Supporting Information for:

Regioselectivity and stereoselectivity of Intramolecular [2+2] Photocycloaddition Catalyzed by Chiral Thioxanthone: A Quantum Chemical Study

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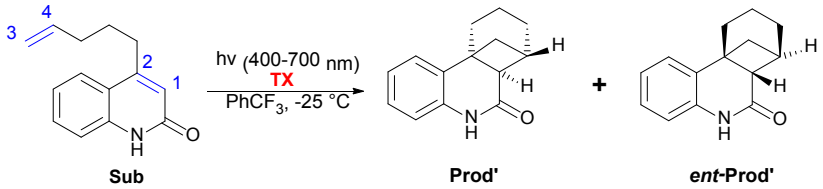
Contents

I. Reaction equation for Prod' and *ent*-Prod'.



Sub **Prod'** ***ent*-Prod'**

Scheme S1. *[2+2] cycloaddition of 4-(pent-4-en-1-yl)quinolin-2(1H)-one produce Prod' and ent-Prod'.*

II. Structures for ^{1}Sub, ^{3}Sub, Prod and ent-Prod.

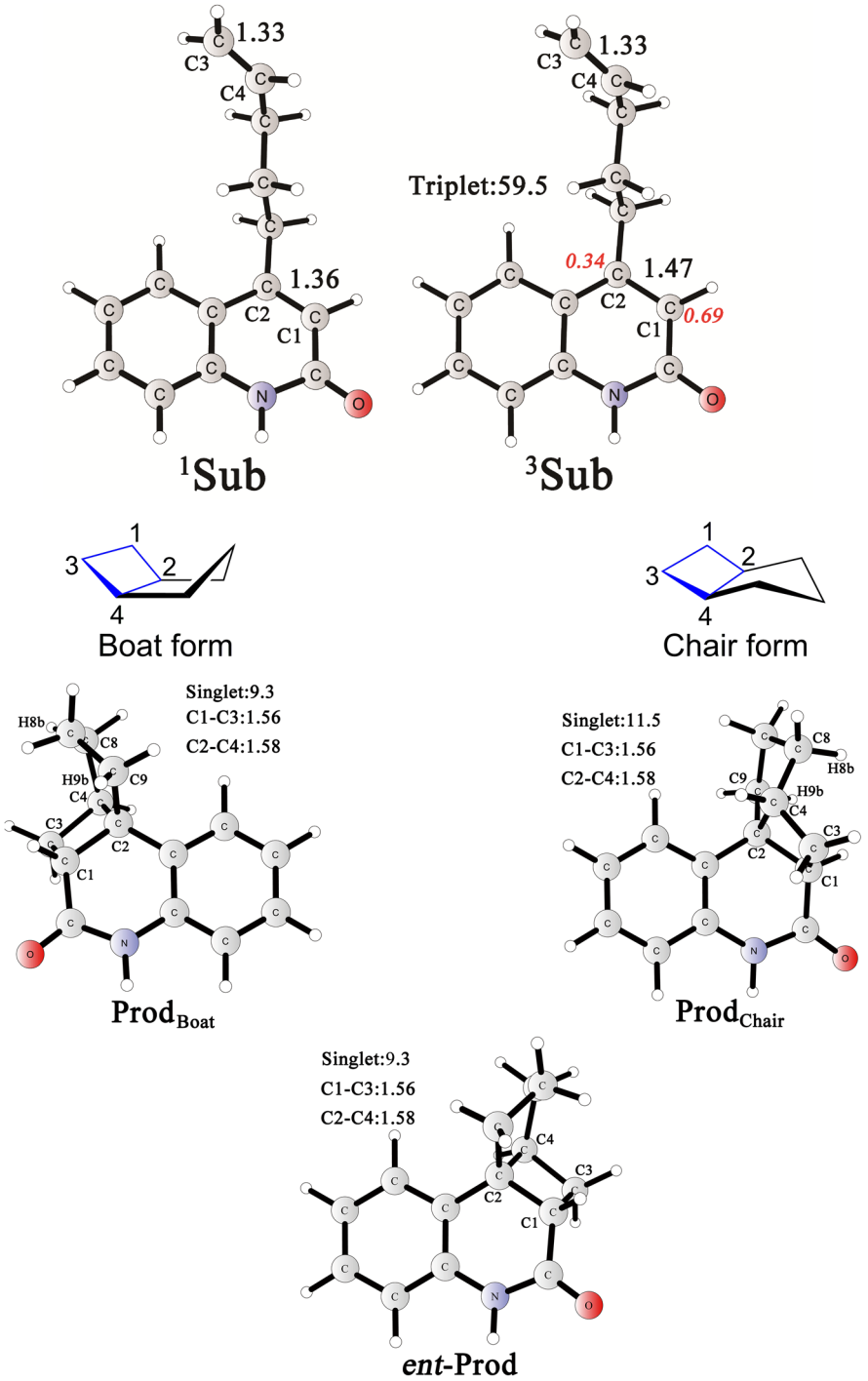


Figure S1. *Optimized structures of ^{1}Sub (closed-shell singlet), ^{3}Sub (triplet), Prod (closed-shell singlet) and ent-Prod (closed-shell singlet). The boat and chair conformation of Prod are also given. Distances are given in Å. Spin densities on selected atoms are indicated in red italics.*

III. Structures for $^3Int1_A$ and $^3Int1_B$.

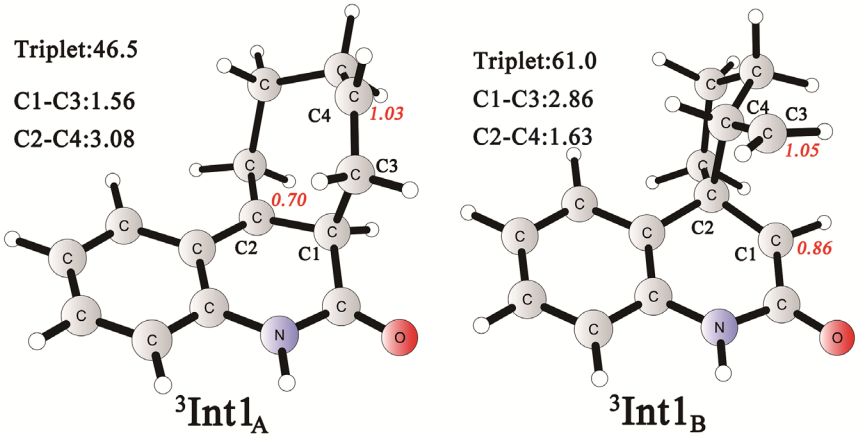


Figure S2. *Optimized structures of $^3Int1_A$ (triplet), $^3Int1_B$ (triplet). Distances are given in Å. Atomic spin population on selected atoms are indicated in red italics*.

IV. Structures for Prod' and *ent*-Prod'.

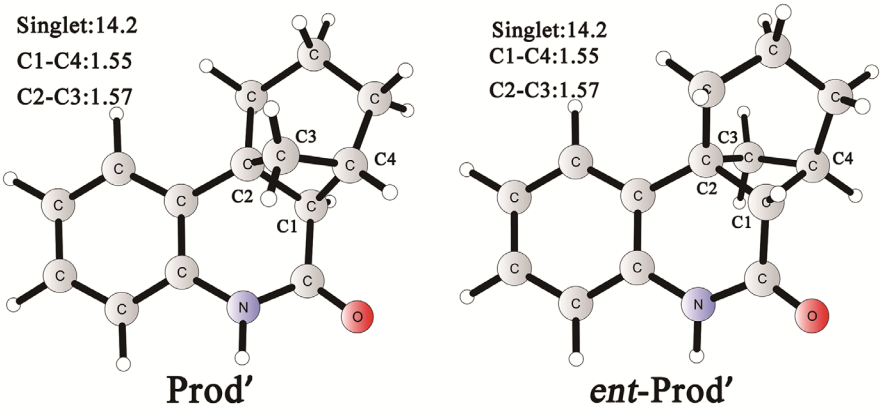


Figure S3. *Optimized structures of Prod' (closed-shell singlet), ent-Prod' (closed-shell singlet). Distances are given in Å.*

V. Gibbs energy diagram for pathway C and D at the B3LPY-D3 level.

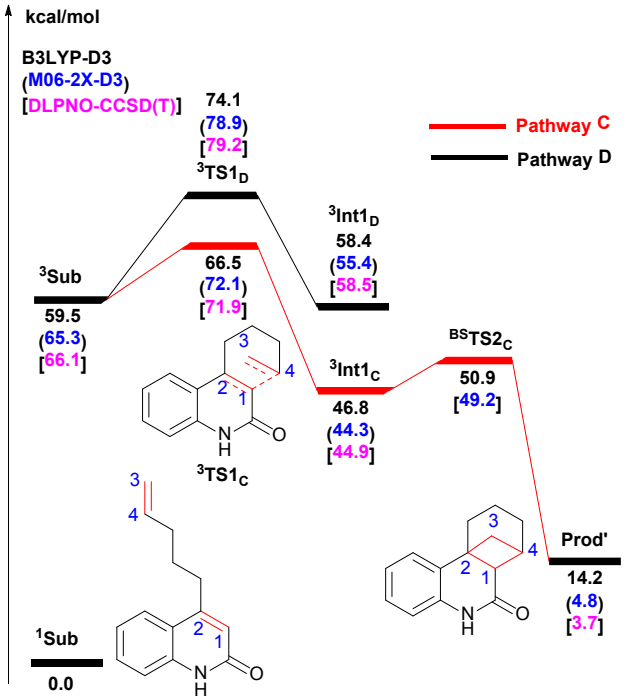


Figure S4. *Gibbs free energy diagram (kcal/mol) for the uncatalyzed cyclization of quinolone, pathway C and D. The numbers 1 and 3 indicate the closed-shell singlet and triplet, and BS represents the broken-symmetry open-shell singlet. The B3LYP-D3, M06-2X-D3 and DLPNO-CCSD(T) results were shown in black, blue (parentheses) and pink color (brackets), respectively.*

VI. Gibbs energy diagram for pathway A and B at the DLPNO-CCSD(T) level.

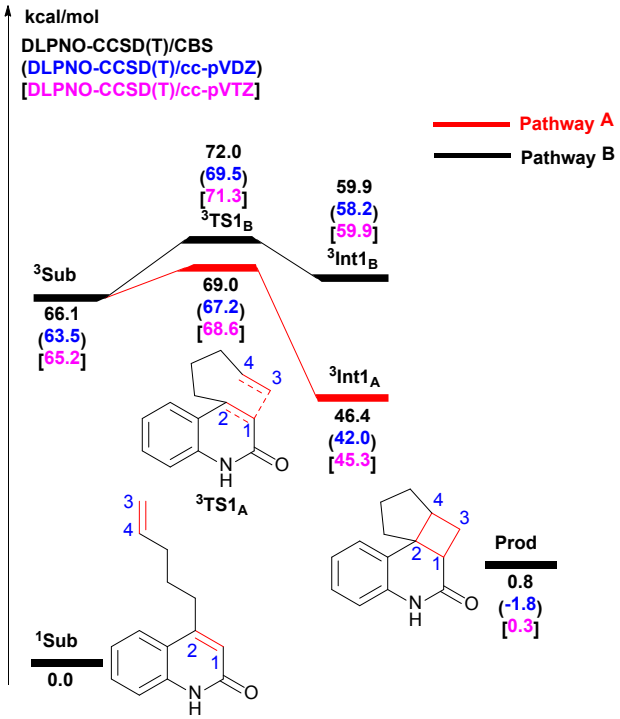


Figure S5. *Gibbs free energy diagram (kcal/mol) for the uncatalyzed cyclization of quinolone, pathway A and B. The numbers 1 and 3 indicate the closed-shell singlet and triplet, and BS represents the broken-symmetry open-shell singlet. The DLPNO-CCSD(T)/CBS, DLPNO-CCSD(T)/cc-pVDZ and DLPNO-CCSD(T)/cc-pVTZ results were shown in black, blue (parentheses) and pink color (brackets), respectively.*

VII. Minimum Energy Crossing Point analysis on ^{3}TX-Int2$_{ex}$.

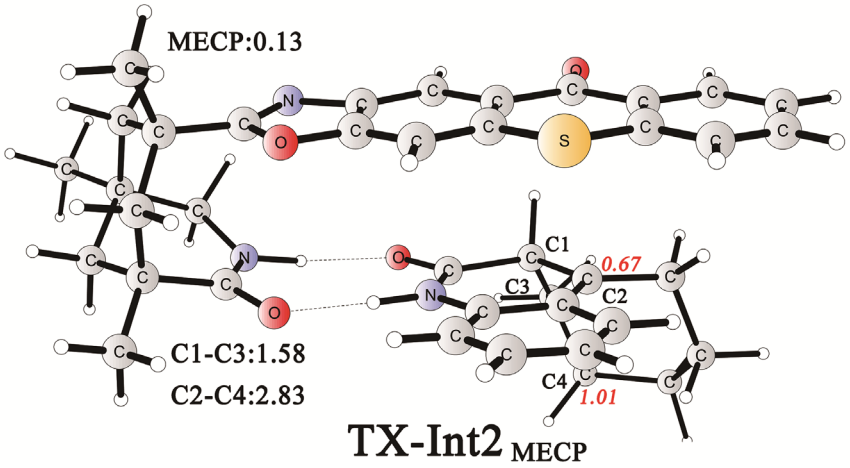


Figure S6. *The minimum energy crossing point of ^{3}TX-Int2$_{ex}$ found with the sobMECP software.*

VIII. Structure for ^{1}TX-Sub.

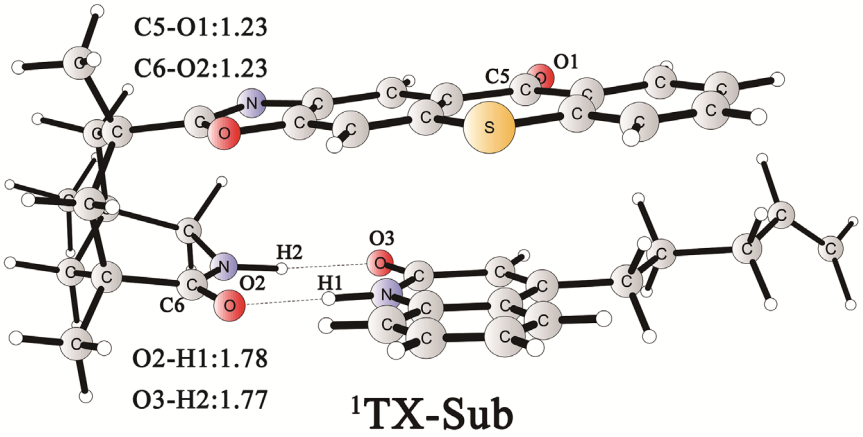


Figure S7. *Optimized structure of ^{1}TX-Sub (closed-shell singlet). Distances are given in Å.*

IX. Atomic spin density figures for ^{3}Sub、^{3}TX-Sub、^{3}TX-Int1$_{ex}$.

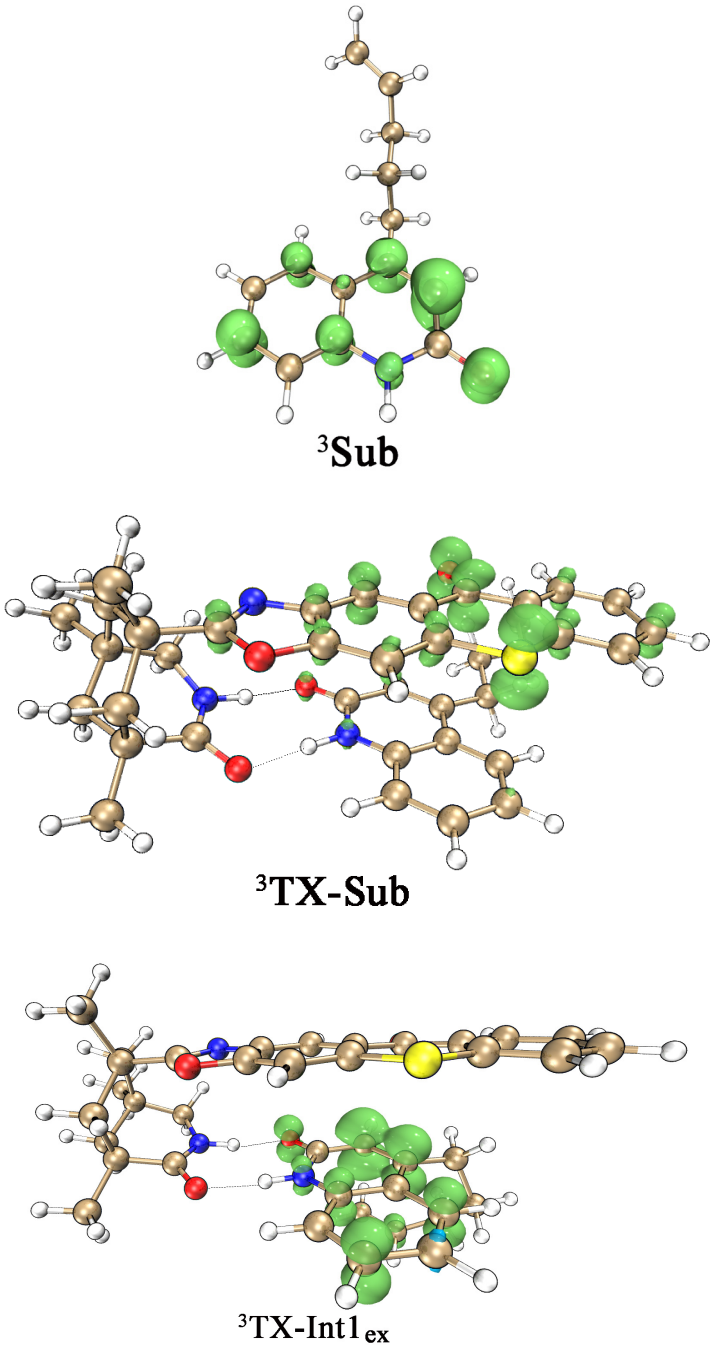


Figure S8. *Atomic spin density figures for ^{3}Sub、^{3}TX-Sub、^{3}TX-Int1$_{ex}$. The green and blue correspond to the positive and negative spin density parts.*

X. Electronic structure of ^{3}Sub、^{3}TX-Sub、^{3}TX-Int1ex.

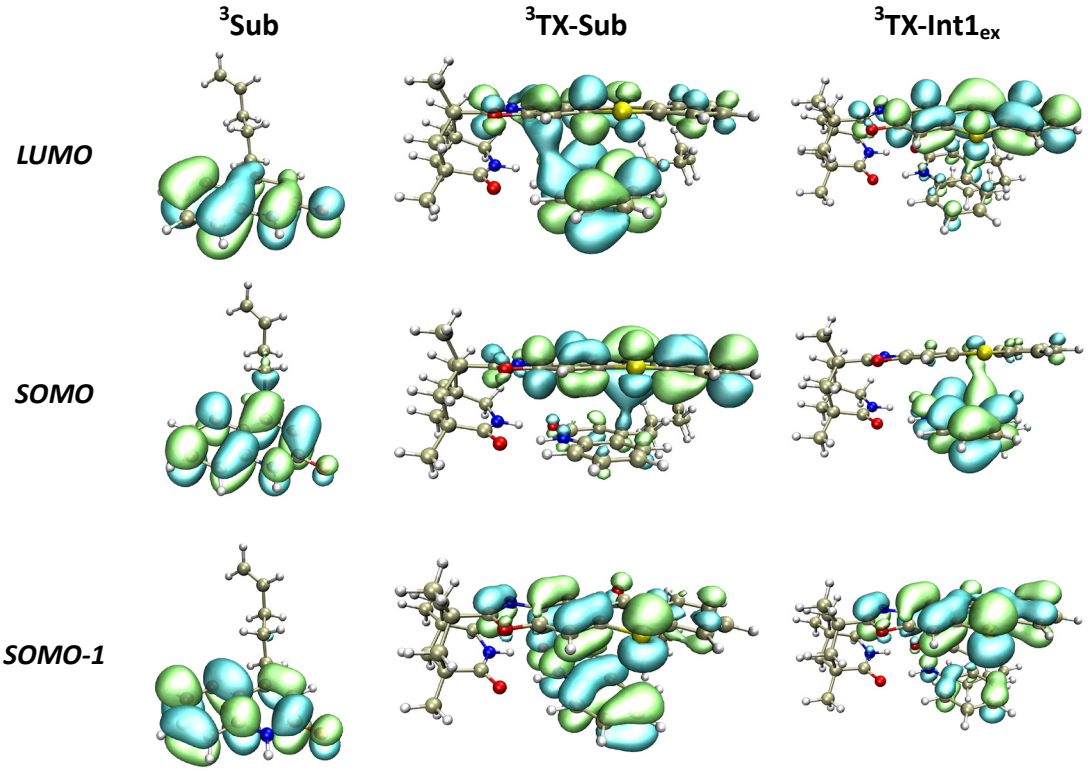


Figure S9. *Lowest unoccupied molecular orbital (LUMO) and single occupied molecular orbitals (SOMOs) of ^{3}Sub、^{3}TX-Sub、^{3}TX-Int1$_{ex}$.*

XI. Structures for TX and ^{3}TX-Int1$_{en}$.

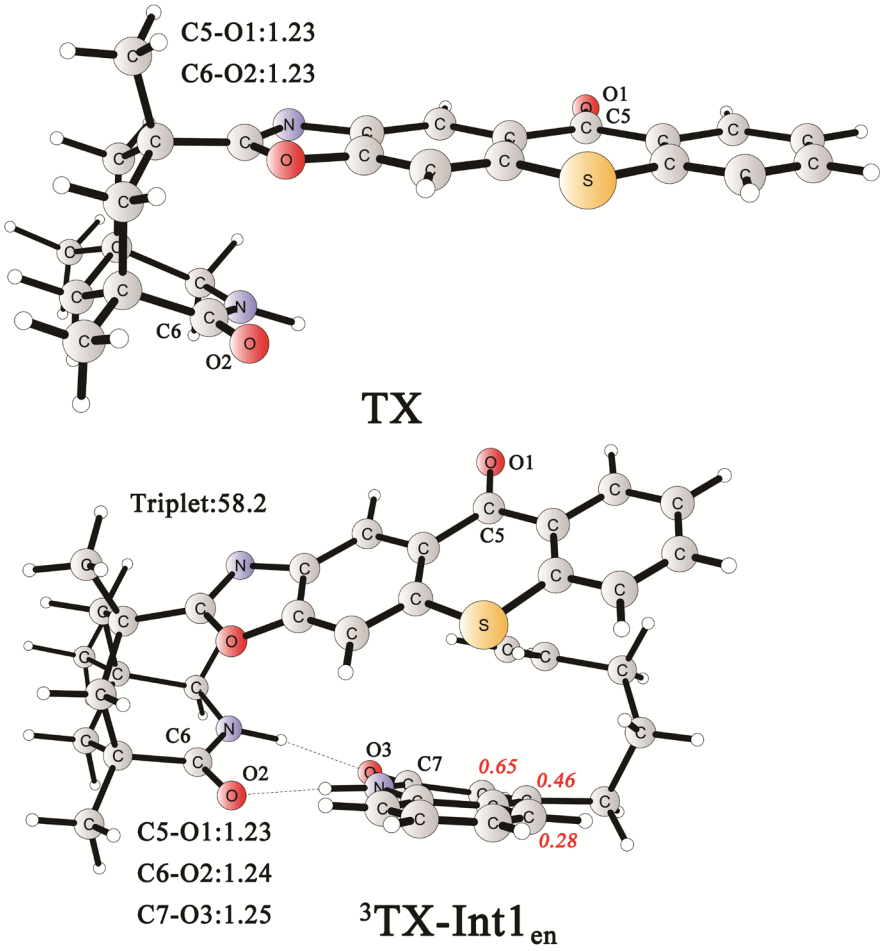


***Figure S10**. Optimized structures of TX (closed-shell singlet), ^{3}TX-Int1$_{en}$ (triplet). Distances are given in Å. Atomic spin population on selected atoms are indicated in red italics.*

