68189709 au

Spin expectation value = 0.7545

C	-1.36499100	-0.23167900	-0.55115000
C	-2.42075800	-0.46810100	-1.63809900

C	-3.12132300	1.16277100	-0.03191200
C	-2.19514600	3.39034700	0.04939800
O	-1.13298700	3.45046400	0.88116200
O	-2.10283300	3.90498100	-1.03846900
C	-1.23298500	3.02526100	2.24784400
H	-0.24381700	3.19805500	2.67345400
H	-1.96851200	3.62864200	2.78558500
H	-1.47974400	1.96393800	2.31357100
O	-1.99260500	0.57461800	0.46454200
H	-1.05581400	-1.16694000	-0.08046200
C	-0.17232600	0.55152900	-1.10662600
H	0.42943100	-0.10822500	-1.73987400
H	-0.54278200	1.36619500	-1.74293100
N	0.65392000	1.12623100	-0.05601400
H	0.29402900	1.97130700	0.37976600
P	2.15122300	0.66449300	0.38715000
O	2.66108800	1.34403200	1.59431900
O	2.13758400	-0.95774400	0.44131100
O	3.05334200	0.82185600	-0.94187300
C	1.19799700	-1.66480300	1.17355900
C	0.85389300	-2.91989000	0.67951800
C	0.60983300	-1.15358100	2.32769400
C	-0.12140900	-3.66388300	1.33723400
H	1.33921700	-3.28508900	-0.21989500
C	-0.37194300	-1.90720600	2.96916700
H	0.91146400	-0.18584400	2.71595000
C	-0.74523500	-3.15604100	2.47710300
H	-0.39889800	-4.63975800	0.95116600
H	-0.84326500	-1.51019900	3.86290300
H	-1.51277600	-3.73374200	2.98189700
C	4.35083000	0.31382800	-0.96592200
C	5.34559000	0.90569600	-0.19507200
C	4.61929800	-0.75553000	-1.81213500
C	6.64316400	0.40484800	-0.27807700
H	5.09667500	1.73938500	0.45276400
C	5.92203000	-1.24180600	-1.88892900
H	3.81324900	-1.18879400	-2.39546500
C	6.93435500	-0.66498800	-1.12285000
H	7.42845100	0.85791100	0.31888700
H	6.14404900	-2.07515700	-2.54815100
H	7.94800600	-1.04770700	-1.18516200
C	-3.52661500	0.57898300	-1.34539000
H	-1.98583200	-0.37037800	-2.63680800
H	-3.65702900	1.33596400	-2.12416500

O	-3.07252600	-1.71645400	-1.55791600
O	-4.72371800	-0.19289700	-1.30861700
C	-4.37591600	-1.53460100	-1.00655200
C	-4.35300600	-1.79451800	0.49598400
H	-5.33336000	-1.57321900	0.92772500
H	-4.11418900	-2.84625100	0.68094100
H	-3.59908800	-1.17903700	0.99375200
C	-5.33857500	-2.44826000	-1.73635400
H	-5.05041000	-3.49205800	-1.58620400
H	-6.35311700	-2.30538000	-1.35462100
H	-5.31901100	-2.21795100	-2.80430300
C	-3.39669000	2.54898400	0.45685000
H	-3.57955300	2.57042800	1.53475500
H	-4.27235400	2.94788700	-0.05759200

17^T

E (M06-2X-SMD/BS1) = -1976.4413331 au

H (M06-2X-SMD/BS1) = -1975.916742 au

G (M06-2X-SMD/BS1) = -1976.02562 au

E (M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -2263.44781575 au

Spin expectation value = 2.0166

C	1.79302400	-0.64786800	2.00891200
C	3.02254400	-0.19211300	1.19480300
C	1.55009300	-1.56281800	-0.06357700
C	0.96235600	-3.85117700	-0.95752100
O	0.10027700	-4.61949000	-1.64876900
O	1.82319400	-4.39095400	-0.30852100
C	-0.99690000	-4.03997700	-2.35856700
H	-1.46486200	-4.86582100	-2.89505800
H	-1.72284300	-3.60180400	-1.66630200
H	-0.66108300	-3.28850400	-3.07812600
O	1.14061300	-1.66248000	1.23354300
H	2.11094800	-1.09607900	2.95476900
C	0.80591300	0.48239700	2.28724600
H	-0.07728200	0.07621600	2.78723800
H	1.27604200	1.19898100	2.97039800
N	0.38571400	1.16708500	1.07059900
H	1.10887200	1.57501800	0.47051300
P	-1.08377600	1.10443400	0.38030200
O	-1.20537300	1.86642400	-0.87986300
O	-1.46648600	-0.46792500	0.26948700
O	-2.05458000	1.58272000	1.59094300
C	-2.45770700	-0.98962700	-0.55194700
C	-2.48266400	-0.71746100	-1.91756300