XII. Structures for ^{3}TX-Int2$_{ex}$ and ^{3}TX-Int2$_{en}$.

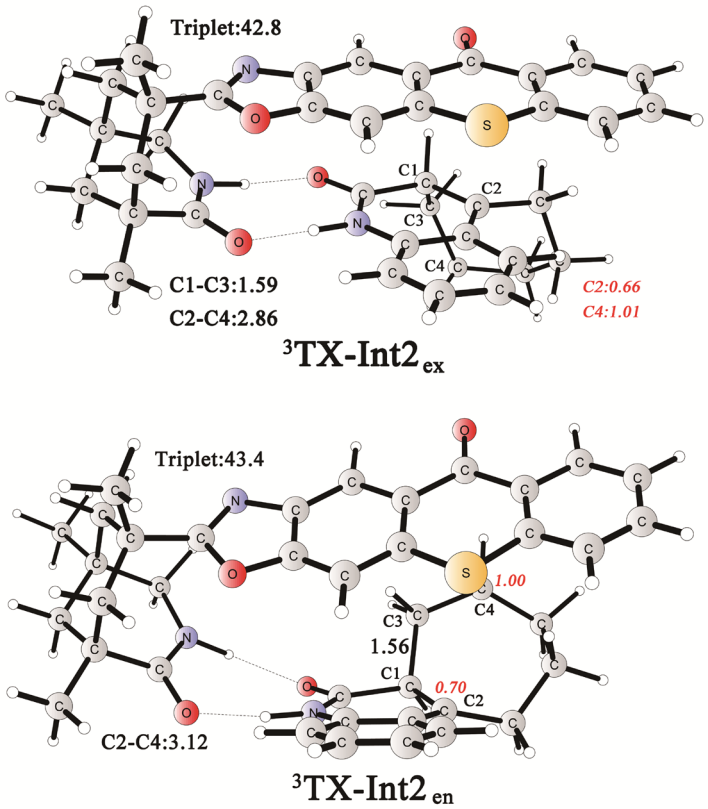


Figure S11. *Optimized structures of ^{3}TX-Int2$_{ex}$ (triplet), ^{3}TX-Int2$_{en}$ (triplet). Distances are given in Å. Atomic spin population on selected atoms are indicated in red italics***.**

XIII. Different conformations for ^{3}TX-TS1$_{en}$, ^{BS}TX-TS2$_{en}$, and ^{3}TX-TS1$_{ex}$.

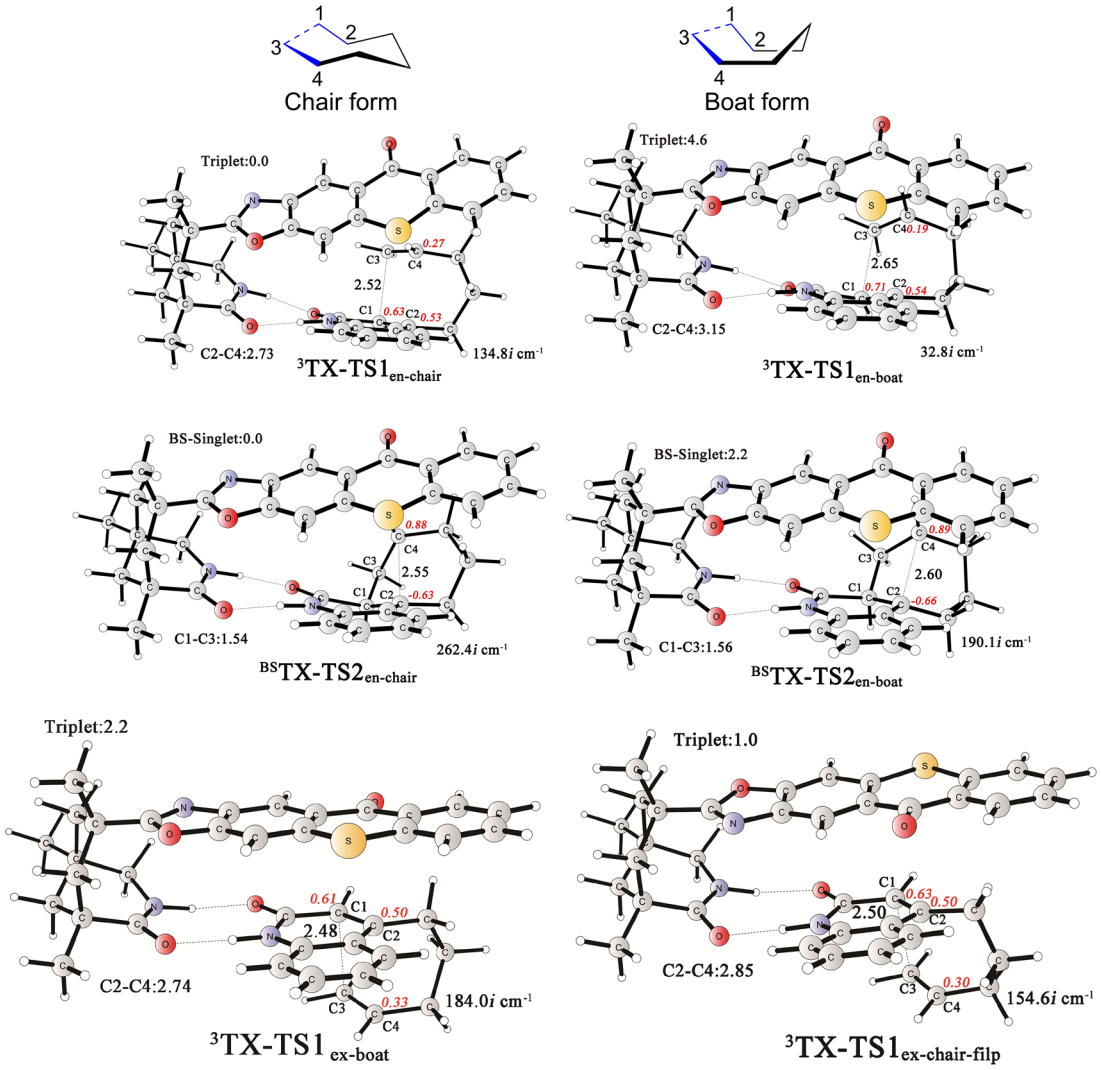


Figure S12. *Optimized structures of ^{3}TX-TS1$_{en\text{-}chair}$, ^{3}TX-TS1$_{en\text{-}boat}$, ^{BS}TX-TS2$_{en\text{-}chair}$, ^{BS}TX-TS2$_{en\text{-}boat}$ ^{3}TX-TS1$_{ex\text{-}boat}$, ^{3}TX-TS1$_{ex\text{-}chair\text{-}flip}$. Distances are given in Å. Relative energies of ^{3}TX-TS1$_{ex\text{-}boat}$ and ^{3}TX-TS1$_{ex\text{-}chair\text{-}flip}$ are given in kcal/mol relative to complexation ^{3}TX-TS1$_{ex}$. The imaginary frequencies are also indicated. Atomic spin population densities on selected atoms are indicated in red italics.*

XIV. Structures for TX-Prod$_{RSR}$ and TX-Prod$_{SRS}$.

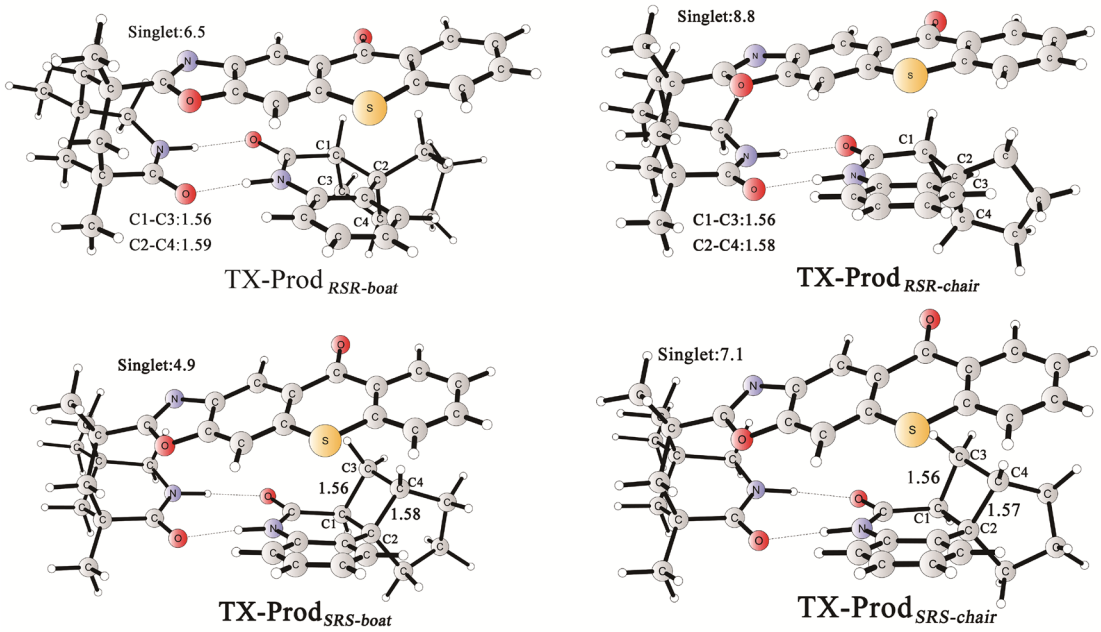


***Figure S13**. Optimized structures of TX-Prod$_{RSR}$ (closed-shell singlet), TX-Prod$_{SRS}$ (closed-shell singlet). Boat and chair conformation of the product are also exhibited. Distances are given in Å.*

XV. Distortion/interaction analysis for TX-Prod$_{RSR\text{-}boat}$ and TX-Prod$_{SRS\text{-}boat}$.

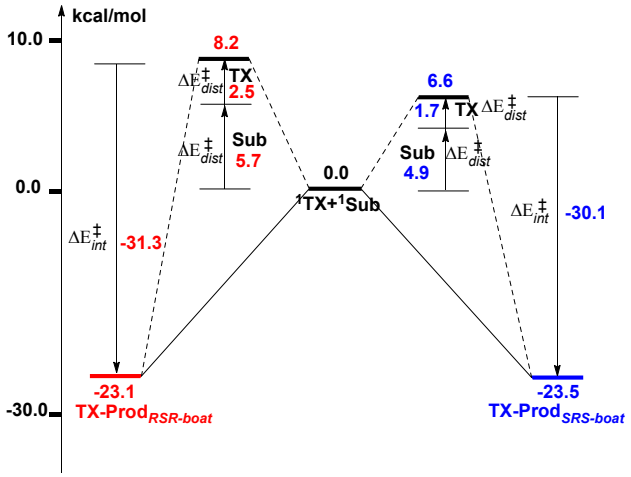


Figure S14. *Distortion/interaction analysis for TX-Prod calculated at the B3LYP-D3 level.*

XVI. Gibbs energy diagram for the formation of Prod'.

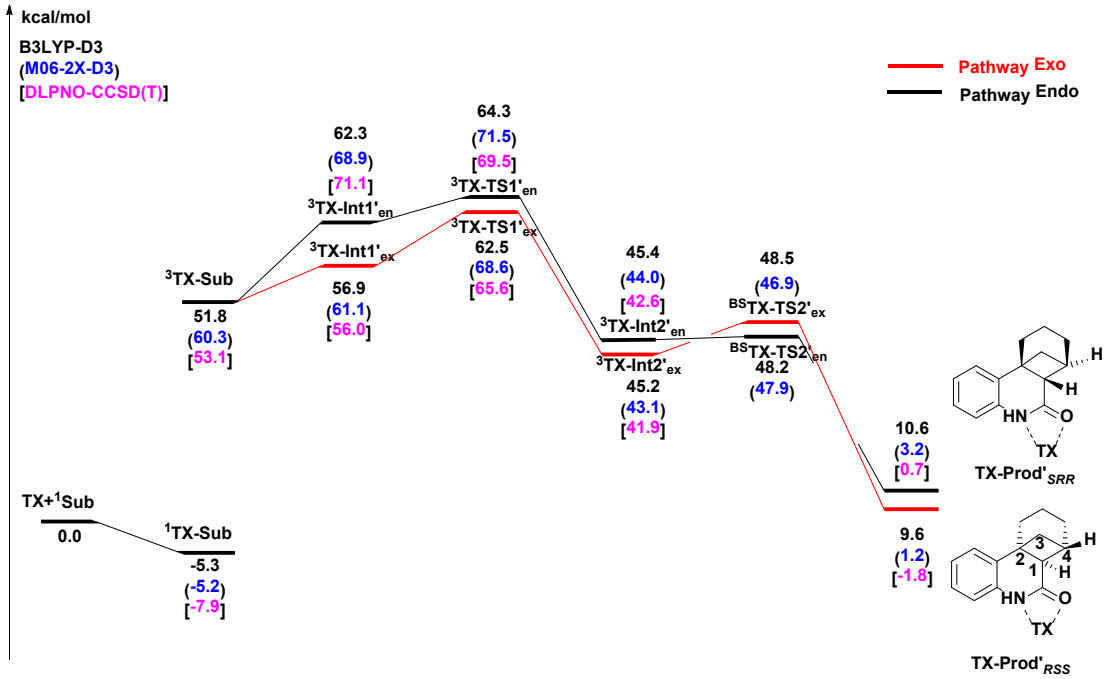


Figure S15. *Gibbs free energy diagram (kcal/mol) for the catalyzed cyclization of quinolone. The numbers 1 and 3 indicate the closed-shell singlet and triplet, and BS represents the broken-symmetry open-shell singlet. The B3LYP-D3, DLPNO-CCSD(T) and M06-2X-D3 results were shown in black, blue (parentheses) and pink color (brackets), respectively.*

XVII. Details of the DLPNO-CCSD(T) calculations.

Domain-based local pair natural orbital coupled cluster single-point energy calculations in the gas phase on the basis of the B3LYP-D3 geometries were performed for selected key stationary points at the DLPNO-CCSD(T) level by using ORCA 4.2.0.[S1-S2] Extrapolate to the complete basis set by calculating the single point energy to obtain the CCSD(T) specified goal[S3-S6]. To solve the slow convergence problem with respect to the basis set limit, the basis set limit was extrapolated using cc-pVDZ and cc-pVTZ energies, treating the convergence of the HF energies and the correlation energies separately.

(a) The convergence of the HF energy to the basis set limit is calculated by

$$E_{SCF}^{(X)} = E_{SCF}^{(\infty)} + A\exp\left(-\alpha\sqrt{X}\right) \quad (1.1)$$

Here, $E_{SCF}^{(X)}$ is the SCF energy calculated with the basis set with cardinal number *X*, $E_{SCF}^{(X)}$ is the basis set limit SCF energy, α=4.42(empirically optimized for cc/pVDZ//cc/pVTZ), and A is a parameter to be determined.

(b) The correlation energy is supposed to converge as

$$E_{corr}^{(X)} = \frac{X^{\beta}E_{corr}^{(X)} - Y^{\beta}E_{corr}^{(Y)}}{X^{\beta} - Y^{\beta}} \quad (1.2)$$

Here, $E_{corr}^{(X)}$ is the correlation energy and the value of X and Y is 2 and 3 in our case, β= 2.46 (empirically optimized for cc/pVDZ//cc/pVTZ).[S7]

Gibbs free energy correction and the solvation effects were taken from the B3LYP-D3. The INP files of pyridine for the DLPNO-CCSD(T) calculation are shown here as examples. The cc-pvtz/jk auxiliary basis set was used with the RIJK acceleration, but without the RIJCOSX acceleration.

For Local Energy Decomposition calculations, two fragments (TX and Sub) are defined and the !LED keywords was specified in the input line. The ^{3}TX-TS1$_{ex}$ structure input file is as follows.

```
[1]Sub ORCA Input File
%pal nprocs 4
end
!UHF DLPNO-CCSD(T) Extrapolate(2/3,cc)  cc-pvtz/jk  tightscf  GRIDX5 KDIIS
```

```
%maxcore 18000
%mdci
      maxiter 200
      density 0
end
%scf maxiter 500
end
* XYZ 0 1
C                0.99348900       2.94001700       0.28613200
C                2.30256800       2.89977200      -0.21713200
C                2.92557500       1.68381500      -0.45423400
C                2.24448800       0.48205000      -0.19321400
C                0.91818600       0.50086600       0.31276000
C                0.31892100       1.75579300       0.54486600
N                2.85541000      -0.73365700      -0.42275500
C                2.28748900      -1.98921900      -0.19680200
C                0.92486000      -1.93443600       0.32319800
C                0.25874000      -0.77370700       0.56683700
O                2.91898000      -3.01455800      -0.43303300
C               -2.18736500      -0.53567300      -0.07651200
C               -3.64036100      -0.53216900       0.43091300
C               -4.63357000      -0.31889800      -0.67789700
C               -5.46970100       0.71520500      -0.77085100
H                0.50968900       3.89329300       0.47283600
H                2.83572400       3.82337700      -0.42189400
H                3.94040400       1.64770300      -0.84140600
H               -0.69212800       1.79744800       0.93439600
H                3.80079800      -0.75869300      -0.78420900
H                0.46358300      -2.89936600       0.50440400
H               -1.96822000       0.42478900      -0.55608700
H               -2.06532100      -1.30078000      -0.85339700
H               -3.84185400      -1.49379600       0.92607900
H               -3.76188000       0.24550500       1.19614100
H               -4.63430400      -1.07654000      -1.46315900
H               -6.15899600       0.82202900      -1.60334900
H               -5.49782400       1.49363800      -0.01126200
C               -1.17219400      -0.80898800       1.05181200
H               -1.31736400      -0.08004400       1.85882300
H               -1.37875400      -1.79306000       1.48637100
*
```

^{3}TX-TS1$_{ex}$ ORCA Input File

```
%pal nprocs 4
end
!UHF DLPNO-CCSD(T) cc-pvtz cc-pvtz/c rijk cc-pvtz/jk tightscf    normalPNO LED
%maxcore 28000
%mdci
      dodidplot true
      LED 1
      PrintLevel 3
      maxiter 200
      density 0
end
%scf maxiter 500
end
* XYZ 0 3
C(1)          4.94851200      0.68110600      1.19069900
C(1)          5.97062800      1.13996500      0.13797900
C(1)          5.55687800      0.63732200     -1.25302700
C(1)          5.45087200     -0.91237200     -1.23808300
C(1)          4.67466100     -1.58261800     -0.07677100
C(1)          4.98039100     -0.86532400      1.26705100
C(1)          4.23489000      1.34379200     -1.61126000
C(1)          6.60454500      1.02534400     -2.30974900
C(1)          5.27014400      1.26843400      2.57192000
C(1)          5.11068400     -3.06717100      0.03448700
C(1)          3.52662100      1.10953800      0.78822600
N(1)          3.31570500      1.47655900     -0.48515200
O(1)          2.60512700      1.07978100      1.62816900
C(1)          3.18991900     -1.60468000     -0.33604700
N(1)          2.52114400     -1.31612600     -1.40342700
C(1)          1.18108500     -1.53466500     -1.05937000
C(1)          1.13677800     -1.99667100      0.26843400
O(1)          2.41839400     -2.04910800      0.73142100
C(1)         -0.00137200     -1.33884400     -1.75149000
C(1)         -1.21996500     -1.63974100     -1.10713300
C(1)         -1.21749100     -2.15036500      0.21924200
C(1)         -0.02181900     -2.32242800      0.93774700
C(1)         -2.46119600     -1.33790700     -1.86483900
C(1)         -3.78778500     -1.67062300     -1.28570800
C(1)         -3.97964100     -2.18530000      0.01063700
C(1)         -4.92353400     -1.40122200     -2.07589800
C(1)         -6.20527100     -1.61971500     -1.59810700
C(1)         -6.38331500     -2.11119700     -0.29606300
```

C(1)	-5.28241800	-2.39073700	0.50172600
O(1)	-2.39501500	-0.78536800	-2.96751300
H(1)	6.96505000	0.75857100	0.40609200
H(1)	6.04026300	2.23549500	0.12932700
H(1)	5.04600000	-1.26297400	-2.19309100
H(1)	6.47826800	-1.29218800	-1.17257500
H(1)	3.71386600	0.79612100	-2.40298800
H(1)	4.46114600	2.34879900	-1.99228800
H(1)	7.56764000	0.54791900	-2.10001100
H(1)	6.28700900	0.71553000	-3.31200200
H(1)	6.76360200	2.10882300	-2.32586300
H(1)	5.29226000	2.36252700	2.53362200
H(1)	4.51009600	0.97189000	3.29744600
H(1)	6.25077500	0.91962100	2.91353100
H(1)	4.56354900	-3.57443300	0.83388000
H(1)	4.92059900	-3.59716000	-0.90423600
H(1)	6.18118300	-3.12861700	0.25436900
H(1)	2.33704800	1.66951200	-0.74579000
H(1)	-0.02699500	-0.93129200	-2.75386500
H(1)	-0.01310300	-2.66592400	1.96546900
H(1)	-4.74848800	-1.00280600	-3.06904600
H(1)	-7.06600200	-1.40550900	-2.22399400
H(1)	-7.38313200	-2.27562500	0.09509200
H(1)	-5.42193100	-2.77130000	1.50968800
H(1)	5.99007500	-1.15889900	1.58093500
H(1)	4.28694500	-1.21080900	2.03808100
S(1)	-2.67002300	-2.60312300	1.10352800
C(2)	-3.10331000	0.28590300	3.44937100
C(2)	-1.75202700	0.21703400	3.81886600
C(2)	-0.75369000	0.55557500	2.89634400
C(2)	-1.09299000	0.96265200	1.60892400
C(2)	-2.47237900	1.02966500	1.19418900
C(2)	-3.45677000	0.67857000	2.16895700
N(2)	-0.08277300	1.31450300	0.71770900
C(2)	-0.29055900	1.63047200	-0.60645900
C(2)	-1.66298500	1.72006600	-1.04258400
C(2)	-2.78162500	1.43534700	-0.12014100
O(2)	0.67259300	1.84878900	-1.37075500
C(2)	-4.88465900	2.89688600	-0.10403100
C(2)	-4.19488100	4.18226700	-0.60330700
C(2)	-1.69595600	4.21827600	-0.96081500
C(2)	-2.77462400	4.28029500	-0.13751600

H(2)	-3.87646700	0.02017000	4.16432800
H(2)	-1.47294500	-0.09587100	4.82031700
H(2)	0.29739800	0.51002700	3.16729400
H(2)	-4.50318000	0.70070600	1.88663200
H(2)	0.89493900	1.26566200	1.04309500
H(2)	-4.89056300	2.89222800	0.99282100
H(2)	-5.93366500	2.89759000	-0.42740500
H(2)	-4.23129700	4.21649000	-1.69963900
H(2)	-1.81045200	4.23084000	-2.04051900
H(2)	-0.68288100	4.30505200	-0.58490500
H(2)	-4.76568300	5.04757000	-0.23624900
C(2)	-4.19332100	1.60851100	-0.60899400
H(2)	-4.80396700	0.75104900	-0.30438300
H(2)	-4.19683400	1.60298600	-1.70536300
H(2)	-1.82796900	1.69106100	-2.11228900
H(2)	-2.61726200	4.32719700	0.93909000

*

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S2. C. Riplinger, P. Pinski, U. Becker, E. F. Valeev and F. Neese, *J. Chem. Phys.*, 2016, **144**, 024109.

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S5. J. Rezac and P. Hobza, J. Chem. *Theory. Comput.*, 2013, **9**, 2151-2155.

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XVIII. Table statistics for TX-Prod$_{RSR}$.

***Table S1**. Mulliken Atomic Spin Population on the TX, Sub Fragment and selected atoms of Relevant Stationary Point Involved in Figure 4.*

Compound	Mulliken atomic spin population					
	TX	Sub	C1	C2	C3	C4
^{3}**TX-Sub**	1.75	0.25	0.04	-0.01	0.01	-0.00
^{3}**TX-Int1$_{ex}$**	0.11	1.89	0.71	0.45	0.04	0.12
^{3}**TX-TS1$_{ex}$**	0.07	1.93	0.63	0.51	0.03	0.30
^{3}**TX-Int2$_{ex}$**	0.03	1.97	-0.02	0.63	-0.07	1.04
TX-Int2$_{MECP}$	-0.03	0.03	0.12	-0.67	-0.11	1.01
^{BS}**TX-TS2$_{ex}$**	-0.01	0.01	0.12	-0.68	-0.14	0.97

***Table S2**. Key Bond Distances on the TX, Sub Fragment and selected atoms of Relevant Stationary Point Involved in Figure 4.*

Compound	Bond length (Å)				
	C5=O1	C1-C2	C3-C4	C1-C3	C2-C4
^{3}**TX-Sub**	1.28	1.36	1.33	6.33	5.10
^{3}**TX-Int1$_{ex}$**	1.24	1.47	1.34	2.79	2.94
^{3}**TX-TS1$_{ex}$**	1.24	1.47	1.36	2.50	2.85
^{3}**TX-Int2$_{ex}$**	1.24	1.51	1.49	1.59	2.86
TX-Int2$_{MECP}$	1.24	1.51	1.50	1.58	2.83
^{BS}**TX-TS2$_{ex}$**	1.23	1.52	1.51	1.56	2.553

XIX. Local energy decomposition (LED) analysis.

Table S3. *LED Analysis of* ^{3}***TX-TS1***$_{ex}$ *and* ^{3}***TX-TS1***$_{en}$ *at the DLPNO-CCSD(T)/cc-pVTZ level.*

ΔE	^{3}*TX-TS1*$_{ex}$		^{3}*TX-TS1*$_{en}$	
	Hartree	kcal/mol	Hartree	kcal/mol
$\Delta E_{geo\text{-}prep}$	0.005505	3.5	0.005504	3.5
$\Delta E_{el\text{-}prep}$	0.239951	150.6	0.203899	127.9
ΔE_{elstat}	-0.198795	-124.7	-0.172351	-108.2
ΔE_{exch}	-0.047510	-29.8	-0.038503	-24.2
$\Delta E^{C-CCSD}_{non-dispersion}$	0.006186	3.9	0.005599	3.5
$\Delta E^{C-CCSD}_{dispersion}$	-0.041735	-26.2	-0.034366	-21.6
$\Delta E^{C-(T)}_{int}$	-0.002784	-1.7	-0.002115	-1.3

In the LED scheme, the binding energy Δ*E* of the two non-interacting fragments (i.e **TX** and **Sub**) can be expressed as

$$\Delta E = \Delta E_{geo-prep} + \Delta E_{int} \quad (1)$$

where the $\Delta E_{geo\text{-}prep}$ term is the geometric preparation energy (also called "strain" energy), and the ΔE_{int} term is the interaction energy of the two fragments. ΔE_{int} can be divided into the Hartree-Fock (HF) interaction term ΔE^{HF}_{int}, the perturbative triples correlation interaction term $\Delta E^{C-(T)}_{int}$ and the CCSD correlation interaction term ΔE^{C-CCSD}_{int}.

$$\Delta E_{int} = \Delta E^{HF}_{int} + \Delta E^{C-(T)}_{int} + \Delta E^{C-CCSD}_{int} \quad (2)$$

ΔE^{HF}_{int} includes the static electronic preparation energy term $\Delta E_{el\text{-}prep}$, the electrostatic energy term ΔE_{elstat} and the exchange energy term ΔE_{exch}.

$$\Delta E^{HF}_{int} = \Delta E_{el-prep} + \Delta E_{elstat} + \Delta E_{exch} \quad (3)$$

ΔE^{C-CCSD}_{int} can be divided into the non-dispersive term $\Delta E^{C-CCSD}_{non-dispersion}$ and the dispersive term $\Delta E^{C-CCSD}_{dispersion}$.

Table S4. *Energies of* ^{3}***TX-TS1***$_{ex}$ *and* ^{3}***TX-TS1***$_{en}$ *at the DLPNO-CCSD(T)/cc-pVTZ level. All values are given in hartree. The superscript "opt" denotes energies of optimized structures, while "fixed" denotes energies of isolated fragments.*

	Sub^{opt}	**TX**^{opt}	**Sub**^{fixed}	**TX**^{fixed}	^{3}**TX-TS1**$_{ex}$
E_{HF}	-668.315512	-1692.185049	-668.299316	-1692.180182	-2360.485852
E_c(CCSD)	-2.742469	-5.377661	-2.754791	-5.378200	-8.078504
E_c(T)	-0.130479	-0.260192	-0.132971	-0.260399	-0.396153
E_{tot}	-671.188460	-1697.822902	-671.187077	-1697.818781	-2369.059104
	Sub^{opt}	**TX**^{opt}	**Sub**^{fixed}	**TX**^{fixed}	^{3}**TX-TS1**$_{en}$
E_{HF}	-668.315512	-1692.185049	-668.298337	-1692.182097	-2360.487389
E_c(CCSD)	-2.742469	-5.377661	-2.754660	-5.377549	-8.169834
E_c(T)	-0.130479	-0.260192	-0.133018	-0.260198	-0.395331
E_{tot}	-671.188460	-1697.822902	-671.186015	-1697.819844	-2369.052555

Table S5. *Geometric preparation term* $\Delta E_{geo-prep}$ *of* ^{3}***TX-TS1***$_{ex}$ *and* ^{3}***TX-TS1***$_{en}$ *(in hartree).*

	TX	Sub	Total
^{3}***TX-TS1***$_{ex}$	0.0041205	0.001383	0.005504
^{3}***TX-TS1***$_{en}$	0.004200	0.002446	0.005504

Table S6. *Electronic preparation term* $\Delta E_{el\text{-}prep}$ *of* ^{3}*TX-TS1*$_{ex}$ *and* ^{3}*TX-TS1*$_{en}$ *(in hartree).*

		$\Delta E_{el\text{-}prep}$
^{3}***TX-TS1***$_{ex}$	Sub^{fixed}	0.126926
	TX^{fixed}	0.113025
^{3}***TX-TS1***$_{en}$	Sub^{fixed}	0.103708
	TX^{fixed}	0.100190

Table S7. *Fragment electrostatic term* ΔE_{elstat} *and exchange interaction* ΔE_{exch} *of* ^{3}***TX-TS1***$_{ex}$ *and* ^{3}***TX-TS1***$_{en}$ *(in hartree).*

	ΔE_{elstat}	ΔE_{exch}
^{3}TX-TS1$_{ex}$	-0.198795	-0.047510
^{3}TX-TS1$_{en}$	-0.172351	-0.038503

Table S8. *Dispersion term* $\Delta E_{dispersion}^{C-CCSD}$ *of* ^{3}***TX-TS1***$_{ex}$ *and* ^{3}***TX-TS1***$_{en}$ *(in hartree).*

	Strong pairs	Weak pairs	Total
^{3}**TX-TS1**$_{ex}$	-0.017319	-0.024417	-0.041735
^{3}**TX-TS1**$_{en}$	-0.013393	-0.020973	-0.034366

Table S9. *Non-dispersion term* $\Delta E_{non-dispersion}^{C-CCSD}$ *of* ^{3}***TX-TS1***$_{ex}$ *and* ^{3}***TX-TS1***$_{en}$ *(in hartree).*

		$\Delta E_{non-dispersion}^{C-CCSD}$
^{3}**TX-TS1**$_{ex}$	Strong pairs	-8.061185
	Weak pairs	-0.065620
	Total of strong and weak pairs	-8.126805
	CCSD correction[a] (Sub^{fixed} + TX^{fixed})	-8.132991
	Non-dispersion	0.006186
^{3}**TX-TS1**$_{en}$	Strong pairs	-8.060786
	Weak pairs	-0.065824
	Total of strong and weak pairs	-8.126610
	CCSD correction[a] (Sub^{fixed} + TX^{fixed})	-8.132209
	Non-dispersion	0.005599

[a]Derived from Ec(CCSD) in Table S4.

XX. UV-Vis Spectrum for Sub, TX, OX and SeX.

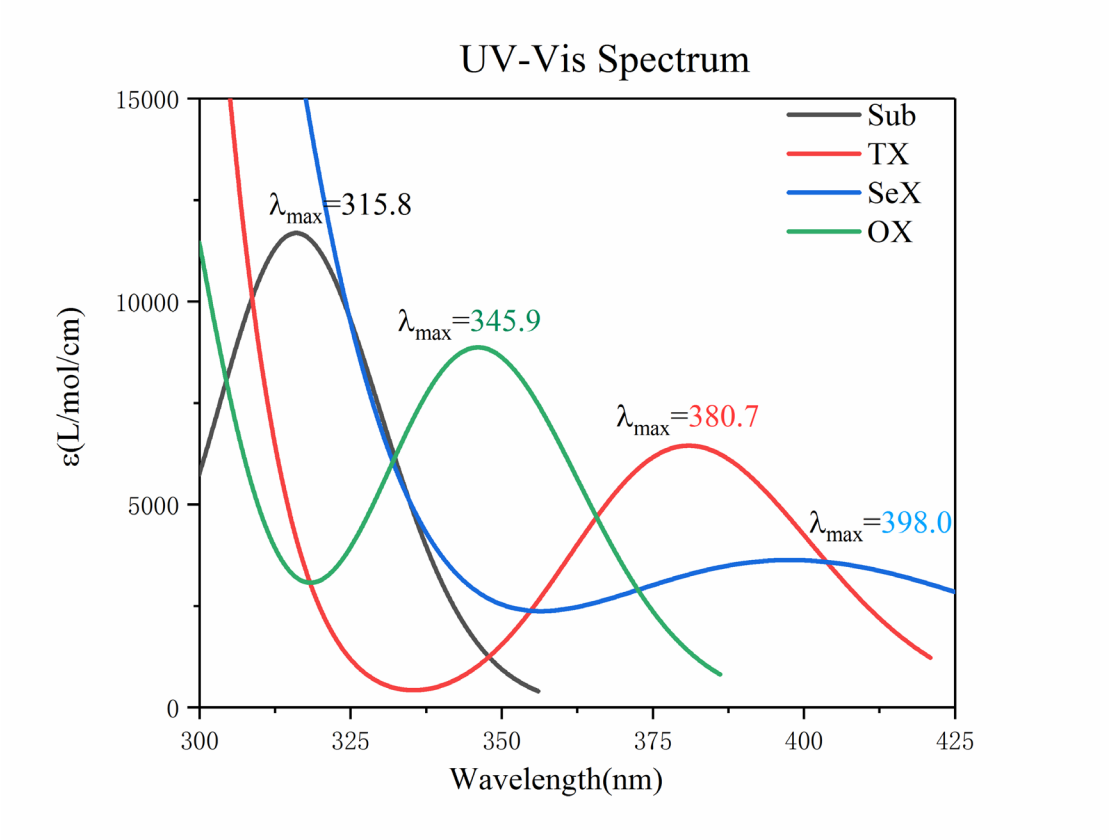


Figure S16. *Calculated UV-Vis spectrum of Sub, TX, OX and SeX in toluene at the B3LYP-D3 Level.*

XXI. Calculated optical transitions for ^{1}Sub, ^{1}TX, ^{1}OX and ^{1}SeX.

Table S10. *The main calculated optical transition for ^{1}Sub, with oscillator strength f >0.02[a]* (nstate=15).

Excitation	*w* (nm)	*f*	Energy(eV)	Composition
57 -> 58	315.83	0.1733	3.9257	94.2%(HOMO→LUMO)
56 -> 58	271.58	0.1131	4.5652	81.1%(HOMO-1→LUMO)
57 -> 59				14.8%(HOMO→LUMO+1)
54 -> 58	246.83	0.0273	5.023	55.8%(HOMO-3→LUMO)
55 -> 58				42.3%(HOMO-2→LUMO)
56 -> 59	238.29	0.0758	5.2031	12.2%(HOMO-1→LUMO+1)
57 -> 59				36.5%(HOMO→LUMO+1)
57 -> 60				33.8%(HOMO→LUMO+2)
57 -> 59	229.51	0.5379	5.4021	37.7%(HOMO→LUMO+1)
57 -> 60				32.1%(HOMO→LUMO+2)
57 -> 61				11.2%(HOMO→LUMO+3)
57 -> 61	226.74	0.1078	5.468	46.9%(HOMO→LUMO+3)
57 -> 62				33.9%(HOMO→LUMO+4)
56 -> 59	219.06	0.2677	5.6599	57.7%(HOMO-1→LUMO+1)
57 -> 60				16.5%(HOMO→LUMO+2)
53 -> 58	209.95	0.1407	5.9055	15.4%(HOMO-4→LUMO)
56 -> 60				51.7%(HOMO-1→LUMO+2)

Table S11. *The main calculated optical transition for ^{1}TX, with oscillator strength f >0.02[a]* (nstate=15).

Excitation	*w* (nm)	*f*	Energy(eV)	Composition
114 -> 115	380.67	0.0957	3.257	97.1%(HOMO→LUMO)
111 -> 115	301.11	0.0358	4.1176	17.2%(HOMO-3→LUMO)
112 -> 115				18.0%(HOMO-2→LUMO)
114 -> 116				48.8%(HOMO→LUMO+1)
112 -> 115	295.1	0.0541	4.2015	13.4%(HOMO-2→LUMO)
113 -> 115				74.2%(HOMO-1→LUMO)
112 -> 115	292.35	0.084	4.2409	65.1%(HOMO-2→LUMO)
113 -> 115				22.5%(HOMO-1→LUMO)
111 -> 115	281.9	0.5755	4.3982	34.7%(HOMO-3→LUMO)
114 -> 116				29.1%(HOMO→LUMO+1)
114 -> 117				19.6%(HOMO→LUMO+2)
111 -> 115	273.44	0.5288	4.5343	27.3%(HOMO-3→LUMO)
114 -> 117				64.2%(HOMO→LUMO+2)
108 -> 115	265.55	0.346	4.669	62.4%(HOMO-6→LUMO)

109 -> 115				29.1%(HOMO-5→LUMO)
114 -> 118	261.92	0.0386	4.7337	85.3%(HOMO→LUMO+3)

Table S12. *The main calculated optical transition for ^{1}OX, with oscillator strength f >0.02*[a] (nstate=15).

Excitation	*w* (nm)	*f*	Energy(eV)	Composition
110 -> 111	345.9	0.1315	3.5844	96.5%(HOMO→LUMO)
108 -> 111	294.85	0.0497	4.2049	48.9%(HOMO-2→LUMO)
109 -> 111				44.4%(HOMO-1→LUMO)
108 -> 111	292.84	0.0436	4.2338	38.5%(HOMO-2→LUMO)
109 -> 111				54.5%(HOMO-1→LUMO)
106 -> 111	285.53	0.1759	4.3422	18.1%(HOMO-4→LUMO)
107 -> 111				57.9%(HOMO-3→LUMO)
108 -> 111				10.7%(HOMO-2→LUMO)
104 -> 111	263.12	0.4367	4.7121	23.5%(HOMO-6→LUMO)
105 -> 111				12.9%(HOMO-5→LUMO)
110 -> 112				50.8%(HOMO→LUMO+1)
104 -> 111	259.39	0.6407	4.7798	46.4%(HOMO-6→LUMO)
105 -> 111				11.4%(HOMO-5→LUMO)
110 -> 112				37.6%(HOMO→LUMO+1)
110 -> 113	250.57	0.3974	4.9481	79.7%(HOMO→LUMO+2)
107 -> 112	225.67	0.0398	5.4941	31.9%(HOMO-3→LUMO+1)
110 -> 114				12.2%(HOMO→LUMO+3)

Table S13. *The main calculated optical transition for ^{1}SeX, with oscillator strength f >0.02*[a] (nstate=15).

Excitation	*w* (nm)	*f*	Energy(eV)	Composition
123 -> 124	397.95	0.0894	3.1156	97.7%HOMO→LUMO)
120 -> 124	304.46	0.0567	4.0723	15.8%(HOMO-3→LUMO)
121 -> 124				11.9%(HOMO-2→LUMO)
123 -> 125				55.7%(HOMO→LUMO+1)
121 -> 124	296.11	0.1549	4.1871	21.2%(HOMO-2→LUMO)
122 -> 124				57.8%(HOMO-1→LUMO)
123 -> 125				16.2%(HOMO→LUMO+1)
121 -> 124	292.62	0.0823	4.2371	53.8%(HOMO-2→LUMO)
122 -> 124				36.5%(HOMO-1→LUMO)
120 -> 124	288.05	0.1356	4.3042	27.8%(HOMO-3→LUMO)
123 -> 125				16.5%(HOMO→LUMO+1)
123 -> 126				38.9%(HOMO→LUMO+2)
120 -> 124	278.41	0.7498	4.4533	48.0%(HOMO-3→LUMO)

123 -> 126				43.7%(HOMO→LUMO+2)
123 -> 127	269.93	0.1211	4.5932	84.1%(HOMO→LUMO+3)
118 -> 124	268.5	0.2385	4.6177	15.3%(HOMO-5→LUMO)

[a] *Only orbital percentages larger than 10% are reported*

XXII. Key molecular orbitals for Sub.

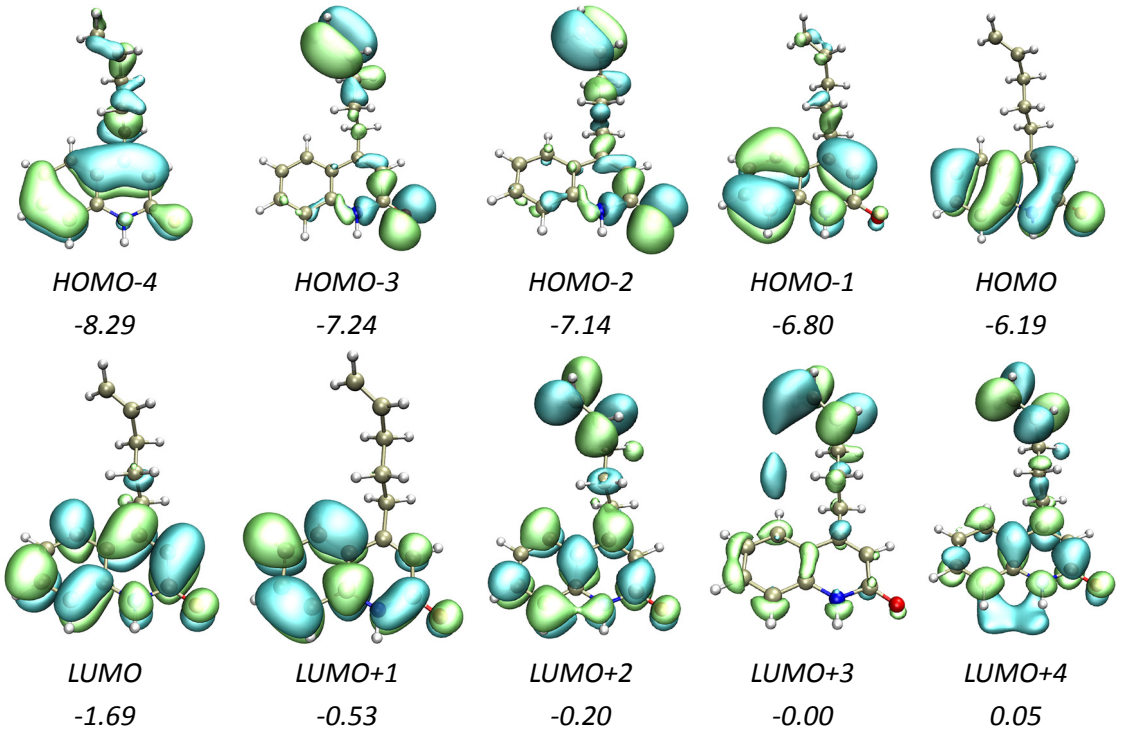


Figure S17. *Several important molecular orbitals of Sub. Numbers below of molecular orbitals are orbitals energies (in eV).*

XXIII. Key molecular orbitals for TX.

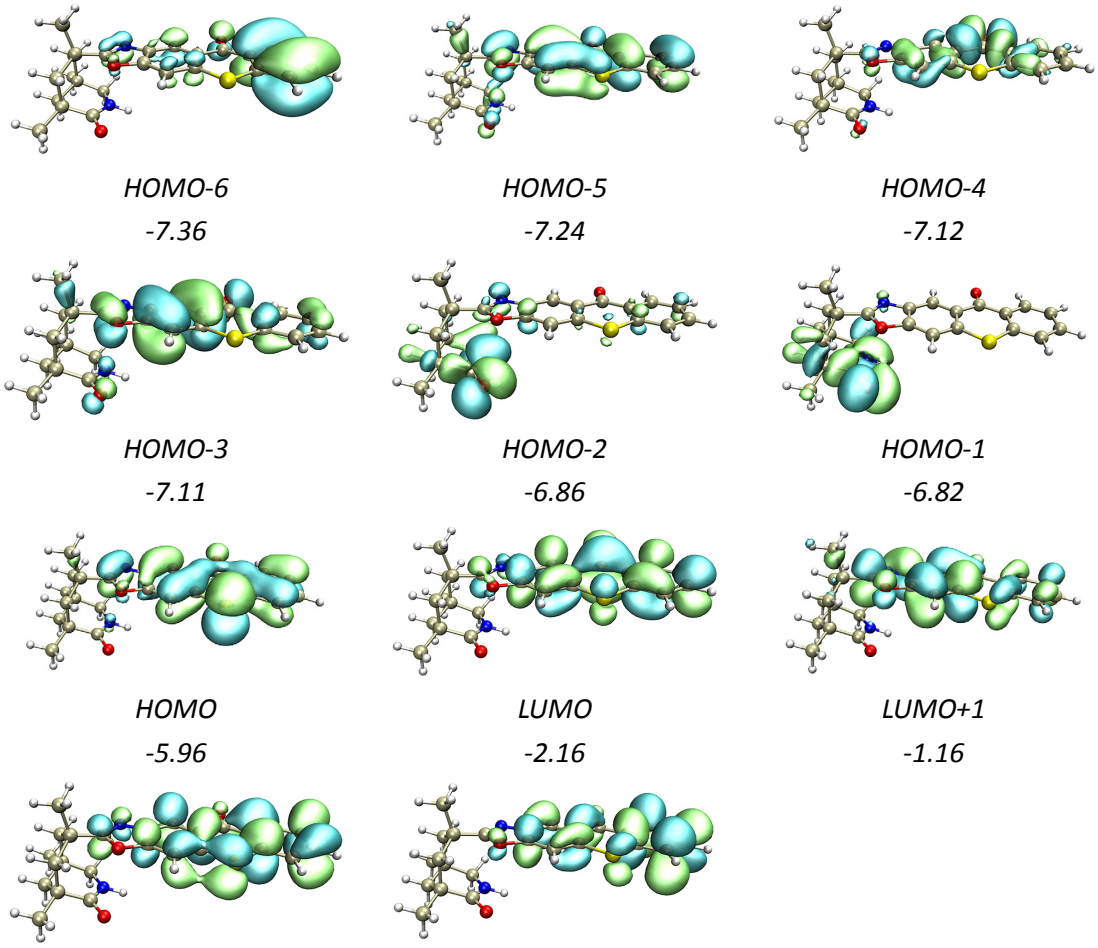


Figure S18. *Several important molecular orbitals of TX. Numbers below of molecular orbitals are orbitals energies (in eV).*