C	-3.36774600	-1.86656400	0.03124600
C	-3.45758200	-1.32880800	-2.70453200
H	-1.75510600	-0.03581900	-2.34329900
C	-4.33386900	-2.47056500	-0.76920600
H	-3.31155700	-2.05721300	1.09797600
C	-4.38333900	-2.20306100	-2.13742600
H	-3.48692400	-1.11984100	-3.76958300
H	-5.04982000	-3.15117800	-0.31887300
H	-5.13844200	-2.67494700	-2.75786700
C	-3.39315300	1.20518500	1.58144300
C	-4.22241700	1.55574600	0.51970300
C	-3.86621300	0.47535300	2.66566300
C	-5.54962400	1.13297500	0.53761200
H	-3.82342000	2.13332100	-0.30844700
C	-5.19922400	0.07106600	2.67647800
H	-3.18851200	0.22532400	3.47581100
C	-6.03987000	0.39022600	1.61064200
H	-6.20099500	1.38848400	-0.29227300
H	-5.57736800	-0.50209400	3.51731600
H	-7.07501800	0.06445300	1.61855700
C	2.83046400	-0.82587600	-0.20587600
H	3.10823700	0.89866100	1.17242300
H	2.81646900	-0.10578100	-1.02958100
O	4.24678100	-0.70697500	1.66605200
O	4.00990600	-1.62015000	-0.38756300
C	4.60953000	-1.84040400	0.87615300
C	4.10841600	-3.12312900	1.52653200
H	4.39194800	-3.98433500	0.91597000
H	4.55560400	-3.22608800	2.52014600
H	3.01982500	-3.12134500	1.61281500
C	6.11458400	-1.82912300	0.69972400
H	6.60772100	-1.93741400	1.66970500
H	6.42113100	-2.65781000	0.05583100
H	6.42057000	-0.88492500	0.24245300
O	2.20724800	2.29651200	-0.87894100
I	1.65959000	4.13271800	-1.07356500
C	0.79418500	-2.33966400	-1.06768800
H	-0.27191600	-2.10446600	-0.98931500
H	1.10872600	-2.04491300	-2.07748000

MECP3

E (M06-2X-SMD/BS1) = -1976.44129538 au

C	1.79209700	-0.64888990	2.00875830
C	3.02200530	-0.19297790	1.19456630

C	1.54798670	-1.55893840	-0.06522020
C	0.96255320	-3.85056600	-0.95771210
O	0.10006660	-4.61993610	-1.64878560
O	1.82303810	-4.39145920	-0.30906680
C	-0.99676890	-4.04029610	-2.35850070
H	-1.46503740	-4.86584430	-2.89518980
H	-1.72279120	-3.60179720	-1.66648870
H	-0.66110830	-3.28858720	-3.07796010
O	1.14149270	-1.66527390	1.23687790
H	2.11172670	-1.09443720	2.95540540
C	0.80632050	0.48218400	2.28788000
H	-0.07725590	0.07629920	2.78737760
H	1.27593680	1.19940990	2.97080470
N	0.38449580	1.16864280	1.07245900
H	1.10805620	1.57281840	0.47226600
P	-1.08379350	1.10411740	0.38046780
O	-1.20407410	1.86663600	-0.87966460
O	-1.46694130	-0.46768020	0.26953710
O	-2.05488940	1.58292810	1.59076920
C	-2.45782260	-0.98959050	-0.55202530
C	-2.48275020	-0.71742300	-1.91759250
C	-3.36776600	-1.86653760	0.03119630
C	-3.45764520	-1.32878040	-2.70456030
H	-1.75508730	-0.03587870	-2.34329440
C	-4.33389720	-2.47054300	-0.76923030
H	-3.31151150	-2.05720440	1.09793330
C	-4.38338790	-2.20304880	-2.13744460
H	-3.48693060	-1.11986780	-3.76961880
H	-5.04980820	-3.15117990	-0.31888410
H	-5.13845530	-2.67496950	-2.75788140
C	-3.39323630	1.20517120	1.58144980
C	-4.22248420	1.55572510	0.51972130
C	-3.86623100	0.47536210	2.66568450
C	-5.54965060	1.13299070	0.53760300
H	-3.82342280	2.13328290	-0.30843570
C	-5.19922200	0.07109180	2.67647670
H	-3.18849290	0.22528680	3.47579690
C	-6.03989000	0.39022970	1.61064720
H	-6.20101240	1.38848330	-0.29228980
H	-5.57736660	-0.50210390	3.51730020
H	-7.07501990	0.06445350	1.61855750
C	2.83006070	-0.82719520	-0.20623340
H	3.10818230	0.89787260	1.17298040
H	2.81852220	-0.10698180	-1.02980590