XXIV. Key molecular orbitals for OX.

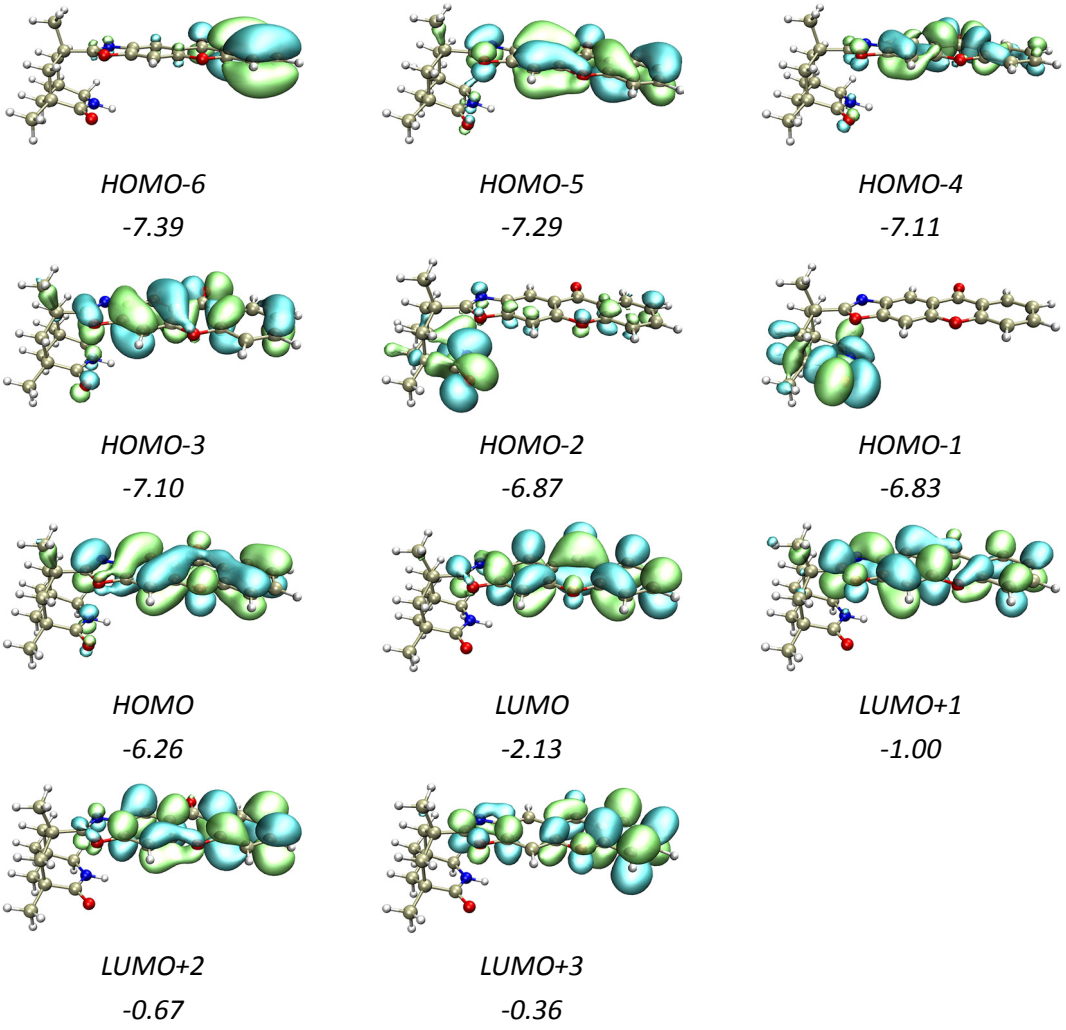
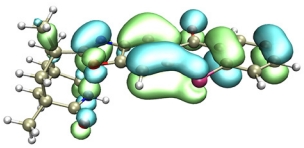


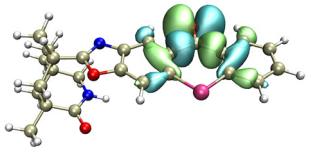
Figure S19. *Several important molecular orbitals of OX. Numbers below of molecular orbitals are orbitals energies (in eV).*

XXV. Key molecular orbitals for SeX.



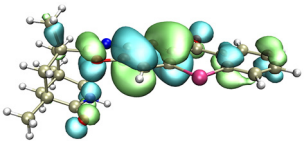
HOMO-5

-7.15



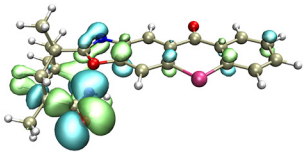
HOMO-4

-7.10



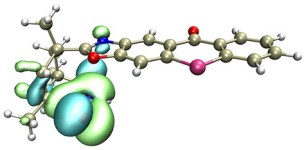
HOMO-3

-7.07



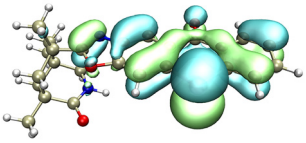
HOMO-2

-6.84



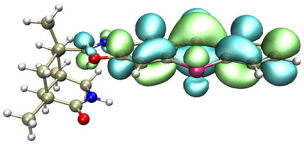
HOMO-1

-6.81



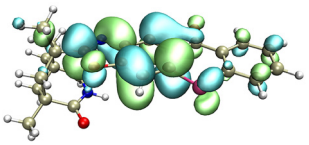
HOMO

-5.81



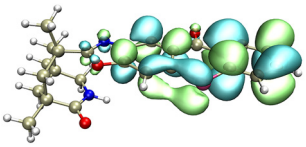
LUMO

-2.15



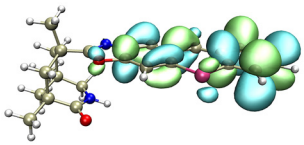
LUMO+1

-1.09



LUMO+2

-0.81



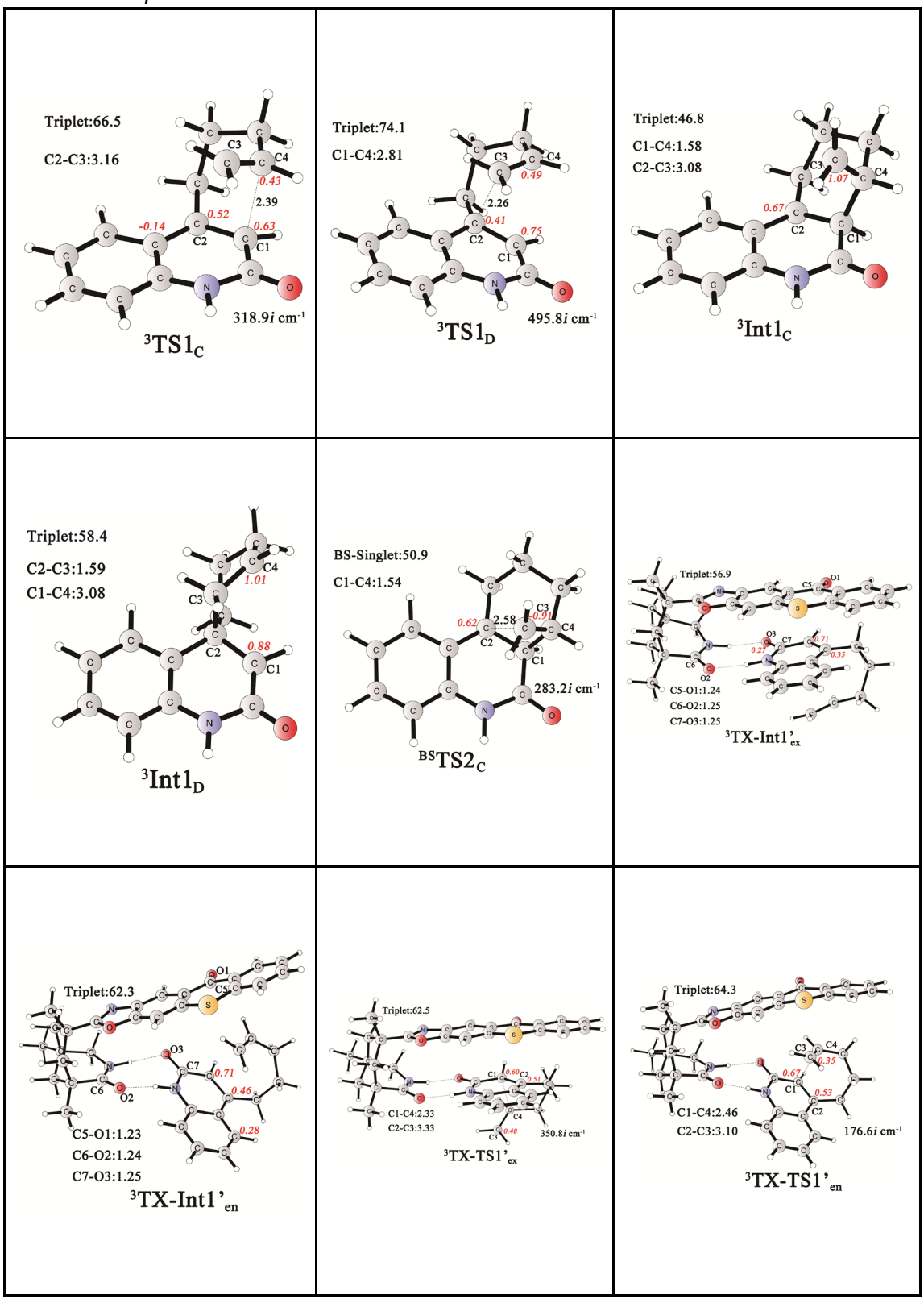
LUMO+3

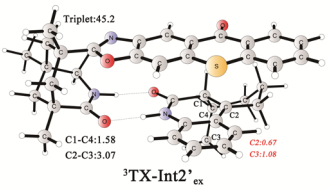
-0.55

Figure S20. *Several important molecular orbitals of SeX. Numbers below of molecular orbitals are orbitals energies (in eV).*

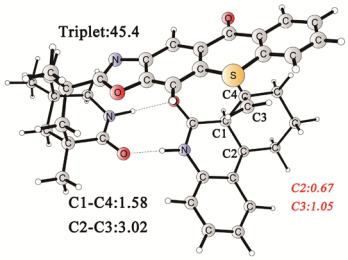
XXVI. Other optimized structures.

Table S14. *Optimized structures.*

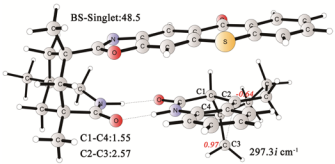




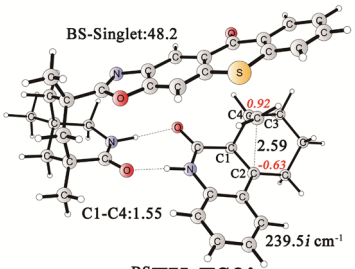
^{3}TX-Int2'$_{ex}$



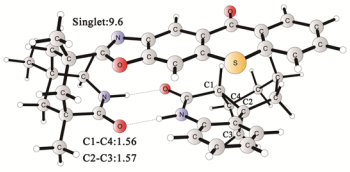
^{3}TX-Int2'$_{en}$



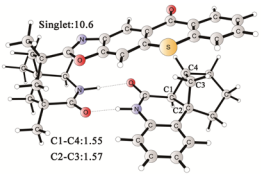
^{BS}TX-TS2'$_{ex}$



^{BS}TX-TS2'$_{en}$



TX-Prod'$_{RSS}$



TX-Prod'$_{SRR}$

XXVII. Table of energies.

Table S15. *Calculated energies* (in hartree) *and imaginary frequencies.*

Stationary point	Geometry optimization energy	Gibbs free energy correction	B3LYP-D3 large basis set Singlet-point energy	M06-2X-D3 large basis set Singlet-point energy	Imaginary frequencies
^{1}Sub	-672.5445064	0.217552	-672.7609702	-672.4440145	
^{3}Sub	-672.4443203	0.210278	-672.6588761	-672.3326167	
$^{3}TS1_{A}$	-672.4470103	0.215651	-672.6593491	-672.3325107	224.6*i*
$^{3}TS1_{B}$	-672.440988	0.215869	-672.6527417	-672.3273188	317.6*i*
$^{3}TS1_{C}$	-672.4402159	0.215009	-672.6523748	-672.3266317	318.9*i*
$^{3}TS1_{D}$	-672.4272944	0.214677	-672.6400556	-672.3154353	495.8*i*
$^{3}Int1_{A}$	-672.4782395	0.217909	-672.6872736	-672.3721705	
$^{3}Int1_{B}$	-672.452728	0.215463	-672.6617365	-672.349223	
$^{3}Int1_{C}$	-672.4773833	0.21666	-672.685461	-672.3725602	
$^{3}Int1_{D}$	-672.4578335	0.216778	-672.6671844	-672.3548791	
$^{BS}Int1_{A}$	-672.4783987	0.218906	-672.6879656	-672.3190436	
$^{BS}Int1_{C}$	-672.4784322	0.218105	-672.6862863	-672.3155023	
$^{BS}TS2_{A}$	-672.4757377	0.219614	-672.6844802	-672.3689511	293.6*i*
$^{BS}TS2_{C}$	-672.4750529	0.220227	-672.6825037	-672.3682865	283.2*i*
Prod	-672.547374	0.224973	-672.7535517	-672.4488821	
Prod’	-672.5419957	0.226356	-672.7470854	-672.4451581	
TX	-1700.615256	0.392704	-1701.042098	-1700.447273	
^{1}TX-Sub	-2373.220451	0.638286	-2373.839518	-2372.927631	
^{3}TX-Sub	-2373.122617	0.634189	-2373.744496	-2372.819062	
$^{3}TX\text{-}Int1_{ex}$	-2373.120063	0.632728	-2373.736792	-2372.81706	
$^{3}TX\text{-}Int1_{en}$	-2373.114703	0.633166	-2373.733252	-2372.811149	
$^{3}TX\text{-}Int1'_{ex}$	-2373.117771	0.632375	-2373.734573	-2372.816053	

^{3}TX-Int1'$_{en}$	-2373.101519	0.629751	-2373.723255	-2372.801044	
^{3}TX-TS1$_{ex}$	-2373.11978	0.634576	-2373.736164	-2372.814724	155.7*i*
^{3}TX-TS1$_{en}$	-2373.114432	0.634953	-2373.733128	-2372.808799	134.8*i*
^{3}TX-TS1'$_{ex}$	-2373.111734	0.633863	-2373.727058	-2372.805498	350.8*i*
^{3}TX-TS1'$_{en}$	-2373.101566	0.632144	-2373.72247	-2372.799236	176.6*i*
^{3}TX-TS1$_{ex\text{-}isomer}$	-2373.151819	0.634958	-2373.733061		184.0*i*
^{3}TX-TS1$_{ex\text{-}flip}$	-2373.117271	0.634423	-2373.73447		154.6*i*
^{3}TX-Int2$_{ex}$	-2373.152031	0.639558	-2373.764117	-2372.854207	
^{3}TX-Int2$_{en}$	-2373.147551	0.63769	-2373.761288	-2372.849407	
^{3}TX-Int2'$_{ex}$	-2373.147212	0.637399	-2373.75815	-2372.849794	
^{3}TX-Int2'$_{en}$	-2373.139938	0.635291	-2373.75576	-2372.846203	
^{BS}TX-Int2$_{ex}$	-2373.151907	0.640011	-2373.763965	-2372.85389	
^{BS}TX-Int2$_{en}$	-2373.146096	0.63937	-2373.758848	-2372.847815	
^{BS}TX-Int2'$_{ex}$	-2373.145249	0.638146	-2373.758999	-2372.849318	
^{BS}TX-Int2'$_{en}$	-2373.139898	0.63566	-2373.755752	-2372.845833	
^{BS}TX-TS2$_{ex}$	-2373.150691	0.64025	-2373.762654	-2372.851584	293.5*i*
^{BS}TX-TS2$_{en}$	-2373.146466	0.639507	-2373.760135	-2372.847738	262.4*i*
^{BS}TX-TS2'$_{en}$	-2373.138092	0.637578	-2373.753544	-2372.842273	239.5*i*
^{BS}TX-TS2'$_{ex}$	-2373.145249	0.640222	-2373.755763	-2372.846561	297.3*i*
TX-Prod$_{RSR}$	-2373.215338	0.64368	-2373.8261127	-2372.92455	
TX-Prod$_{SRS}$	-2373.215449	0.643497	-2373.828488	-2372.92566	
TX-Prod'$_{RSS}$	-2373.215866	0.646884	-2373.8244504	-2372.92608	
TX-Prod'$_{SRR}$	-2373.206808	0.64373	-2373.8196305	-2372.919583	
OX	-1377.650441	0.397385	-1378.069763		
SeX	-3701.352077	0.391251	-3704.363347		
^{3}OX-TS1$_{ex}$	-2050.155513	0.639182	-2050.763996		171.2*i*
^{3}OX-TS1$_{en}$	-2050.147386	0.63784	-2050.120413		151.4*i*
^{3}SeX-TS1$_{ex}$	-4373.857076	0.633143	-4377.058114		150.2*i*

^{3}SeX-TS1$_{en}$	-4373.853268	0.633821	-4377.056351	145.3*i*

Table S16. *Calculated DLPNO-CCSD(T) energies (in hartree).*

Stationary point	DLPNO-CCSD(T) /cc-pVDZ	DLPNO-CCSD(T) /cc-pVTZ	Final energy DLPNO-CCSD(T)
^{1}Sub	-670.6430737	-671.2988761	-671.6382112
^{3}Sub	-670.5359942	-671.1891247	-671.527001
^{3}TS1$_{A}$	-670.5354401	-671.1890656	-671.5277878
^{3}TS1$_{B}$	-670.5321456	-671.1849852	-671.5233434
^{3}TS1$_{C}$	-670.5307756	-671.1842652	-671.5230075
^{3}TS1$_{D}$	-670.5186268	-671.1717477	-671.5102611
^{3}Int1$_{A}$	-670.5778382	-671.2284018	-671.5659955
^{3}Int1$_{B}$	-670.5552232	-671.2054667	-671.5426583
^{3}Int1$_{C}$	-670.5796037	-671.2303674	-671.5680586
^{3}Int1$_{D}$	-670.5585361	-671.2084104	-671.5454518
Prod	-670.6547461	-671.30717	-671.6458
Prod’	-670.652471	-671.3043838	-671.6428259
TX	-1696.510631	-1697.824326	-1698.50518
^{1}TX-Sub	-2367.202409	-2369.174045	-2370.197444271
^{3}TX-Sub	-2367.070988	-2369.041175	-2370.095514182
^{3}TX-Int1$_{ex}$	-2367.040185	-2369.062048	-2370.095663
^{3}TX-Int1$_{en}$	-2367.088317	-2369.055898	-2370.078048
^{3}TX-Int1’$_{ex}$	-2367.048666	-2369.061078	-2370.089907
^{3}TX-Int1’$_{en}$	-2367.077945	-2369.041298	-2370.060672
^{3}TX-TS1$_{ex}$	-2367.092294	-2369.060812	-2370.083038
^{3}TX-TS1$_{en}$	-2367.086226	-2369.054602	-2370.076213
^{3}TX-TS1’$_{ex}$	-2367.085079	-2369.0537	-2370.077102
^{3}TX-TS1’$_{en}$	-2367.07697	-2369.044151	-2370.06521
^{3}TX-Int2$_{ex}$	-2367.13463	-2369.10091	-2370.12247
^{3}TX-Int2$_{en}$	-2367.128098	-2369.093355	-2370.11415
^{3}TX-Int2’$_{ex}$	-2367.132038	-2369.098066	-2370.119475

^{3}TX-Int2'$_{en}$	-2367.126581	-2369.091537	-2370.11229
TX-Prod$_{RSR}$	-2367.205726	-2369.173501	-2370.195651
TX-Prod$_{SRS}$	-2367.206184	-2369.173227	-2370.19483
TX-Prod'$_{RSS}$	-2367.20871	-2369.175516	-2370.197324
TX-Prod'$_{SRR}$	-2367.201573	-2369.166847	-2370.187515

XXVIII. Cartesian coordinates of optimized structures.

^{1}Sub E(opt)= -672.5445064 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.993489	-2.940017	0.286132
2	6	0	-2.302568	-2.899772	-0.217132
3	6	0	-2.925575	-1.683815	-0.454234
4	6	0	-2.244488	-0.482050	-0.193214
5	6	0	-0.918186	-0.500866	0.312760
6	6	0	-0.318921	-1.755793	0.544866
7	7	0	-2.855410	0.733657	-0.422755
8	6	0	-2.287489	1.989219	-0.196802
9	6	0	-0.924860	1.934436	0.323198
10	6	0	-0.258740	0.773707	0.566837
11	8	0	-2.918980	3.014558	-0.433033
12	6	0	2.187365	0.535673	-0.076512
13	6	0	3.640361	0.532169	0.430913
14	6	0	4.633570	0.318898	-0.677897
15	6	0	5.469701	-0.715205	-0.770851
16	1	0	-0.509689	-3.893293	0.472836
17	1	0	-2.835724	-3.823377	-0.421894
18	1	0	-3.940404	-1.647703	-0.841406
19	1	0	0.692128	-1.797448	0.934396
20	1	0	-3.800798	0.758693	-0.784209
21	1	0	-0.463583	2.899366	0.504404
22	1	0	1.968220	-0.424789	-0.556087
23	1	0	2.065321	1.300780	-0.853397
24	1	0	3.841854	1.493796	0.926079
25	1	0	3.761880	-0.245505	1.196141
26	1	0	4.634304	1.076540	-1.463159
27	1	0	6.158996	-0.822029	-1.603349
28	1	0	5.497824	-1.493638	-0.011262
29	6	0	1.172194	0.808988	1.051812
30	1	0	1.317364	0.080044	1.858823
31	1	0	1.378754	1.793060	1.486371

^{3}Sub E(opt)= -672.4443203 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.236945	2.946293	0.214530
2	6	0	2.559875	2.796976	-0.264757
3	6	0	3.082686	1.512260	-0.464241
4	6	0	2.319295	0.383988	-0.192589
5	6	0	0.947898	0.501313	0.316509
6	6	0	0.455507	1.849974	0.492499
7	7	0	2.836891	-0.885185	-0.393055

8	6	0	2.133576	-2.077289	-0.174336
9	6	0	0.802913	-1.945576	0.320423
10	6	0	0.203812	-0.637190	0.599536
11	8	0	2.693711	-3.160866	-0.417166
12	6	0	-2.244610	-0.437153	-0.043753
13	6	0	-3.696292	-0.403246	0.466283
14	6	0	-4.695023	-0.284866	-0.651297
15	6	0	-5.532539	0.737306	-0.828443
16	1	0	0.831624	3.943406	0.361226
17	1	0	3.166746	3.669270	-0.481706
18	1	0	4.095920	1.386694	-0.837279
19	1	0	-0.558296	1.988477	0.848793
20	1	0	3.776764	-0.998155	-0.747585
21	1	0	0.252489	-2.863597	0.485413
22	1	0	-2.029073	0.483605	-0.599065
23	1	0	-2.120258	-1.261868	-0.757759
24	1	0	-3.889006	-1.324168	1.036911
25	1	0	-3.819988	0.431478	1.168486
26	1	0	-4.697865	-1.105433	-1.370722
27	1	0	-6.224272	0.773594	-1.665029
28	1	0	-5.558697	1.576918	-0.137017
29	6	0	-1.215521	-0.595524	1.096481
30	1	0	-1.351210	0.220306	1.817493
31	1	0	-1.433936	-1.520908	1.645489

$^{3}TS1_{A}$ E(opt)= -672.4470103 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.801993	-1.867620	0.075890
2	6	0	3.502361	-0.760341	0.574911
3	6	0	2.895663	0.501694	0.580440
4	6	0	1.600093	0.670700	0.100785
5	6	0	0.848479	-0.451642	-0.405738
6	6	0	1.510714	-1.717575	-0.403297
7	7	0	1.007421	1.932192	0.112944
8	6	0	-0.236229	2.249235	-0.437469
9	6	0	-1.024206	1.113654	-0.861361
10	6	0	-0.475127	-0.259196	-0.854995
11	8	0	-0.604454	3.425263	-0.501344
12	6	0	-1.903985	-2.277396	-0.204533
13	6	0	-2.808114	-1.485743	0.762628
14	6	0	-2.357381	0.965286	1.193447
15	6	0	-2.079615	-0.351225	1.415706
16	1	0	3.271491	-2.846715	0.061967
17	1	0	4.513333	-0.872821	0.953377
18	1	0	3.436175	1.364932	0.960948
19	1	0	0.986156	-2.582683	-0.793284
20	1	0	1.551293	2.731085	0.409952
21	1	0	-1.068019	-2.710938	0.357094
22	1	0	-2.468854	-3.115091	-0.633222

23	1	0	-3.682674	-1.104545	0.219998
24	1	0	-3.242184	1.266302	0.640887
25	1	0	-1.824644	1.754559	1.711565
26	1	0	-3.184267	-2.177192	1.530358
27	6	0	-1.342974	-1.389164	-1.341492
28	1	0	-0.783060	-2.027893	-2.037650
29	1	0	-2.184914	-0.979375	-1.913051
30	1	0	-1.894593	1.343251	-1.463944
31	1	0	-1.231588	-0.614337	2.045634

$^{3}TS1_{B}$ E(opt)= -672.440988 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.562799	-2.067806	0.033379
2	6	0	3.393113	-1.022385	0.447038
3	6	0	2.909573	0.284287	0.464173
4	6	0	1.592845	0.560213	0.077705
5	6	0	0.724732	-0.491250	-0.331236
6	6	0	1.251445	-1.798226	-0.347099
7	7	0	1.126452	1.872679	0.085659
8	6	0	-0.091033	2.300197	-0.455990
9	6	0	-0.981276	1.234610	-0.847062
10	6	0	-0.663674	-0.178115	-0.661755
11	8	0	-0.337244	3.503992	-0.560960
12	6	0	-2.191930	-2.159165	-0.357349
13	6	0	-2.770186	-1.287117	0.763667
14	6	0	-2.001481	0.994900	1.594963
15	6	0	-1.709754	-0.340360	1.265343
16	1	0	2.935454	-3.087064	0.007524
17	1	0	4.417042	-1.219936	0.749519
18	1	0	3.554626	1.103891	0.770887
19	1	0	0.619599	-2.618240	-0.669800
20	1	0	1.765660	2.621507	0.316397
21	1	0	-1.442854	-2.839618	0.064104
22	1	0	-2.960576	-2.779848	-0.830734
23	1	0	-3.627528	-0.714035	0.388133
24	1	0	-2.939598	1.453137	1.300687
25	1	0	-1.289814	1.614083	2.127903
26	1	0	-3.139038	-1.911394	1.589370
27	6	0	-1.530792	-1.204620	-1.371342
28	1	0	-0.947421	-1.762595	-2.113991
29	1	0	-2.319859	-0.680906	-1.923137
30	1	0	-1.920323	1.534790	-1.294965
31	1	0	-0.858862	-0.805437	1.759554

$^{3}TS1_{C}$ E(opt)= -672.4402159 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	3.144317	-1.575206	0.147180
2	6	0	3.685869	-0.330752	0.505544
3	6	0	2.888974	0.820805	0.425880
4	6	0	1.571908	0.745529	-0.007268
5	6	0	0.986586	-0.520629	-0.398071
6	6	0	1.835735	-1.670650	-0.291268
7	7	0	0.773488	1.891934	-0.025785
8	6	0	-0.503955	1.981287	-0.572055
9	6	0	-1.099517	0.713889	-0.939904
10	6	0	-0.348058	-0.557078	-0.822648
11	8	0	-1.066283	3.074157	-0.674747
12	6	0	-2.135554	-2.111608	0.088724
13	6	0	-3.118905	-0.966116	0.388776
14	6	0	-2.500847	0.300468	0.950847
15	6	0	-1.576066	0.313131	1.952972
16	1	0	3.755777	-2.470579	0.211157
17	1	0	4.713172	-0.253259	0.846304
18	1	0	3.296552	1.786060	0.716768
19	1	0	1.438222	-2.640782	-0.567767
20	1	0	1.182827	2.779562	0.234003
21	1	0	-1.953094	0.776261	-1.606573
22	1	0	-2.711244	-3.008515	-0.169847
23	1	0	-1.559277	-2.360873	0.987105
24	1	0	-3.672550	-0.720930	-0.525716
25	1	0	-3.871888	-1.322714	1.106397
26	1	0	-3.004067	1.234253	0.710946
27	1	0	-1.232537	1.249317	2.379665
28	1	0	-1.093761	-0.592051	2.306490
29	6	0	-1.151037	-1.800902	-1.067512
30	1	0	-0.511235	-2.672779	-1.227846
31	1	0	-1.737745	-1.672771	-1.989796

$^{3}TS1_{D}$ E(opt)= -672.4272944 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.722860	-2.077595	0.021421
2	6	0	3.568361	-1.014292	0.347622
3	6	0	3.068988	0.291473	0.361737
4	6	0	1.733043	0.543584	0.050760
5	6	0	0.854737	-0.525154	-0.308606
6	6	0	1.390249	-1.833182	-0.297245
7	7	0	1.231984	1.847675	0.116885
8	6	0	-0.013654	2.263577	-0.360403
9	6	0	-0.890665	1.193569	-0.759685
10	6	0	-0.535698	-0.226494	-0.559872
11	8	0	-0.297009	3.464744	-0.411982
12	6	0	-2.620625	-1.795245	-0.316597
13	6	0	-3.448217	-0.713990	0.402123
14	6	0	-2.592721	0.200838	1.236790

15	6	0	-1.300234	-0.160060	1.568435
16	1	0	3.101061	-3.095382	0.015800
17	1	0	4.610255	-1.193805	0.593961
18	1	0	3.719653	1.123048	0.621237
19	1	0	0.742797	-2.669635	-0.539655
20	1	0	1.863792	2.603495	0.345552
21	1	0	-1.831299	1.473656	-1.216215
22	1	0	-3.283927	-2.399420	-0.945578
23	1	0	-2.193870	-2.485925	0.419955
24	1	0	-3.992322	-0.113698	-0.341435
25	1	0	-4.229501	-1.192582	1.014663
26	1	0	-2.931972	1.217425	1.413343
27	1	0	-0.638091	0.552176	2.050679
28	1	0	-1.001395	-1.198085	1.662135
29	6	0	-1.486745	-1.226591	-1.207208
30	1	0	-0.925474	-2.067788	-1.625460
31	1	0	-1.955601	-0.727785	-2.066938

$^{3}Int1_{A}$ E(opt)= -672.4782395 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.902745	-1.937322	0.210282
2	6	0	3.656107	-0.792407	0.506721
3	6	0	3.064917	0.469925	0.418456
4	6	0	1.730051	0.598500	0.041775
5	6	0	0.929190	-0.553156	-0.256867
6	6	0	1.573770	-1.819364	-0.165634
7	7	0	1.165317	1.868976	-0.108878
8	6	0	-0.149069	2.141972	-0.416179
9	6	0	-1.089993	0.946029	-0.353223
10	6	0	-0.422348	-0.372458	-0.639168
11	8	0	-0.530842	3.280848	-0.641177
12	6	0	-2.305607	-2.067792	-0.227922
13	6	0	-3.318322	-1.035380	0.331705
14	6	0	-1.739474	0.975637	1.069551
15	6	0	-2.758612	-0.084368	1.343816
16	1	0	3.357869	-2.920591	0.281224
17	1	0	4.696600	-0.879940	0.803006
18	1	0	3.645718	1.363324	0.634615
19	1	0	0.997616	-2.714965	-0.371773
20	1	0	1.770217	2.680343	-0.080914
21	1	0	-1.778478	-2.545969	0.606190
22	1	0	-2.859757	-2.855471	-0.754647
23	1	0	-3.745994	-0.488108	-0.525974
24	1	0	-2.174048	1.979940	1.206000
25	1	0	-0.927996	0.904743	1.811266
26	1	0	-4.151990	-1.581179	0.786723
27	6	0	-1.278852	-1.463583	-1.212606
28	1	0	-0.658963	-2.266555	-1.623787
29	1	0	-1.839181	-1.045553	-2.062851

30	1	0	-1.880141	1.143028	-1.086150
31	1	0	-3.128979	-0.140052	2.364391

$^{3}Int1_{B}$ E(opt)= -672.452728 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.343218	-2.280247	0.054676
2	6	0	3.338669	-1.312804	0.212192
3	6	0	3.007494	0.037067	0.176386
4	6	0	1.675593	0.437736	-0.015560
5	6	0	0.658924	-0.524767	-0.175823
6	6	0	1.022999	-1.875956	-0.134039
7	7	0	1.365724	1.798052	-0.050065
8	6	0	0.120321	2.331195	-0.360083
9	6	0	-0.926878	1.357525	-0.566654
10	6	0	-0.795281	-0.108084	-0.323485
11	8	0	-0.044399	3.550831	-0.448437
12	6	0	-2.735874	-1.659318	-0.727309
13	6	0	-3.014787	-0.827026	0.528625
14	6	0	-1.536320	0.549289	2.105098
15	6	0	-1.611448	-0.479287	1.042822
16	1	0	2.591757	-3.336472	0.079995
17	1	0	4.373173	-1.607668	0.360888
18	1	0	3.777877	0.795074	0.294037
19	1	0	0.248474	-2.630115	-0.247882
20	1	0	2.104108	2.479369	0.062703
21	1	0	-2.407589	-2.663811	-0.431262
22	1	0	-3.611386	-1.783011	-1.371803
23	1	0	-3.558673	0.092018	0.272227
24	1	0	-2.248956	1.367520	2.132452
25	1	0	-0.665678	0.617032	2.748452
26	1	0	-3.605758	-1.356864	1.282338
27	6	0	-1.588006	-0.906573	-1.431148
28	1	0	-0.922849	-1.570430	-1.987935
29	1	0	-1.994979	-0.195284	-2.156581
30	1	0	-1.899200	1.770333	-0.812461
31	1	0	-1.136949	-1.403198	1.398588

$^{3}Int1_{C}$ E(opt)= -672.4773833 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.254016	-1.506819	0.187399
2	6	0	3.780366	-0.226625	0.413730
3	6	0	2.950817	0.891495	0.299078
4	6	0	1.608101	0.743985	-0.037180
5	6	0	1.035509	-0.551975	-0.273566
6	6	0	1.919385	-1.664478	-0.147661
7	7	0	0.796597	1.876141	-0.157427

8	6	0	-0.542057	1.902144	-0.469083
9	6	0	-1.222809	0.555158	-0.632115
10	6	0	-0.328799	-0.653401	-0.615383
11	8	0	-1.149228	2.958575	-0.579947
12	6	0	-2.221586	-2.117159	0.151106
13	6	0	-3.143652	-0.889139	0.167874
14	6	0	-2.361731	0.410006	0.446587
15	6	0	-1.825575	0.463019	1.839338
16	1	0	3.893282	-2.380123	0.275628
17	1	0	4.825474	-0.098357	0.676657
18	1	0	3.349214	1.888443	0.471763
19	1	0	1.532395	-2.662975	-0.315892
20	1	0	1.215742	2.790738	-0.041132
21	1	0	-1.745394	0.611738	-1.600181
22	1	0	-2.793431	-3.019883	-0.093212
23	1	0	-1.792068	-2.264483	1.149493
24	1	0	-3.649926	-0.799868	-0.802783
25	1	0	-3.928757	-1.013617	0.923380
26	1	0	-3.028070	1.273702	0.281759
27	1	0	-1.008951	1.127101	2.101489
28	1	0	-2.335987	-0.052736	2.646240
29	6	0	-1.068250	-1.937745	-0.865329
30	1	0	-0.411934	-2.810547	-0.844254
31	1	0	-1.506357	-1.901512	-1.876171

$^{3}Int1_{D}$ E(opt)= -672.4578335 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.167629	-2.492144	0.053349
2	6	0	3.290649	-1.666346	0.140649
3	6	0	3.139457	-0.284099	0.130641
4	6	0	1.861975	0.291064	0.037824
5	6	0	0.718576	-0.526995	-0.049215
6	6	0	0.902333	-1.914475	-0.039091
7	7	0	1.735013	1.681281	0.026016
8	6	0	0.549614	2.380562	-0.166847
9	6	0	-0.634355	1.561799	-0.284172
10	6	0	-0.682907	0.074688	-0.103131
11	8	0	0.543322	3.613443	-0.228682
12	6	0	-2.745946	-1.386092	-0.794945
13	6	0	-3.659623	-0.558416	0.123499
14	6	0	-2.865397	0.075646	1.222613
15	6	0	-1.400135	-0.193658	1.288295
16	1	0	2.275291	-3.572157	0.057266
17	1	0	4.285136	-2.096541	0.213002
18	1	0	4.010086	0.364110	0.191895
19	1	0	0.029248	-2.557933	-0.107182
20	1	0	2.564308	2.256882	0.081138
21	1	0	-1.565910	2.100379	-0.419671
22	1	0	-3.305430	-1.749353	-1.663958

23	1	0	-2.395814	-2.277113	-0.258638
24	1	0	-4.172793	0.214037	-0.475185
25	1	0	-4.468402	-1.187569	0.529772
26	1	0	-3.356732	0.682503	1.976258
27	1	0	-0.906694	0.403093	2.060862
28	1	0	-1.206218	-1.248032	1.547717
29	6	0	-1.549642	-0.549860	-1.271498
30	1	0	-0.898155	-1.144453	-1.917566
31	1	0	-1.932955	0.265591	-1.896191

$^{BS}TS2_A$ E(opt)= -672.4757377 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.244257	-1.582349	0.135328
2	6	0	3.829799	-0.315906	0.247979
3	6	0	3.031351	0.825566	0.156730
4	6	0	1.656931	0.712200	-0.044378
5	6	0	1.029160	-0.566657	-0.164163
6	6	0	1.876216	-1.701116	-0.067318
7	7	0	0.875324	1.870592	-0.122876
8	6	0	-0.477762	1.942719	-0.357048
9	6	0	-1.200896	0.623112	-0.576706
10	6	0	-0.384306	-0.634264	-0.345678
11	8	0	-1.057728	3.018657	-0.391332
12	6	0	-2.489184	-2.021759	-0.020576
13	6	0	-3.268194	-0.698338	-0.022575
14	6	0	-2.375793	0.479766	0.415148
15	6	0	-1.690802	0.182846	1.722171
16	1	0	3.858183	-2.475093	0.205368
17	1	0	4.899018	-0.214330	0.404935
18	1	0	3.477217	1.813707	0.240845
19	1	0	1.441113	-2.690534	-0.149641
20	1	0	1.325907	2.769754	-0.004933
21	1	0	-1.576789	0.671989	-1.613510
22	1	0	-3.078676	-2.814553	-0.495128
23	1	0	-2.308200	-2.331814	1.014420
24	1	0	-3.664369	-0.490044	-1.025359
25	1	0	-4.131588	-0.774255	0.649686
26	1	0	-2.975816	1.402673	0.441488
27	1	0	-0.861051	0.802473	2.046237
28	1	0	-2.196506	-0.386647	2.497571
29	6	0	-1.122662	-1.892071	-0.724019
30	1	0	-0.531835	-2.791473	-0.535862
31	1	0	-1.290732	-1.857759	-1.814701

$^{BS}TS2_C$ E(opt)= -672.4750529 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	3.244257	-1.582349	0.135328
2	6	0	3.829799	-0.315906	0.247979
3	6	0	3.031351	0.825566	0.156730
4	6	0	1.656931	0.712200	-0.044378
5	6	0	1.029160	-0.566657	-0.164163
6	6	0	1.876216	-1.701116	-0.067318
7	7	0	0.875324	1.870592	-0.122876
8	6	0	-0.477762	1.942719	-0.357048
9	6	0	-1.200896	0.623112	-0.576706
10	6	0	-0.384306	-0.634264	-0.345678
11	8	0	-1.057728	3.018657	-0.391332
12	6	0	-2.489184	-2.021759	-0.020576
13	6	0	-3.268194	-0.698338	-0.022575
14	6	0	-2.375793	0.479766	0.415148
15	6	0	-1.690802	0.182846	1.722171
16	1	0	3.858183	-2.475093	0.205368
17	1	0	4.899018	-0.214330	0.404935
18	1	0	3.477217	1.813707	0.240845
19	1	0	1.441113	-2.690534	-0.149641
20	1	0	1.325907	2.769754	-0.004933
21	1	0	-1.576789	0.671989	-1.613510
22	1	0	-3.078676	-2.814553	-0.495128
23	1	0	-2.308200	-2.331814	1.014420
24	1	0	-3.664369	-0.490044	-1.025359
25	1	0	-4.131588	-0.774255	0.649686
26	1	0	-2.975816	1.402673	0.441488
27	1	0	-0.861051	0.802473	2.046237
28	1	0	-2.196506	-0.386647	2.497571
29	6	0	-1.122662	-1.892071	-0.724019
30	1	0	-0.531835	-2.791473	-0.535862
31	1	0	-1.290732	-1.857759	-1.814701

Prod E(opt)= -672.547374 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.739183	-1.995003	0.162377
2	6	0	3.579579	-0.880154	0.161036
3	6	0	3.038319	0.396811	0.045654
4	6	0	1.652716	0.571142	-0.077697
5	6	0	0.792148	-0.542161	-0.100846
6	6	0	1.362865	-1.813334	0.033528
7	7	0	1.138807	1.875492	-0.167818
8	6	0	-0.185443	2.246909	-0.205182
9	6	0	-1.193055	1.122203	-0.198602
10	6	0	-0.700316	-0.361884	-0.215731
11	8	0	-0.514207	3.424825	-0.231760
12	6	0	-2.833347	-1.382019	-0.831753
13	6	0	-2.673731	-1.587499	0.687942
14	6	0	-1.914589	0.878759	1.161181

15	6	0	-1.545900	-0.629059	1.097552
16	1	0	3.150118	-2.994629	0.263440
17	1	0	4.654582	-1.000876	0.255887
18	1	0	3.686686	1.269611	0.055129
19	1	0	0.708511	-2.680854	0.043360
20	1	0	1.788078	2.651849	-0.152897
21	1	0	-1.895973	1.345346	-1.006241
22	1	0	-3.422373	-0.478253	-1.030672
23	1	0	-3.346517	-2.212366	-1.326205
24	1	0	-2.363117	-2.621204	0.886284
25	1	0	-1.450519	1.409829	1.996496
26	1	0	-0.976551	-0.989041	1.958149
27	1	0	-2.984255	1.107509	1.161627
28	1	0	-3.599809	-1.412075	1.246567
29	6	0	-1.384657	-1.197352	-1.321594
30	1	0	-1.311070	-0.710866	-2.300302
31	1	0	-0.898412	-2.175194	-1.409009

Prod’ E(opt)= -672.5419957 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.184734	-1.633848	0.056450
2	6	0	3.809635	-0.387415	0.034718
3	6	0	3.041725	0.774042	-0.012427
4	6	0	1.644495	0.694187	-0.034523
5	6	0	0.994045	-0.557847	-0.013821
6	6	0	1.790351	-1.705521	0.030401
7	7	0	0.894127	1.882942	-0.060322
8	6	0	-0.464240	2.009660	-0.251633
9	6	0	-1.218814	0.719558	-0.493033
10	6	0	-0.513440	-0.575596	0.014949
11	8	0	-1.007012	3.105400	-0.246933
12	6	0	-2.683116	-1.891118	-0.314980
13	6	0	-3.346960	-0.526429	-0.010255
14	6	0	-2.316437	0.452075	0.572441
15	6	0	-1.224842	-0.301041	1.389798
16	1	0	3.774585	-2.544376	0.094333
17	1	0	4.892971	-0.314181	0.051806
18	1	0	3.522232	1.749111	-0.035618
19	1	0	1.313820	-2.679981	0.054928
20	1	0	1.383730	2.763472	0.039007
21	1	0	-1.549632	0.727739	-1.539812
22	1	0	-3.230621	-2.425715	-1.097776
23	1	0	-2.758829	-2.515643	0.581492
24	1	0	-3.778260	-0.084307	-0.916997
25	1	0	-4.176080	-0.672594	0.691926
26	1	0	-2.779556	1.336466	1.016079
27	1	0	-0.635308	0.385127	2.004227
28	1	0	-1.513492	-1.161779	2.000127
29	6	0	-1.184753	-1.774736	-0.692072

30	1	0	-0.689502	-2.714345	-0.428195
31	1	0	-1.053159	-1.648615	-1.773891

TX E(opt)= -1700.615256 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.297218	-1.228801	-0.551765
2	6	0	-5.148696	-0.032485	-1.012020
3	6	0	-4.405125	1.289002	-0.764270
4	6	0	-4.107475	1.427699	0.750596
5	6	0	-3.380685	0.238697	1.423155
6	6	0	-4.020064	-1.099107	0.970161
7	6	0	-3.133590	1.281179	-1.641987
8	6	0	-5.266454	2.488730	-1.191306
9	6	0	-5.016119	-2.555911	-0.823980
10	6	0	-3.504229	0.361599	2.964139
11	6	0	-2.947067	-1.238313	-1.289236
12	7	0	-2.464386	-0.018275	-1.674486
13	8	0	-2.300261	-2.265210	-1.464958
14	6	0	-1.904306	0.299629	1.123208
15	7	0	-1.176967	1.346190	0.896173
16	6	0	0.116718	0.846433	0.718266
17	6	0	0.079542	-0.551085	0.876936
18	8	0	-1.210513	-0.897745	1.161340
19	6	0	1.316368	1.467387	0.417579
20	6	0	2.473594	0.675429	0.276569
21	6	0	2.394864	-0.733341	0.441565
22	6	0	1.178393	-1.372052	0.747511
23	6	0	3.730569	1.404065	-0.050654
24	6	0	5.004358	0.653577	-0.214800
25	6	0	5.123520	-0.743167	-0.090207
26	6	0	6.159705	1.402474	-0.515595
27	6	0	7.390927	0.791977	-0.687351
28	6	0	7.495309	-0.601111	-0.560661
29	6	0	6.374326	-1.363279	-0.265184
30	8	0	3.716043	2.628045	-0.185415
31	1	0	-6.103822	-0.034808	-0.469850
32	1	0	-5.388707	-0.132361	-2.078896
33	1	0	-3.546045	2.348094	0.938595
34	1	0	-5.075128	1.533499	1.257775
35	1	0	-2.424220	2.029059	-1.272430
36	1	0	-3.415375	1.561276	-2.667019
37	1	0	-6.176760	2.548511	-0.585723
38	1	0	-4.719705	3.430633	-1.068820
39	1	0	-5.567074	2.404997	-2.241190
40	1	0	-5.251253	-2.658854	-1.888079
41	1	0	-4.381591	-3.398045	-0.541520
42	1	0	-5.953668	-2.603207	-0.259598
43	1	0	-2.982048	-0.461385	3.462147
44	1	0	-3.071540	1.304842	3.310091