O	4.24674340	-0.70697110	1.66616810
O	4.01193410	-1.61961080	-0.38754300
C	4.60980100	-1.84029950	0.87572260
C	4.10830830	-3.12301150	1.52641990
H	4.39191090	-3.98434510	0.91603360
H	4.55563360	-3.22603240	2.52004100
H	3.01964820	-3.12083270	1.61235090
C	6.11491180	-1.82920760	0.70016300
H	6.60817850	-1.93749000	1.67001850
H	6.42128350	-2.65777750	0.05596040
H	6.42069450	-0.88504770	0.24259030
O	2.20825040	2.30042200	-0.88287940
I	1.65932430	4.13257730	-1.07380120
C	0.79388680	-2.33979220	-1.06768820
H	-0.27233480	-2.10539670	-0.99049080
H	1.10788990	-2.04546910	-2.07802190

19

E (M06-2X-SMD/BS1) = -1976.5650399 au

H (M06-2X-SMD/BS1) = -1976.038388 au

G (M06-2X-SMD/BS1) = -1976.143905 au

E (M06-2X-SMD/BS2//M06-2X-SMD/BS1) = -2263.56249831 au

C	-2.23932900	-0.94351300	-2.28150000
C	-3.19278300	0.06649800	-1.62286700
C	-1.76474100	-1.22421400	-0.21649900
C	-0.44329900	-3.03001000	0.96074900
O	0.02665500	-3.54868400	2.10304300
O	0.03072300	-3.41059100	-0.08384300
C	-0.36826100	-3.00892500	3.36533900
H	0.11879400	-3.63304100	4.11429800
H	-0.01776800	-1.97824600	3.46306900
H	-1.45145200	-3.06191800	3.50272900
O	-2.18898100	-1.99996600	-1.31631700
H	-2.55731100	-1.31976100	-3.25187200
C	-0.80763500	-0.39485000	-2.21673900
H	-0.11304900	-1.02810900	-2.77493200
H	-0.73729000	0.64020000	-2.56427300
N	-0.57832700	-0.50732500	-0.76083800
H	-0.39661800	2.10665100	-0.82154700
P	0.90028100	-0.36870500	-0.08639600
O	0.99734200	-0.66935900	1.35652500
O	1.92782300	-1.16402800	-1.03810300
O	1.22265300	1.17962700	-0.49425100
C	3.14871300	-1.67663600	-0.59147400

C	3.18380700	-2.70367300	0.34473600
C	4.30926600	-1.16178800	-1.15827400
C	4.42376700	-3.21301400	0.72669900
H	2.25889500	-3.09787500	0.75108100
C	5.53952000	-1.68446700	-0.76843800
H	4.23880900	-0.35735400	-1.88392800
C	5.60030200	-2.70815400	0.17600500
H	4.46478900	-4.01468600	1.45763100
H	6.45031700	-1.28485600	-1.20346000
H	6.56068000	-3.11225600	0.47995800
C	2.53572200	1.65176800	-0.50781800
C	3.31784300	1.58822200	0.63989300
C	3.01134300	2.19040500	-1.69677600
C	4.62841000	2.05755100	0.57748200
H	2.90773300	1.16699300	1.55233400
C	4.31987800	2.66619800	-1.73928800
H	2.36255700	2.22225800	-2.56651200
C	5.13145100	2.59258300	-0.60723600
H	5.25527300	2.00460500	1.46188600
H	4.70585600	3.08849500	-2.66163700
H	6.15267000	2.95747000	-0.64731700
C	-2.86626600	-0.14149200	-0.12561000
H	-3.05144700	1.09013000	-1.97834500
H	-2.52343600	0.74954800	0.40325100
O	-4.53903100	-0.32142500	-1.76127500
O	-4.04701800	-0.64110700	0.44823000
C	-5.06567500	-0.81472700	-0.53480200
C	-5.39744800	-2.29051000	-0.67301000
H	-5.77044600	-2.68041100	0.27865800
H	-6.16882100	-2.43009800	-1.43590400
H	-4.49787800	-2.83806300	-0.96349400
C	-6.26664500	0.02842400	-0.14399400
H	-7.04911900	-0.05758400	-0.90309100
H	-6.66801100	-0.30855200	0.81581300
H	-5.96443800	1.07607100	-0.05856200
O	-1.22612300	2.60795200	-0.69621000
I	-1.06931700	3.31842200	1.18994500
C	-1.57120400	-2.02357200	1.04785000
H	-1.41435900	-1.33063600	1.87651400
H	-2.50981200	-2.55545600	1.24339900