45	1	0	-4.557265	0.330408	3.261987
46	1	0	-1.559000	-0.067868	-2.124684
47	1	0	1.400611	2.539176	0.284798
48	1	0	1.103399	-2.447475	0.862681
49	1	0	6.041309	2.476565	-0.606471
50	1	0	8.268851	1.387049	-0.918439
51	1	0	8.455122	-1.091876	-0.693198
52	1	0	6.459168	-2.442036	-0.168010
53	1	0	-4.987221	-1.182675	1.481886
54	1	0	-3.407282	-1.941469	1.302643
55	16	0	3.777722	-1.818970	0.279860

[1]TX-Sub E(opt)= -2373.220451 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.375836	0.929906	0.469777
2	6	0	-6.184060	-0.104748	1.270370
3	6	0	-5.486819	-1.472871	1.233904
4	6	0	-5.354200	-1.933802	-0.239792
5	6	0	-4.740271	-0.933126	-1.251067
6	6	0	-5.314610	0.487845	-1.017114
7	6	0	-4.132148	-1.313389	1.949526
8	6	0	-6.308163	-2.526949	1.993287
9	6	0	-6.016198	2.320947	0.560934
10	6	0	-5.095719	-1.392321	-2.690015
11	6	0	-3.932710	1.002259	0.989717
12	7	0	-3.423743	-0.087248	1.596456
13	8	0	-3.246092	2.018397	0.781648
14	6	0	-3.230326	-0.896015	-1.205372
15	8	0	-0.654784	-0.138935	2.180225
16	6	0	0.063239	0.722129	1.629492
17	7	0	-0.490679	1.766411	0.935169
18	6	0	1.515972	0.697658	1.669798
19	6	0	2.289028	1.615132	1.021988
20	6	0	1.644353	2.660938	0.244893
21	6	0	0.228556	2.700645	0.224447
22	6	0	2.342122	3.626550	-0.511149
23	6	0	1.666496	4.583621	-1.249654
24	6	0	0.260506	4.602446	-1.258105
25	6	0	-0.459186	3.671132	-0.529017
26	6	0	4.429012	0.416568	1.849796
27	6	0	5.965756	0.430621	1.760262
28	6	0	6.587139	-0.764261	2.427297
29	6	0	7.431218	-0.723102	3.458350
30	7	0	-2.456493	-0.010546	-1.742722
31	6	0	-1.159696	-0.478847	-1.514965
32	6	0	-1.243981	-1.691612	-0.809395
33	8	0	-2.569900	-1.974358	-0.629122
34	6	0	0.083176	0.029528	-1.854511
35	6	0	1.232950	-0.686903	-1.468841

36	6	0	1.105265	-1.896681	-0.734893
37	6	0	-0.152341	-2.421843	-0.393955
38	6	0	2.540622	-0.099439	-1.862141
39	6	0	3.804849	-0.832979	-1.573889
40	6	0	3.877308	-2.028740	-0.836635
41	6	0	5.000953	-0.274854	-2.067706
42	6	0	6.228703	-0.872732	-1.833384
43	6	0	6.287927	-2.059271	-1.086782
44	6	0	5.125273	-2.633778	-0.593947
45	8	0	2.587478	0.988711	-2.436525
46	1	0	-7.195717	-0.181186	0.849905
47	1	0	-6.295821	0.228382	2.310640
48	1	0	-4.814159	-2.885214	-0.284952
49	1	0	-6.371694	-2.139173	-0.595406
50	1	0	-3.478758	-2.160704	1.718754
51	1	0	-4.302670	-1.320534	3.035248
52	1	0	-7.283468	-2.677390	1.518539
53	1	0	-5.791051	-3.493268	2.011475
54	1	0	-6.483577	-2.218176	3.029310
55	1	0	-6.086907	2.649313	1.602887
56	1	0	-5.416813	3.054448	0.018770
57	1	0	-7.027002	2.299231	0.139694
58	1	0	-4.674594	-0.701330	-3.424894
59	1	0	-4.696852	-2.392583	-2.888864
60	1	0	-6.182532	-1.425006	-2.818516
61	1	0	-2.427974	-0.044350	1.873713
62	1	0	-1.524020	1.835576	0.915076
63	1	0	1.940395	-0.117379	2.241379
64	1	0	3.425578	3.611066	-0.528094
65	1	0	2.223123	5.312029	-1.830839
66	1	0	-0.267904	5.348333	-1.844809
67	1	0	-1.545013	3.657820	-0.530381
68	1	0	4.126743	0.467312	2.902558
69	1	0	4.059958	-0.539694	1.462642
70	1	0	6.248326	0.436045	0.698400
71	1	0	6.358709	1.355748	2.201166
72	1	0	6.292087	-1.730470	2.015730
73	1	0	7.840451	-1.626575	3.901516
74	1	0	7.746026	0.221056	3.897823
75	1	0	0.203495	0.963843	-2.388696
76	1	0	-0.258635	-3.340586	0.171446
77	1	0	4.917327	0.646043	-2.634448
78	1	0	7.138240	-0.425997	-2.222265
79	1	0	7.244178	-2.534592	-0.890087
80	1	0	5.173914	-3.555023	-0.020110
81	1	0	-6.341720	0.501026	-1.403484
82	1	0	-4.734378	1.213268	-1.593810
83	6	0	3.800873	1.566052	1.059144
84	1	0	4.168071	2.523134	1.455985
85	1	0	4.160576	1.521218	0.023294
86	16	0	2.477916	-2.832549	-0.135772

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^{3}TX-Sub E(opt)= -2373.122617 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.404752	0.896229	0.455058
2	6	0	-6.222258	-0.169910	1.203166
3	6	0	-5.500080	-1.525111	1.163844
4	6	0	-5.309584	-1.952241	-0.313008
5	6	0	-4.667965	-0.921151	-1.274517
6	6	0	-5.272467	0.486561	-1.036799
7	6	0	-4.171824	-1.357755	1.925422
8	6	0	-6.327559	-2.607999	1.874051
9	6	0	-6.075781	2.272403	0.547291
10	6	0	-4.954809	-1.352555	-2.739045
11	6	0	-3.983569	0.983398	1.027260
12	7	0	-3.470060	-0.116586	1.612567
13	8	0	-3.311645	2.017839	0.870393
14	6	0	-3.162603	-0.874612	-1.172250
15	8	0	-0.712627	-0.157229	2.216215
16	6	0	0.002735	0.704288	1.659899
17	7	0	-0.558844	1.762490	0.993090
18	6	0	1.453660	0.671424	1.673142
19	6	0	2.221831	1.585972	1.008213
20	6	0	1.566822	2.613595	0.222142
21	6	0	0.149638	2.673209	0.244026
22	6	0	2.254629	3.550141	-0.582454
23	6	0	1.569032	4.501567	-1.317418
24	6	0	0.164053	4.543486	-1.277154
25	6	0	-0.546805	3.639002	-0.505524
26	6	0	4.378757	0.422681	1.842635
27	6	0	5.916194	0.491549	1.794420
28	6	0	6.561546	-0.703592	2.437476
29	6	0	7.355008	-0.671142	3.508373
30	7	0	-2.377127	0.033637	-1.673473
31	6	0	-1.088506	-0.437188	-1.452710
32	6	0	-1.183989	-1.678514	-0.782107
33	8	0	-2.517594	-1.963627	-0.622953
34	6	0	0.151807	0.095427	-1.788639
35	6	0	1.315763	-0.625704	-1.445639
36	6	0	1.160700	-1.883110	-0.741316
37	6	0	-0.093125	-2.424067	-0.403433
38	6	0	2.611541	-0.070081	-1.799526
39	6	0	3.850141	-0.762893	-1.540256
40	6	0	3.949568	-2.022683	-0.870393
41	6	0	5.076751	-0.181472	-1.959777
42	6	0	6.292107	-0.802911	-1.724093
43	6	0	6.361947	-2.042825	-1.059828
44	6	0	5.181112	-2.646805	-0.635305
45	8	0	2.650878	1.092118	-2.371674
46	1	0	-7.216500	-0.254879	0.744590
47	1	0	-6.377744	0.139107	2.245211
48	1	0	-4.758130	-2.896936	-0.359893

49	1	0	-6.310679	-2.158770	-0.711692
50	1	0	-3.498511	-2.191735	1.703471
51	1	0	-4.376768	-1.383931	3.004898
52	1	0	-7.283858	-2.764759	1.364045
53	1	0	-5.794749	-3.565757	1.890276
54	1	0	-6.542483	-2.323430	2.909528
55	1	0	-6.192912	2.578688	1.591714
56	1	0	-5.471130	3.028083	0.042785
57	1	0	-7.069011	2.239305	0.086926
58	1	0	-4.514205	-0.639132	-3.440116
59	1	0	-4.534270	-2.342793	-2.942629
60	1	0	-6.034989	-1.396394	-2.911480
61	1	0	-2.481102	-0.066397	1.913677
62	1	0	-1.591049	1.840693	0.997517
63	1	0	1.886608	-0.136116	2.249088
64	1	0	3.335180	3.511539	-0.639443
65	1	0	2.116047	5.204652	-1.937249
66	1	0	-0.372268	5.284859	-1.862484
67	1	0	-1.632130	3.641335	-0.474729
68	1	0	4.050016	0.444136	2.888537
69	1	0	4.053504	-0.538318	1.428847
70	1	0	6.224234	0.542192	0.741420
71	1	0	6.263239	1.414321	2.276927
72	1	0	6.331842	-1.661240	1.968676
73	1	0	7.786115	-1.574333	3.931028
74	1	0	7.605682	0.265522	4.001969
75	1	0	0.257245	1.045454	-2.294561
76	1	0	-0.189429	-3.364701	0.126876
77	1	0	5.016972	0.770973	-2.472737
78	1	0	7.208452	-0.321745	-2.055024
79	1	0	7.317460	-2.521353	-0.876031
80	1	0	5.210987	-3.603600	-0.120347
81	1	0	-6.281576	0.492077	-1.467830
82	1	0	-4.679446	1.232695	-1.572728
83	6	0	3.732797	1.562336	1.052941
84	1	0	4.074832	2.525155	1.459316
85	1	0	4.100080	1.531024	0.020282
86	16	0	2.528737	-2.848049	-0.251173

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^{3}TX-Int1$_{ex}$ E(opt)= -2373.120063 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.961620	0.583916	1.219136
2	6	0	5.995970	1.066550	0.189092
3	6	0	5.572583	0.637960	-1.223715
4	6	0	5.425190	-0.907467	-1.280203
5	6	0	4.641935	-1.614938	-0.145629
6	6	0	4.963219	-0.964138	1.228358
7	6	0	4.270612	1.394093	-1.550789
8	6	0	6.632299	1.046045	-2.260767

9	6	0	5.290556	1.104836	2.625203
10	6	0	5.056202	-3.109488	-0.103366
11	6	0	3.550231	1.059032	0.832923
12	7	0	3.355846	1.501837	-0.418721
13	8	0	2.622086	1.002492	1.664321
14	6	0	3.154906	-1.603662	-0.394154
15	7	0	2.476641	-1.235389	-1.430938
16	6	0	1.138357	-1.474869	-1.090553
17	6	0	1.105767	-2.029632	0.200925
18	8	0	2.391232	-2.118036	0.647080
19	6	0	-0.051892	-1.232955	-1.756649
20	6	0	-1.264631	-1.582320	-1.124673
21	6	0	-1.248805	-2.186581	0.161410
22	6	0	-0.046761	-2.404484	0.855613
23	6	0	-2.513586	-1.224031	-1.843178
24	6	0	-3.832345	-1.615144	-1.286754
25	6	0	-4.013468	-2.228917	-0.032256
26	6	0	-4.975679	-1.305148	-2.051817
27	6	0	-6.252352	-1.579644	-1.589233
28	6	0	-6.419019	-2.171472	-0.328173
29	6	0	-5.310841	-2.492582	0.443821
30	8	0	-2.457066	-0.579582	-2.897460
31	1	0	6.980623	0.650011	0.440229
32	1	0	6.091419	2.159370	0.230243
33	1	0	5.004361	-1.201808	-2.247295
34	1	0	6.442877	-1.315832	-1.242349
35	1	0	3.735146	0.894690	-2.364645
36	1	0	4.523004	2.408319	-1.888279
37	1	0	7.582341	0.535034	-2.071776
38	1	0	6.309153	0.789958	-3.276307
39	1	0	6.819148	2.124692	-2.227867
40	1	0	5.334934	2.198895	2.634222
41	1	0	4.522380	0.792476	3.335429
42	1	0	6.262798	0.721733	2.953753
43	1	0	4.505515	-3.644493	0.674998
44	1	0	4.854186	-3.593821	-1.064059
45	1	0	6.126728	-3.196056	0.107602
46	1	0	2.384803	1.732576	-0.670595
47	1	0	-0.087651	-0.758782	-2.728986
48	1	0	-0.027515	-2.823934	1.854672
49	1	0	-4.810181	-0.831450	-3.013001
50	1	0	-7.118102	-1.333376	-2.196220
51	1	0	-7.414805	-2.382424	0.050687
52	1	0	-5.441106	-2.952178	1.419641
53	1	0	5.966873	-1.290836	1.528525
54	1	0	4.262982	-1.329612	1.983877
55	16	0	-2.692674	-2.709408	1.022346
56	6	0	-3.139862	0.147872	3.347023
57	6	0	-1.793982	0.048634	3.738560
58	6	0	-0.774107	0.423641	2.853851
59	6	0	-1.082714	0.895803	1.581679
60	6	0	-2.458941	0.991203	1.140835
61	6	0	-3.467352	0.603022	2.083609

62	7	0	-0.055734	1.295673	0.734482
63	6	0	-0.246319	1.694214	-0.572931
64	6	0	-1.603425	1.770107	-1.035792
65	6	0	-2.742335	1.460577	-0.150527
66	8	0	0.727203	1.978064	-1.303599
67	6	0	-4.805564	2.982015	-0.087635
68	6	0	-4.085361	4.286812	-0.476985
69	6	0	-1.578882	4.531113	-0.624320
70	6	0	-2.702698	4.385685	0.097867
71	1	0	-3.927224	-0.146794	4.034542
72	1	0	-1.537782	-0.315766	4.728508
73	1	0	0.270495	0.358367	3.144596
74	1	0	-4.507326	0.646420	1.781563
75	1	0	0.916537	1.231943	1.074017
76	1	0	-4.848013	2.906878	1.006244
77	1	0	-5.843639	3.024268	-0.441042
78	1	0	-4.043089	4.377223	-1.569957
79	1	0	-1.606509	4.624963	-1.706356
80	1	0	-0.599889	4.580185	-0.159361
81	1	0	-4.688327	5.131385	-0.112093
82	6	0	-4.137706	1.705075	-0.651787
83	1	0	-4.779567	0.851654	-0.406251
84	1	0	-4.119032	1.757155	-1.746593
85	1	0	-1.755087	1.930167	-2.094131
86	1	0	-2.628508	4.296605	1.181648

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^{3}TX-Int1$_{en}$ E(opt)= -2373.110031 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.049292	1.043268	-0.487886
2	6	0	-5.978995	0.622721	0.663675
3	6	0	-5.419289	-0.616055	1.377855
4	6	0	-5.298330	-1.779101	0.360414
5	6	0	-4.539762	-1.478082	-0.954302
6	6	0	-4.975615	-0.106171	-1.524094
7	6	0	-4.070368	-0.214826	2.013381
8	6	0	-6.359447	-1.069665	2.506572
9	6	0	-5.565751	2.314444	-1.175867
10	6	0	-4.862717	-2.582177	-1.996193
11	6	0	-3.636396	1.313009	0.052367
12	7	0	-3.269911	0.687334	1.188488
13	8	0	-2.855647	2.057020	-0.566650
14	6	0	-3.049160	-1.561430	-0.739083
15	7	0	-2.398881	-2.334420	0.070391
16	6	0	-1.050886	-2.114566	-0.233804
17	6	0	-0.978607	-1.163271	-1.267994
18	8	0	-2.257892	-0.822206	-1.603331
19	6	0	0.117197	-2.664194	0.266652
20	6	0	1.350315	-2.233879	-0.264726
21	6	0	1.380038	-1.236790	-1.276062

22	6	0	0.196961	-0.693686	-1.808391
23	6	0	2.569654	-2.880465	0.293716
24	6	0	3.917748	-2.399436	-0.118141
25	6	0	4.141308	-1.383697	-1.067046
26	6	0	5.030277	-2.974272	0.526848
27	6	0	6.321580	-2.553865	0.251175
28	6	0	6.530755	-1.535563	-0.691340
29	6	0	5.453339	-0.955972	-1.345672
30	8	0	2.466441	-3.796773	1.108296
31	1	0	-6.980357	0.411513	0.265443
32	1	0	-6.087076	1.449149	1.378193
33	1	0	-4.849276	-2.652818	0.843145
34	1	0	-6.319869	-2.061545	0.075182
35	1	0	-3.474712	-1.110935	2.220980
36	1	0	-4.263064	0.283248	2.972912
37	1	0	-7.328780	-1.382870	2.104565
38	1	0	-5.934588	-1.917105	3.056552
39	1	0	-6.537921	-0.258157	3.220088
40	1	0	-5.650271	3.137599	-0.459410
41	1	0	-4.880526	2.628625	-1.965271
42	1	0	-6.555832	2.133194	-1.607828
43	1	0	-4.321937	-2.403942	-2.931013
44	1	0	-4.576377	-3.565866	-1.613318
45	1	0	-5.935185	-2.590279	-2.215982
46	1	0	-2.375927	0.994773	1.594863
47	1	0	0.121254	-3.419221	1.043336
48	1	0	0.212772	0.073680	-2.572249
49	1	0	4.829367	-3.751672	1.255736
50	1	0	7.165053	-3.006702	0.762791
51	1	0	7.537484	-1.192919	-0.911920
52	1	0	5.616981	-0.164540	-2.071781
53	1	0	-5.982831	-0.231289	-1.940987
54	1	0	-4.320312	0.185080	-2.349373
55	16	0	2.862896	-0.552592	-1.945728
56	6	0	2.794613	3.262711	-2.476113
57	6	0	1.470146	3.048016	-2.891589
58	6	0	0.487037	2.711119	-1.946974
59	6	0	0.812031	2.580409	-0.601338
60	6	0	2.165228	2.818142	-0.135663
61	6	0	3.135814	3.154536	-1.139965
62	7	0	-0.169099	2.188631	0.302814
63	6	0	0.022177	2.117152	1.669497
64	6	0	1.332054	2.439494	2.155913
65	6	0	2.457540	2.714402	1.229784
66	8	0	-0.916536	1.767841	2.420033
67	6	0	4.767926	1.656258	1.521976
68	6	0	4.320621	0.388228	2.269738
69	6	0	1.941208	-0.288898	2.801019
70	6	0	2.921919	-0.023906	1.922880
71	1	0	3.555671	3.522529	-3.206250
72	1	0	1.199959	3.145156	-3.938343
73	1	0	-0.543422	2.545436	-2.249746
74	1	0	4.159197	3.340492	-0.834448

75	1	0	-1.142216	2.106078	-0.030382
76	1	0	1.463371	2.497422	3.227755
77	1	0	0.952194	-0.590738	2.473628
78	1	0	2.699534	-0.088072	0.863978
79	1	0	2.103980	-0.221213	3.873860
80	6	0	3.847190	2.874200	1.785431
81	1	0	4.410065	0.535265	3.353798
82	1	0	5.005702	-0.427855	1.998554
83	1	0	4.784678	1.446533	0.445959
84	1	0	5.796724	1.904270	1.812154
85	1	0	4.323971	3.767783	1.360323
86	1	0	3.790125	3.044657	2.867628

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^{3}TX-Int1'$_{ex}$ E(opt)= -2373.117771 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.953387	0.595042	1.186624
2	6	0	6.008671	1.009065	0.147578
3	6	0	5.588972	0.528548	-1.249742
4	6	0	5.397480	-1.012993	-1.241457
5	6	0	4.599778	-1.655108	-0.078345
6	6	0	4.927235	-0.950062	1.267099
7	6	0	4.312265	1.303789	-1.625317
8	6	0	6.670400	0.861067	-2.291486
9	6	0	5.275580	1.175668	2.570893
10	6	0	4.992828	-3.152474	0.030168
11	6	0	3.557223	1.081707	0.761263
12	7	0	3.395147	1.492251	-0.505904
13	8	0	2.613025	1.073278	1.576696
14	6	0	3.111789	-1.634461	-0.323442
15	7	0	2.426272	-1.284106	-1.362752
16	6	0	1.089177	-1.517685	-1.008929
17	6	0	1.066533	-2.044400	0.293403
18	8	0	2.354661	-2.124186	0.732918
19	6	0	-0.108888	-1.297638	-1.673139
20	6	0	-1.316615	-1.637595	-1.024771
21	6	0	-1.287924	-2.209564	0.275905
22	6	0	-0.080244	-2.407227	0.964910
23	6	0	-2.572472	-1.297519	-1.738205
24	6	0	-3.885523	-1.652989	-1.149337
25	6	0	-4.055213	-2.228571	0.126015
26	6	0	-5.039916	-1.360391	-1.906239
27	6	0	-6.311647	-1.596721	-1.410244
28	6	0	-6.464609	-2.138255	-0.125420
29	6	0	-5.346340	-2.454747	0.634529
30	8	0	-2.523560	-0.694578	-2.821242
31	1	0	6.980793	0.581805	0.427392
32	1	0	6.128936	2.100139	0.141521
33	1	0	4.966550	-1.334821	-2.195347
34	1	0	6.403644	-1.447076	-1.189261

35	1	0	3.767983	0.779026	-2.417374
36	1	0	4.594191	2.292825	-2.010270
37	1	0	7.604129	0.334067	-2.068417
38	1	0	6.351391	0.567885	-3.298275
39	1	0	6.885986	1.934732	-2.304875
40	1	0	5.340865	2.267915	2.529301
41	1	0	4.493368	0.911011	3.285238
42	1	0	6.236325	0.790397	2.929266
43	1	0	4.435399	-3.645216	0.831017
44	1	0	4.783907	-3.675808	-0.908369
45	1	0	6.062200	-3.244175	0.244615
46	1	0	2.438514	1.751612	-0.774438
47	1	0	-0.154630	-0.855395	-2.660078
48	1	0	-0.051520	-2.805770	1.972367
49	1	0	-4.887518	-0.940048	-2.893902
50	1	0	-7.184336	-1.362999	-2.012359
51	1	0	-7.456246	-2.318851	0.279125
52	1	0	-5.464733	-2.882431	1.626301
53	1	0	5.923265	-1.280251	1.587945
54	1	0	4.216667	-1.268879	2.033923
55	16	0	-2.721977	-2.724085	1.159445
56	6	0	-3.222008	0.313088	3.104914
57	6	0	-1.885955	0.206301	3.546465
58	6	0	-0.836227	0.536876	2.683735
59	6	0	-1.097806	0.960694	1.383310
60	6	0	-2.464498	1.045058	0.883123
61	6	0	-3.507085	0.717499	1.820064
62	7	0	-0.042382	1.341145	0.569443
63	6	0	-0.196623	1.725960	-0.747328
64	6	0	-1.530725	1.754997	-1.269150
65	6	0	-2.692644	1.453509	-0.431824
66	8	0	0.793983	2.036178	-1.443374
67	6	0	-4.273656	3.245805	-1.316739
68	6	0	-3.958242	4.169925	-0.117519
69	6	0	-2.509063	4.574184	-0.042219
70	6	0	-1.691022	4.380124	0.995280
71	1	0	-4.033753	0.061159	3.780992
72	1	0	-1.669323	-0.123097	4.557526
73	1	0	0.197833	0.478677	3.011027
74	1	0	-4.537737	0.769129	1.492108
75	1	0	0.918926	1.296628	0.944536
76	1	0	-1.644322	1.993297	-2.317662
77	1	0	-5.321169	3.365139	-1.617287
78	1	0	-3.672363	3.562206	-2.178426
79	1	0	-4.265429	3.690208	0.820005
80	1	0	-4.562265	5.082981	-0.216984
81	1	0	-2.121962	5.076812	-0.930203
82	1	0	-2.021847	3.860316	1.890747
83	1	0	-0.657457	4.712026	0.976709
84	6	0	-4.031806	1.739851	-1.036198
85	1	0	-4.099710	1.196846	-1.988491
86	1	0	-4.838453	1.360647	-0.405621

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^{3}TX-Int1'$_{en}$ E(opt)= -2373.101519 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.879154	0.840213	0.716255
2	6	0	5.835894	0.860992	-0.486912
3	6	0	5.382798	-0.159120	-1.541905
4	6	0	5.342774	-1.577177	-0.910455
5	6	0	4.627584	-1.745627	0.453053
6	6	0	4.960858	-0.552561	1.390602
7	6	0	4.017424	0.318540	-2.073062
8	6	0	6.365563	-0.197513	-2.723830
9	6	0	5.245962	1.925838	1.737083
10	6	0	5.108383	-3.060231	1.121565
11	6	0	3.426318	1.053695	0.259899
12	7	0	3.134114	0.841349	-1.034353
13	8	0	2.552084	1.365130	1.091051
14	6	0	3.137203	-1.890755	0.280559
15	7	0	2.438510	-2.081758	-0.789497
16	6	0	1.114445	-2.163020	-0.344903
17	6	0	1.109997	-2.036537	1.055930
18	8	0	2.401538	-1.866265	1.459293
19	6	0	-0.082681	-2.320057	-1.020041
20	6	0	-1.275010	-2.399477	-0.271633
21	6	0	-1.234480	-2.303544	1.145989
22	6	0	-0.025091	-2.100735	1.834386
23	6	0	-2.531056	-2.568863	-1.048334
24	6	0	-3.827494	-2.751009	-0.341883
25	6	0	-3.983400	-2.698452	1.054915
26	6	0	-4.970091	-2.966272	-1.137709
27	6	0	-6.224424	-3.121806	-0.572264
28	6	0	-6.366003	-3.063493	0.822215
29	6	0	-5.257866	-2.854406	1.629856
30	8	0	-2.504333	-2.551367	-2.280860
31	1	0	6.854627	0.634352	-0.144828
32	1	0	5.864237	1.864765	-0.930590
33	1	0	4.924116	-2.289356	-1.628927
34	1	0	6.386335	-1.872841	-0.743863
35	1	0	3.495439	-0.504619	-2.570379
36	1	0	4.183253	1.109183	-2.817388
37	1	0	7.356220	-0.531741	-2.397843
38	1	0	6.018353	-0.885374	-3.503271
39	1	0	6.477628	0.794480	-3.174210
40	1	0	5.227024	2.917577	1.273435
41	1	0	4.533502	1.927325	2.564261
42	1	0	6.253829	1.752134	2.129359
43	1	0	4.603091	-3.217097	2.078636
44	1	0	4.901405	-3.919990	0.476526
45	1	0	6.186971	-3.016660	1.302653
46	1	0	2.136605	0.869496	-1.282623
47	1	0	-0.138712	-2.379388	-2.099504

48	1	0	0.015278	-2.004799	2.913564
49	1	0	-4.823774	-2.999660	-2.211634
50	1	0	-7.092161	-3.286905	-1.203232
51	1	0	-7.344748	-3.181671	1.277990
52	1	0	-5.371124	-2.807916	2.709339
53	1	0	5.990550	-0.685999	1.745586
54	1	0	4.309037	-0.575514	2.267847
55	16	0	-2.660598	-2.413123	2.181002
56	6	0	-2.001682	5.095653	2.270398
57	6	0	-0.831505	4.501633	2.776227
58	6	0	-0.156184	3.530422	2.017469
59	6	0	-0.629355	3.155698	0.768171
60	6	0	-1.817403	3.773901	0.198111
61	6	0	-2.486230	4.745143	1.024900
62	7	0	0.035720	2.159235	0.056466
63	6	0	-0.307699	1.759759	-1.217056
64	6	0	-1.473542	2.361667	-1.792580
65	6	0	-2.255342	3.393832	-1.069426
66	8	0	0.393799	0.921691	-1.830642
67	6	0	-4.795983	3.099020	-1.371202
68	6	0	-4.807537	1.662110	-1.916634
69	6	0	-3.904424	0.656027	-1.244201
70	6	0	-3.427564	0.723282	0.004267
71	1	0	-2.531075	5.836595	2.862869
72	1	0	-0.450329	4.783392	3.752516
73	1	0	0.744256	3.054961	2.396094
74	1	0	-3.392189	5.210523	0.652994
75	1	0	0.903397	1.772993	0.455814
76	1	0	-1.741403	2.053918	-2.794995
77	1	0	-5.653702	3.634274	-1.797521
78	1	0	-4.942808	3.099846	-0.284778
79	1	0	-4.563089	1.689534	-2.988042
80	1	0	-5.834787	1.268537	-1.873418
81	1	0	-3.651747	-0.213188	-1.848914
82	1	0	-2.787445	-0.054544	0.402393
83	1	0	-3.624408	1.562061	0.662784
84	6	0	-3.513281	3.902262	-1.714070
85	1	0	-3.682805	4.949923	-1.440607
86	1	0	-3.386544	3.891871	-2.805657

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^{3}TX-TS1$_{ex}$ E(opt)= -2373.11978 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.948512	0.681106	1.190699
2	6	0	5.970628	1.139965	0.137979
3	6	0	5.556878	0.637322	-1.253027
4	6	0	5.450872	-0.912372	-1.238083
5	6	0	4.674661	-1.582618	-0.076771
6	6	0	4.980391	-0.865324	1.267051
7	6	0	4.234890	1.343792	-1.611260

8	6	0	6.604545	1.025344	-2.309749
9	6	0	5.270144	1.268434	2.571920
10	6	0	5.110684	-3.067171	0.034487
11	6	0	3.526621	1.109538	0.788226
12	7	0	3.315705	1.476559	-0.485152
13	8	0	2.605127	1.079781	1.628169
14	6	0	3.189919	-1.604680	-0.336047
15	7	0	2.521144	-1.316126	-1.403427
16	6	0	1.181085	-1.534665	-1.059370
17	6	0	1.136778	-1.996671	0.268434
18	8	0	2.418394	-2.049108	0.731421
19	6	0	-0.001372	-1.338844	-1.751490
20	6	0	-1.219965	-1.639741	-1.107133
21	6	0	-1.217491	-2.150365	0.219242
22	6	0	-0.021819	-2.322428	0.937747
23	6	0	-2.461196	-1.337907	-1.864839
24	6	0	-3.787785	-1.670623	-1.285708
25	6	0	-3.979641	-2.185300	0.010637
26	6	0	-4.923534	-1.401222	-2.075898
27	6	0	-6.205271	-1.619715	-1.598107
28	6	0	-6.383315	-2.111197	-0.296063
29	6	0	-5.282418	-2.390737	0.501726
30	8	0	-2.395015	-0.785368	-2.967513
31	1	0	6.965050	0.758571	0.406092
32	1	0	6.040263	2.235495	0.129327
33	1	0	5.046000	-1.262974	-2.193091
34	1	0	6.478268	-1.292188	-1.172575
35	1	0	3.713866	0.796121	-2.402988
36	1	0	4.461146	2.348799	-1.992288
37	1	0	7.567640	0.547919	-2.100011
38	1	0	6.287009	0.715530	-3.312002
39	1	0	6.763602	2.108823	-2.325863
40	1	0	5.292260	2.362527	2.533622
41	1	0	4.510096	0.971890	3.297446
42	1	0	6.250775	0.919621	2.913531
43	1	0	4.563549	-3.574433	0.833880
44	1	0	4.920599	-3.597160	-0.904236
45	1	0	6.181183	-3.128617	0.254369
46	1	0	2.337048	1.669512	-0.745790
47	1	0	-0.026995	-0.931292	-2.753865
48	1	0	-0.013103	-2.665924	1.965469
49	1	0	-4.748488	-1.002806	-3.069046
50	1	0	-7.066002	-1.405509	-2.223994
51	1	0	-7.383132	-2.275625	0.095092
52	1	0	-5.421931	-2.771300	1.509688
53	1	0	5.990075	-1.158899	1.580935
54	1	0	4.286945	-1.210809	2.038081
55	16	0	-2.670023	-2.603123	1.103528
56	6	0	-3.103310	0.285903	3.449371
57	6	0	-1.752027	0.217034	3.818866
58	6	0	-0.753690	0.555575	2.896344
59	6	0	-1.092990	0.962652	1.608924
60	6	0	-2.472379	1.029665	1.194189

61	6	0	-3.456770	0.678570	2.168957
62	7	0	-0.082773	1.314503	0.717709
63	6	0	-0.290559	1.630472	-0.606459
64	6	0	-1.662985	1.720066	-1.042584
65	6	0	-2.781625	1.435347	-0.120141
66	8	0	0.672593	1.848789	-1.370755
67	6	0	-4.884659	2.896886	-0.104031
68	6	0	-4.194881	4.182267	-0.603307
69	6	0	-1.695956	4.218276	-0.960815
70	6	0	-2.774624	4.280295	-0.137516
71	1	0	-3.876467	0.020170	4.164328
72	1	0	-1.472945	-0.095871	4.820317
73	1	0	0.297398	0.510027	3.167294
74	1	0	-4.503180	0.700706	1.886632
75	1	0	0.894939	1.265662	1.043095
76	1	0	-4.890563	2.892228	0.992821
77	1	0	-5.933665	2.897590	-0.427405
78	1	0	-4.231297	4.216490	-1.699639
79	1	0	-1.810452	4.230840	-2.040519
80	1	0	-0.682881	4.305052	-0.584905
81	1	0	-4.765683	5.047570	-0.236249
82	6	0	-4.193321	1.608511	-0.608994
83	1	0	-4.803967	0.751049	-0.304383
84	1	0	-4.196834	1.602986	-1.705363
85	1	0	-1.827969	1.691061	-2.112289
86	1	0	-2.617262	4.327197	0.939090

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^{3}TX-TS1$_{ex\text{-}isomer}$ E(opt)= -2373.1165643 hartree

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Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.948393	0.537803	1.239205
2	6	0	5.981571	1.064059	0.229257
3	6	0	5.566123	0.679308	-1.198703
4	6	0	5.427871	-0.864263	-1.308639
5	6	0	4.650844	-1.615682	-0.198440
6	6	0	4.969170	-1.009285	1.196542
7	6	0	4.260299	1.437569	-1.503346
8	6	0	6.626482	1.128565	-2.217845
9	6	0	5.266358	1.015473	2.662911
10	6	0	5.074365	-3.108066	-0.207684
11	6	0	3.532721	1.011708	0.862847
12	7	0	3.341800	1.499874	-0.371814
13	8	0	2.599817	0.914594	1.685450
14	6	0	3.162739	-1.604496	-0.440291
15	7	0	2.474407	-1.210142	-1.460625
16	6	0	1.138903	-1.454536	-1.111002
17	6	0	1.120359	-2.040216	0.167725
18	8	0	2.409655	-2.145349	0.595255
19	6	0	-0.059069	-1.194010	-1.755225
20	6	0	-1.265052	-1.551616	-1.114029

21	6	0	-1.234570	-2.182335	0.159479
22	6	0	-0.023835	-2.423747	0.829809
23	6	0	-2.524210	-1.187745	-1.811091
24	6	0	-3.834329	-1.608521	-1.252083
25	6	0	-3.998553	-2.234371	-0.001612
26	6	0	-4.986524	-1.321774	-2.012938
27	6	0	-6.256095	-1.616649	-1.544106
28	6	0	-6.406029	-2.210905	-0.282135
29	6	0	-5.289129	-2.519835	0.481141
30	8	0	-2.488389	-0.519075	-2.850975
31	1	0	6.969320	0.648546	0.469910
32	1	0	6.066805	2.155760	0.306572
33	1	0	5.007338	-1.127011	-2.284992
34	1	0	6.447843	-1.268072	-1.286495
35	1	0	3.730329	0.963617	-2.336033
36	1	0	4.506973	2.464377	-1.805452
37	1	0	7.579511	0.618184	-2.042486
38	1	0	6.308477	0.904044	-3.242459
39	1	0	6.805574	2.206815	-2.148725
40	1	0	5.301008	2.109028	2.707707
41	1	0	4.497176	0.673482	3.358302
42	1	0	6.240282	0.630319	2.984154
43	1	0	4.527364	-3.672927	0.552022
44	1	0	4.875113	-3.560417	-1.184420
45	1	0	6.145460	-3.195109	0.000210
46	1	0	2.368689	1.732234	-0.621953
47	1	0	-0.105711	-0.698148	-2.716341
48	1	0	0.008115	-2.866253	1.818613
49	1	0	-4.835069	-0.854721	-2.979776
50	1	0	-7.128692	-1.387262	-2.147827
51	1	0	-7.396342	-2.437880	0.101934
52	1	0	-5.406354	-2.986497	1.455207
53	1	0	5.977831	-1.334005	1.481870
54	1	0	4.276340	-1.409207	1.941152
55	16	0	-2.665832	-2.705770	1.038986
56	6	0	-3.225809	0.124169	3.280892
57	6	0	-1.890967	-0.000276	3.691499
58	6	0	-0.857117	0.386013	2.831060
59	6	0	-1.143064	0.893039	1.565922
60	6	0	-2.505170	1.018434	1.108631
61	6	0	-3.526129	0.616038	2.021349
62	7	0	-0.089456	1.287397	0.742254
63	6	0	-0.240954	1.745618	-0.545935
64	6	0	-1.595336	1.929036	-1.008494
65	6	0	-2.750634	1.545339	-0.180242
66	8	0	0.748677	2.013133	-1.257227
67	6	0	-4.416374	3.245372	-1.099256
68	6	0	-4.124726	4.165572	0.100640
69	6	0	-1.650238	4.344610	-0.437585
70	6	0	-2.663283	4.207506	0.465633
71	1	0	-4.029859	-0.175951	3.946446
72	1	0	-1.653142	-0.392466	4.675450
73	1	0	0.183058	0.299582	3.132731

74	1	0	-4.562760	0.687417	1.713652
75	1	0	0.874831	1.176520	1.090828
76	1	0	-1.838932	4.562701	-1.483692
77	1	0	-0.616527	4.408452	-0.118016
78	6	0	-4.104311	1.761018	-0.787324
79	1	0	-4.892264	1.353419	-0.150207
80	1	0	-4.147544	1.203121	-1.732388
81	1	0	-1.720926	2.068320	-2.074490
82	1	0	-2.405602	4.079327	1.513966
83	1	0	-4.478035	5.181037	-0.134416
84	1	0	-4.706434	3.830230	0.967252
85	1	0	-3.825876	3.571912	-1.962272
86	1	0	-5.467548	3.335948	-1.397263

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^{3}TX-TS1$_{ex\text{-}iflip}$ E(opt)= -2373.1172711 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.030703	1.201557	0.362303
2	6	0	5.978820	0.723070	-0.750172
3	6	0	5.437050	-0.558467	-1.401681
4	6	0	5.289806	-1.658775	-0.319874
5	6	0	4.546565	-1.289945	0.988431
6	6	0	4.973931	0.120090	1.473770
7	6	0	4.106476	-0.193009	-2.084051
8	6	0	6.402519	-1.074634	-2.480626
9	6	0	5.511357	2.527322	0.966320
10	6	0	4.910603	-2.330555	2.080420
11	6	0	3.607352	1.385797	-0.187307
12	7	0	3.255798	0.673564	-1.276212
13	8	0	2.797168	2.122174	0.401162
14	6	0	3.041459	-1.351090	0.862875
15	7	0	2.182404	-0.913657	1.724158
16	6	0	0.936765	-1.286174	1.214195
17	6	0	1.139519	-1.960551	-0.002690
18	8	0	2.490539	-2.027496	-0.218221
19	6	0	-0.349102	-1.109851	1.696103
20	6	0	-1.428533	-1.596793	0.932435
21	6	0	-1.184529	-2.235066	-0.314286
22	6	0	0.119649	-2.437120	-0.797928
23	6	0	-2.782379	-1.398117	1.510001
24	6	0	-3.986882	-1.828442	0.751055
25	6	0	-3.953436	-2.424668	-0.522557
26	6	0	-5.241777	-1.577909	1.340940
27	6	0	-6.423861	-1.893951	0.689413
28	6	0	-6.375910	-2.475839	-0.585106
29	6	0	-5.152374	-2.740899	-1.186287
30	8	0	-2.914673	-0.870218	2.616530
31	1	0	6.975643	0.543279	-0.325775
32	1	0	6.093445	1.506343	-1.511179
33	1	0	4.840557	-2.554911	-0.760910

34	1	0	6.307552	-1.939162	-0.020995
35	1	0	3.539647	-1.098945	-2.321220
36	1	0	4.323768	0.313949	-3.034906
37	1	0	7.367524	-1.348682	-2.041474
38	1	0	5.997768	-1.961643	-2.981584
39	1	0	6.586142	-0.310228	-3.243192
40	1	0	5.583636	3.302474	0.196503
41	1	0	4.811340	2.875766	1.727829
42	1	0	6.501261	2.400165	1.417530
43	1	0	4.396485	-2.095516	3.015778
44	1	0	4.617087	-3.338885	1.769940
45	1	0	5.990707	-2.328037	2.259979
46	1	0	2.274968	0.752523	-1.584505
47	1	0	-0.557027	-0.601125	2.628659
48	1	0	0.311900	-2.918420	-1.749911
49	1	0	-5.238482	-1.119158	2.323674
50	1	0	-7.379826	-1.690231	1.161884
51	1	0	-7.294276	-2.724277	-1.109035
52	1	0	-5.117877	-3.196273	-2.172252
53	1	0	5.982372	0.037377	1.898958
54	1	0	4.302973	0.445525	2.273233
55	16	0	-2.465566	-2.828444	-1.378414
56	6	0	-2.485028	2.657034	3.076319
57	6	0	-1.099198	2.842221	3.189068
58	6	0	-0.256813	2.514402	2.119940
59	6	0	-0.791087	2.011982	0.936948
60	6	0	-2.209156	1.810316	0.789086
61	6	0	-3.027745	2.148836	1.908568
62	7	0	0.065559	1.711832	-0.120170
63	6	0	-0.315350	1.030047	-1.249986
64	6	0	-1.735327	0.859880	-1.444474
65	6	0	-2.710052	1.287135	-0.421114
66	8	0	0.535214	0.618582	-2.070583
67	6	0	-4.845110	2.547403	-1.042796
68	6	0	-4.294082	3.193367	-2.330348
69	6	0	-1.883206	2.824482	-2.983076
70	6	0	-2.824026	3.467956	-2.244603
71	1	0	-3.135039	2.894608	3.912830
72	1	0	-0.671874	3.231311	4.108050
73	1	0	0.819718	2.637735	2.194125
74	1	0	-4.096309	1.979338	1.845870
75	1	0	1.073924	1.876428	0.021729
76	1	0	-4.686111	3.227603	-0.197227
77	1	0	-5.929707	2.409566	-1.141110
78	1	0	-4.501440	2.538161	-3.186242
79	1	0	-2.164129	2.156038	-3.791611
80	1	0	-0.829580	3.066123	-2.903088
81	1	0	-4.836459	4.133341	-2.507353
82	6	0	-4.180391	1.188176	-0.722341
83	1	0	-4.711890	0.741400	0.124850
84	1	0	-4.335951	0.503728	-1.565065
85	1	0	-2.034948	0.170101	-2.223473
86	1	0	-2.504078	4.175902	-1.481551

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^{3}TX-TS1$_{en}$ E(opt)= -2373.104252 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.056864	0.992012	-0.559845
2	6	0	-5.994344	0.616738	0.601062
3	6	0	-5.425136	-0.575213	1.383613
4	6	0	-5.274455	-1.786262	0.428243
5	6	0	-4.507454	-1.541030	-0.893168
6	6	0	-4.955869	-0.206115	-1.536347
7	6	0	-4.090708	-0.121089	2.013643
8	6	0	-6.372452	-0.985856	2.522834
9	6	0	-5.581602	2.220358	-1.315955
10	6	0	-4.805992	-2.701043	-1.880661
11	6	0	-3.653334	1.307021	-0.018907
12	7	0	-3.293846	0.750934	1.154430
13	8	0	-2.873777	2.024741	-0.670312
14	6	0	-3.017694	-1.595522	-0.663323
15	7	0	-2.364870	-2.310540	0.195891
16	6	0	-1.017669	-2.109716	-0.124145
17	6	0	-0.948085	-1.231003	-1.221045
18	8	0	-2.228066	-0.912714	-1.575013
19	6	0	0.151688	-2.624617	0.409243
20	6	0	1.383582	-2.236388	-0.156924
21	6	0	1.410668	-1.315267	-1.237935
22	6	0	0.226259	-0.804997	-1.799109
23	6	0	2.604359	-2.838807	0.445934
24	6	0	3.951829	-2.395473	-0.008785
25	6	0	4.173514	-1.459579	-1.037196
26	6	0	5.066061	-2.918857	0.676214
27	6	0	6.356960	-2.525060	0.362227
28	6	0	6.564236	-1.587224	-0.660791
29	6	0	5.485221	-1.059411	-1.355174
30	8	0	2.503343	-3.685391	1.333324
31	1	0	-6.987820	0.370674	0.203005
32	1	0	-6.122541	1.476655	1.271321
33	1	0	-4.817089	-2.626885	0.959490
34	1	0	-6.288283	-2.099522	0.147717
35	1	0	-3.484058	-0.996116	2.273329
36	1	0	-4.302808	0.421224	2.944677
37	1	0	-7.331833	-1.334477	2.126081
38	1	0	-5.941607	-1.797312	3.120409
39	1	0	-6.572175	-0.142049	3.191864
40	1	0	-5.685020	3.076806	-0.642281
41	1	0	-4.891217	2.504087	-2.112373
42	1	0	-6.564208	2.004640	-1.749233
43	1	0	-4.258724	-2.563149	-2.818475
44	1	0	-4.510954	-3.660272	-1.445755
45	1	0	-5.876143	-2.734432	-2.109054
46	1	0	-2.412805	1.099425	1.560397

47	1	0	0.157541	-3.322318	1.237788
48	1	0	0.240280	-0.094332	-2.615931
49	1	0	4.866772	-3.635102	1.465716
50	1	0	7.201704	-2.937260	0.905162
51	1	0	7.570787	-1.266427	-0.912800
52	1	0	5.647639	-0.329657	-2.143486
53	1	0	-5.956190	-0.366682	-1.957733
54	1	0	-4.294816	0.052888	-2.367781
55	16	0	2.891947	-0.693543	-1.969508
56	6	0	2.783185	3.131650	-2.566846
57	6	0	1.468893	2.877712	-2.983531
58	6	0	0.481307	2.579905	-2.034909
59	6	0	0.795848	2.523176	-0.678976
60	6	0	2.135399	2.790285	-0.218438
61	6	0	3.108056	3.093939	-1.219575
62	7	0	-0.199580	2.191317	0.235588
63	6	0	-0.032802	2.190608	1.605053
64	6	0	1.293301	2.474534	2.091524
65	6	0	2.415336	2.743923	1.164659
66	8	0	-0.991603	1.917133	2.358730
67	6	0	4.764968	1.809928	1.540128
68	6	0	4.281852	0.550348	2.283243
69	6	0	1.815219	0.064169	2.627924
70	6	0	2.915783	0.140676	1.834932
71	1	0	3.550158	3.365663	-3.299363
72	1	0	1.208691	2.917705	-4.036778
73	1	0	-0.545665	2.392643	-2.337099
74	1	0	4.125872	3.308548	-0.913390
75	1	0	-1.169204	2.104463	-0.107079
76	1	0	5.766471	2.088673	1.891780
77	1	0	4.854641	1.578164	0.472305
78	1	0	4.987677	-0.267882	2.080036
79	1	0	1.877901	0.225204	3.700126
80	1	0	0.865248	-0.289725	2.244637
81	1	0	4.288398	0.724758	3.366671
82	6	0	3.789649	2.998347	1.725164
83	1	0	3.709113	3.220591	2.796518
84	1	0	4.230702	3.889855	1.259176
85	1	0	1.388337	2.691926	3.147539
86	1	0	2.800697	-0.047214	0.775462

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^{3}TX-TS1'$_{ex}$ E(opt)= -2373.111734 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.939138	0.263497	1.257789
2	6	0	5.961189	0.909378	0.308014
3	6	0	5.501309	0.750599	-1.148791
4	6	0	5.324544	-0.756285	-1.481295
5	6	0	4.549654	-1.645454	-0.476625
6	6	0	4.910285	-1.260215	0.985051

7	6	0	4.206648	1.571289	-1.302732
8	6	0	6.546965	1.325282	-2.119008
9	6	0	5.308158	0.513703	2.726662
10	6	0	4.935123	-3.129305	-0.715198
11	6	0	3.529736	0.824026	0.998631
12	7	0	3.316780	1.484694	-0.149411
13	8	0	2.619681	0.636966	1.831126
14	6	0	3.058581	-1.566573	-0.685619
15	7	0	2.366771	-1.011603	-1.625874
16	6	0	1.031249	-1.287047	-1.301905
17	6	0	1.014496	-2.060281	-0.127678
18	8	0	2.306565	-2.245281	0.266013
19	6	0	-0.167860	-0.912258	-1.885540
20	6	0	-1.374396	-1.346450	-1.294664
21	6	0	-1.342934	-2.168614	-0.135355
22	6	0	-0.130940	-2.525846	0.478790
23	6	0	-2.631405	-0.848740	-1.907184
24	6	0	-3.944609	-1.286918	-1.375718
25	6	0	-4.109821	-2.111974	-0.246220
26	6	0	-5.099870	-0.803648	-2.025893
27	6	0	-6.371126	-1.117554	-1.571885
28	6	0	-6.519794	-1.925741	-0.435185
29	6	0	-5.400455	-2.417623	0.222409
30	8	0	-2.585906	-0.043816	-2.846607
31	1	0	6.942770	0.439663	0.456460
32	1	0	6.078012	1.975090	0.544051
33	1	0	4.879987	-0.863800	-2.476208
34	1	0	6.334939	-1.179941	-1.540427
35	1	0	3.645959	1.235895	-2.181188
36	1	0	4.470367	2.626377	-1.456728
37	1	0	7.491281	0.775126	-2.047901
38	1	0	6.198734	1.262503	-3.156388
39	1	0	6.753890	2.377278	-1.895454
40	1	0	5.374755	1.586914	2.933557
41	1	0	4.548893	0.089567	3.386722
42	1	0	6.279187	0.061601	2.956246
43	1	0	4.389320	-3.787809	-0.034150
44	1	0	4.704796	-3.427984	-1.742849
45	1	0	6.007648	-3.269788	-0.547901
46	1	0	2.343436	1.769097	-0.334175
47	1	0	-0.213734	-0.275923	-2.759886
48	1	0	-0.099022	-3.114045	1.388380
49	1	0	-4.947404	-0.170900	-2.893279
50	1	0	-7.245659	-0.736114	-2.089865
51	1	0	-7.510289	-2.170897	-0.063197
52	1	0	-5.516850	-3.042366	1.103588
53	1	0	5.913065	-1.651917	1.197582
54	1	0	4.218119	-1.746080	1.677527
55	16	0	-2.776369	-2.817256	0.652818
56	6	0	-3.132998	-0.433156	3.448403
57	6	0	-1.784288	-0.635848	3.781368
58	6	0	-0.771761	-0.116319	2.964066
59	6	0	-1.095234	0.598639	1.815488

60	6	0	-2.471536	0.807749	1.437450
61	6	0	-3.472436	0.266701	2.303378
62	7	0	-0.074362	1.156110	1.044651
63	6	0	-0.267885	1.754049	-0.174673
64	6	0	-1.643474	1.952702	-0.594255
65	6	0	-2.759367	1.544379	0.276488
66	8	0	0.692410	2.141241	-0.867713
67	6	0	-4.142975	3.224609	-1.044024
68	6	0	-3.371926	4.434546	-0.480037
69	6	0	-1.875027	4.259123	-0.325619
70	6	0	-1.243891	4.454084	0.873295
71	1	0	-3.914767	-0.840673	4.082800
72	1	0	-1.519065	-1.192457	4.674908
73	1	0	0.276229	-0.254130	3.215112
74	1	0	-4.515676	0.385210	2.032079
75	1	0	0.901842	1.015859	1.350444
76	1	0	-1.784169	1.963843	-1.669902
77	1	0	-5.182328	3.522910	-1.222884
78	1	0	-3.736444	2.935897	-2.019661
79	1	0	-3.800887	4.695515	0.495987
80	1	0	-3.542076	5.298149	-1.137335
81	1	0	-1.273956	4.293532	-1.231511
82	1	0	-1.807016	4.555328	1.796544
83	1	0	-0.162130	4.422835	0.948492
84	6	0	-4.138724	2.019289	-0.089420
85	1	0	-4.712335	1.203140	-0.553600
86	1	0	-4.687915	2.285525	0.824251

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^{3}TX-TS1'$_{en}$ E(opt)= -2373.101566 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.834533	0.805410	-0.631594
2	6	0	-5.761354	0.659828	0.587058
3	6	0	-5.263962	-0.464389	1.507921
4	6	0	-5.241767	-1.797824	0.717857
5	6	0	-4.508629	-1.797787	-0.644772
6	6	0	-4.858868	-0.514881	-1.446388
7	6	0	-3.878524	-0.045148	2.039087
8	6	0	-6.203792	-0.641169	2.711384
9	6	0	-5.281784	1.965821	-1.529955
10	6	0	-4.954867	-3.036681	-1.466444
11	6	0	-3.387811	1.048078	-0.176790
12	7	0	-3.029601	0.592688	1.036154
13	8	0	-2.571816	1.590878	-0.945375
14	6	0	-3.021471	-1.958005	-0.454373
15	7	0	-2.370790	-2.398286	0.572598
16	6	0	-1.032819	-2.418588	0.168219
17	6	0	-0.966674	-1.990526	-1.169163
18	8	0	-2.237631	-1.693855	-1.570223
19	6	0	0.131653	-2.753399	0.836826

20	6	0	1.354279	-2.687117	0.140479
21	6	0	1.377693	-2.286393	-1.222432
22	6	0	0.201658	-1.915025	-1.898891
23	6	0	2.578086	-3.010451	0.923894
24	6	0	3.921087	-2.758034	0.331037
25	6	0	4.137121	-2.401989	-1.012904
26	6	0	5.033336	-2.858549	1.188867
27	6	0	6.319196	-2.613629	0.733597
28	6	0	6.521546	-2.263876	-0.609639
29	6	0	5.442237	-2.159959	-1.476694
30	8	0	2.485126	-3.428924	2.077468
31	1	0	-6.782964	0.447464	0.244099
32	1	0	-5.801907	1.606227	1.142213
33	1	0	-4.835561	-2.596056	1.347058
34	1	0	-6.286984	-2.058653	0.507672
35	1	0	-3.342821	-0.917226	2.425695
36	1	0	-4.016958	0.658244	2.871869
37	1	0	-7.202940	-0.948319	2.384567
38	1	0	-5.824826	-1.406560	3.398160
39	1	0	-6.306706	0.294488	3.271315
40	1	0	-5.291922	2.907241	-0.971239
41	1	0	-4.597267	2.084410	-2.371927
42	1	0	-6.292786	1.783013	-1.909649
43	1	0	-4.436291	-3.071703	-2.429037
44	1	0	-4.735335	-3.959931	-0.921484
45	1	0	-6.032172	-2.994129	-1.655710
46	1	0	-2.026615	0.652983	1.267375
47	1	0	0.138531	-3.057211	1.876187
48	1	0	0.211501	-1.582847	-2.930949
49	1	0	4.838720	-3.132716	2.219923
50	1	0	7.163387	-2.691021	1.411537
51	1	0	7.523839	-2.065276	-0.977914
52	1	0	5.601230	-1.877963	-2.513598
53	1	0	-5.879359	-0.639313	-1.830053
54	1	0	-4.198004	-0.422901	-2.312745
55	16	0	2.846983	-2.247784	-2.201598
56	6	0	1.603739	5.944758	-1.323061
57	6	0	0.348029	5.515453	-1.778624
58	6	0	-0.224263	4.348532	-1.248519
59	6	0	0.440759	3.617364	-0.273096
60	6	0	1.731594	4.038986	0.228527
61	6	0	2.279638	5.229643	-0.348244
62	7	0	-0.124929	2.424548	0.187230
63	6	0	0.360069	1.690515	1.241337
64	6	0	1.648260	2.088340	1.752968
65	6	0	2.375775	3.253573	1.196154
66	8	0	-0.274155	0.712248	1.693721
67	6	0	4.753501	2.381211	0.922777
68	6	0	4.352932	0.907682	1.119803
69	6	0	3.041652	0.505567	0.478827
70	6	0	2.656194	0.874602	-0.768881
71	1	0	2.050793	6.845459	-1.734273
72	1	0	-0.182201	6.077117	-2.541199

73	1	0	-1.186782	3.989157	-1.602389
74	1	0	3.247769	5.579333	-0.006193
75	1	0	-1.003665	2.099662	-0.245130
76	1	0	1.941865	1.659811	2.704720
77	1	0	5.769791	2.523884	1.310337
78	1	0	4.793180	2.620891	-0.146092
79	1	0	4.309962	0.685024	2.192834
80	1	0	5.142093	0.258454	0.714280
81	1	0	2.462114	-0.258161	0.987702
82	1	0	1.723040	0.518621	-1.188082
83	1	0	3.220687	1.584596	-1.363632
84	6	0	3.807533	3.392216	1.625096
85	1	0	4.184536	4.403199	1.444713
86	1	0	3.875654	3.224852	2.710511

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^{3}TX-Int2$_{ex}$ E(opt)= -2373.152031 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.921865	0.550886	1.291621
2	6	0	5.940938	1.166512	0.318665
3	6	0	5.543621	0.848923	-1.130574
4	6	0	5.460995	-0.690370	-1.325854
5	6	0	4.698431	-1.525893	-0.266833
6	6	0	4.989275	-0.990098	1.161989
7	6	0	4.213565	1.579288	-1.400747
8	6	0	6.591275	1.390457	-2.117615
9	6	0	5.221129	0.956250	2.741808
10	6	0	5.161847	-3.003566	-0.356202
11	6	0	3.494771	1.005002	0.936983
12	7	0	3.290415	1.551543	-0.270851
13	8	0	2.564798	0.840797	1.752626
14	6	0	3.213833	-1.539873	-0.525490
15	7	0	2.534339	-1.125209	-1.543569
16	6	0	1.199578	-1.404651	-1.223308
17	6	0	1.170365	-2.032851	0.035599
18	8	0	2.455334	-2.129674	0.479154
19	6	0	0.009782	-1.141405	-1.878764
20	6	0	-1.201218	-1.528911	-1.265504
21	6	0	-1.183816	-2.192352	-0.009167
22	6	0	0.020868	-2.447811	0.668695
23	6	0	-2.451357	-1.165266	-1.979924
24	6	0	-3.773287	-1.507108	-1.395813
25	6	0	-3.947604	-2.160306	-0.161081
26	6	0	-4.918675	-1.107236	-2.113024
27	6	0	-6.193680	-1.333432	-1.621776
28	6	0	-6.353473	-1.967264	-0.380177
29	6	0	-5.243054	-2.376805	0.344363
30	8	0	-2.395023	-0.539118	-3.043403
31	1	0	6.940806	0.770425	0.540810
32	1	0	5.989814	2.254187	0.458227

33	1	0	5.060307	-0.914226	-2.319976
34	1	0	6.494147	-1.059479	-1.312472
35	1	0	3.703208	1.132663	-2.260345
36	1	0	4.426491	2.628310	-1.645901
37	1	0	7.560205	0.902802	-1.966805
38	1	0	6.284009	1.214046	-3.154806
39	1	0	6.734066	2.468317	-1.986512
40	1	0	5.219682	2.045862	2.849421
41	1	0	4.463071	0.549910	3.414328
42	1	0	6.206787	0.585292	3.043089
43	1	0	4.623664	-3.624556	0.365220
44	1	0	4.983064	-3.404900	-1.358768
45	1	0	6.232989	-3.074136	-0.142567
46	1	0	2.317367	1.805594	-0.494997
47	1	0	-0.027769	-0.627175	-2.830870
48	1	0	0.041872	-2.913892	1.646772
49	1	0	-4.756600	-0.604464	-3.059914
50	1	0	-7.062707	-1.015578	-2.189219
51	1	0	-7.347588	-2.139609	0.021940
52	1	0	-5.368983	-2.864665	1.306720
53	1	0	6.005646	-1.300002	1.435812
54	1	0	4.304997	-1.451761	1.878292
55	16	0	-2.625084	-2.749517	0.831749
56	6	0	-3.108545	-0.180384	3.452647
57	6	0	-1.754517	-0.333904	3.788643
58	6	0	-0.765260	0.121798	2.915342
59	6	0	-1.120963	0.721973	1.708603
60	6	0	-2.491319	0.871932	1.321686
61	6	0	-3.468777	0.407006	2.251189
62	7	0	-0.114611	1.186563	0.863395
63	6	0	-0.308811	1.787708	-0.337024
64	6	0	-1.729355	1.965872	-0.843208
65	6	0	-2.808550	1.461791	0.076791
66	8	0	0.647511	2.170833	-1.026337
67	6	0	-4.781687	3.030231	0.359476
68	6	0	-4.138635	4.334253	-0.187212
69	6	0	-1.965739	3.471754	-1.282049
70	6	0	-2.643070	4.298083	-0.241013
71	1	0	-3.879600	-0.529343	4.133332
72	1	0	-1.471431	-0.798998	4.727907
73	1	0	0.289229	0.023037	3.157962
74	1	0	-4.518952	0.504121	2.002317
75	1	0	0.865434	1.082792	1.177693
76	1	0	-4.603387	2.959852	1.438568
77	1	0	-5.868941	3.083930	0.215582
78	1	0	-4.525670	4.492870	-1.205527
79	1	0	-2.580230	3.457796	-2.189226
80	1	0	-0.986595	3.871391	-1.564024
81	1	0	-4.488156	5.177874	0.420318
82	6	0	-4.234784	1.745934	-0.313700
83	1	0	-4.876711	0.899783	-0.048518
84	1	0	-4.307325	1.842211	-1.403799
85	1	0	-1.751495	1.390373	-1.781706

86	1	0	-2.071081	4.621618	0.626271

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^{3}TX-Int2$_{en}$ E(opt)= -2373.146072 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.187172	0.749229	-0.322755
2	6	0	-6.065922	-0.077034	0.630965
3	6	0	-5.295118	-1.302018	1.141059
4	6	0	-4.912048	-2.184833	-0.071669
5	6	0	-4.144075	-1.488167	-1.219373
6	6	0	-4.776549	-0.112844	-1.544190
7	6	0	-4.075737	-0.796195	1.945725
8	6	0	-6.168066	-2.144836	2.085163
9	6	0	-5.935940	1.996068	-0.814200
10	6	0	-4.220643	-2.376633	-2.493164
11	6	0	-3.909749	1.186993	0.398064
12	7	0	-3.448325	0.405872	1.393565
13	8	0	-3.309792	2.214181	0.030828
14	6	0	-2.668901	-1.426461	-0.901011
15	7	0	-1.991195	-2.277007	-0.199034
16	6	0	-0.652464	-1.952948	-0.434670
17	6	0	-0.606321	-0.852453	-1.309793
18	8	0	-1.901105	-0.510525	-1.607076
19	6	0	0.525843	-2.535846	-0.001650
20	6	0	1.750269	-2.004017	-0.452016
21	6	0	1.758133	-0.886523	-1.328807
22	6	0	0.563427	-0.285197	-1.770756
23	6	0	2.979389	-2.640100	0.093104
24	6	0	4.315896	-2.088409	-0.249198
25	6	0	4.523284	-1.016730	-1.136576
26	6	0	5.436219	-2.677506	0.369658
27	6	0	6.720208	-2.221338	0.121332
28	6	0	6.914693	-1.155402	-0.770037
29	6	0	5.829236	-0.558811	-1.394622
30	8	0	2.889149	-3.605071	0.855057
31	1	0	-6.976890	-0.395652	0.107231
32	1	0	-6.384970	0.547754	1.475416
33	1	0	-4.343538	-3.057588	0.262887
34	1	0	-5.850131	-2.559625	-0.500749
35	1	0	-3.316855	-1.583493	2.006925
36	1	0	-4.397462	-0.566386	2.969965
37	1	0	-7.036500	-2.549702	1.554945
38	1	0	-5.602489	-2.988831	2.495956
39	1	0	-6.536246	-1.543411	2.923169
40	1	0	-6.234103	2.627677	0.028302
41	1	0	-5.301599	2.594770	-1.470195
42	1	0	-6.839389	1.700393	-1.358053
43	1	0	-3.667258	-1.919091	-3.319059
44	1	0	-3.795688	-3.364987	-2.296526
45	1	0	-5.263329	-2.499255	-2.803114

46	1	0	-2.635628	0.769204	1.909498
47	1	0	0.542444	-3.381800	0.674414
48	1	0	0.564075	0.579888	-2.423155
49	1	0	5.247578	-3.500563	1.050071
50	1	0	7.570028	-2.685520	0.611838
51	1	0	7.916515	-0.788532	-0.973458
52	1	0	5.982589	0.271859	-2.078000
53	1	0	-5.690064	-0.305821	-2.120035
54	1	0	-4.108703	0.465493	-2.189612
55	16	0	3.231702	-0.145706	-1.952781
56	6	0	1.853268	3.490375	-2.416525
57	6	0	0.463106	3.429973	-2.606701
58	6	0	-0.364938	3.033529	-1.554682
59	6	0	0.190960	2.689144	-0.322248
60	6	0	1.602571	2.739241	-0.092002
61	6	0	2.407503	3.161093	-1.189052
62	7	0	-0.657665	2.314669	0.715908
63	6	0	-0.272622	1.843492	1.926412
64	6	0	1.221138	1.697083	2.186122
65	6	0	2.105178	2.399667	1.187735
66	8	0	-1.105267	1.462230	2.761945
67	6	0	4.460903	1.493272	1.709836
68	6	0	4.050056	0.453511	2.777489
69	6	0	1.448057	0.150499	2.256138
70	6	0	2.837056	-0.359732	2.453035
71	1	0	2.500750	3.791506	-3.234720
72	1	0	0.028518	3.692789	-3.566252
73	1	0	-1.443038	2.975802	-1.674113
74	1	0	3.484574	3.188525	-1.069189
75	1	0	-1.677802	2.350544	0.534919
76	1	0	1.407226	2.099502	3.191379
77	1	0	1.039495	-0.280047	1.332590
78	1	0	2.930901	-1.441412	2.471162
79	1	0	0.785882	-0.220151	3.054110
80	6	0	3.511020	2.706729	1.619357
81	1	0	4.891376	-0.230571	2.933181
82	1	0	3.914446	0.993287	3.732793
83	1	0	4.532248	1.003674	0.733572
84	1	0	5.463669	1.866114	1.956570
85	1	0	3.954825	3.458768	0.959781
86	1	0	3.466839	3.169728	2.617977

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^{3}TX-Int2'$_{ex}$ E(opt)= -2373.147212 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.939432	0.119174	1.285391
2	6	0	5.946073	0.914345	0.437602
3	6	0	5.488590	0.950161	-1.028252
4	6	0	5.343301	-0.499570	-1.567814
5	6	0	4.584747	-1.533247	-0.698032

6	6	0	4.945539	-1.351251	0.801652
7	6	0	4.176839	1.758163	-1.068476
8	6	0	6.520848	1.675922	-1.907234
9	6	0	5.303709	0.169636	2.775837
10	6	0	4.986056	-2.963943	-1.143919
11	6	0	3.518321	0.682365	1.105021
12	7	0	3.292199	1.494855	0.061655
13	8	0	2.611874	0.362602	1.900426
14	6	0	3.092737	-1.443146	-0.890963
15	7	0	2.395680	-0.799139	-1.768390
16	6	0	1.062804	-1.103481	-1.462744
17	6	0	1.052510	-1.986851	-0.367149
18	8	0	2.346725	-2.213821	-0.006900
19	6	0	-0.137938	-0.675228	-2.000695
20	6	0	-1.341368	-1.155156	-1.438913
21	6	0	-1.305675	-2.071283	-0.352965
22	6	0	-0.089013	-2.496707	0.207860
23	6	0	-2.601121	-0.620645	-2.013534
24	6	0	-3.914109	-1.077691	-1.494030
25	6	0	-4.070180	-1.965695	-0.412677
26	6	0	-5.070927	-0.544318	-2.098193
27	6	0	-6.337847	-0.858848	-1.635585
28	6	0	-6.478339	-1.723066	-0.538851
29	6	0	-5.357595	-2.272658	0.066504
30	8	0	-2.559240	0.237464	-2.903050
31	1	0	6.938063	0.450730	0.521455
32	1	0	6.038868	1.938941	0.820369
33	1	0	4.902387	-0.477037	-2.569828
34	1	0	6.361874	-0.891532	-1.680706
35	1	0	3.622155	1.535826	-1.986013
36	1	0	4.418161	2.829473	-1.075049
37	1	0	7.476105	1.140338	-1.912601
38	1	0	6.172293	1.751977	-2.943592
39	1	0	6.706855	2.690168	-1.538353
40	1	0	5.346483	1.204442	3.131076
41	1	0	4.554672	-0.359516	3.368285
42	1	0	6.284719	-0.288554	2.942000
43	1	0	4.448734	-3.717994	-0.562098
44	1	0	4.757396	-3.117174	-2.203334
45	1	0	6.060240	-3.114675	-0.997592
46	1	0	2.320975	1.817135	-0.060434
47	1	0	-0.188388	0.031791	-2.819143
48	1	0	-0.051830	-3.161729	1.062634
49	1	0	-4.925945	0.130830	-2.933738
50	1	0	-7.215159	-0.434910	-2.113837
51	1	0	-7.465754	-1.967261	-0.158114
52	1	0	-5.468624	-2.942095	0.914737
53	1	0	5.959005	-1.743951	0.952266
54	1	0	4.270984	-1.947284	1.421387
55	16	0	-2.735464	-2.749409	0.413878
56	6	0	-3.078387	-0.811390	3.554659
57	6	0	-1.724436	-1.088756	3.799358
58	6	0	-0.734927	-0.493893	3.012168

59	6	0	-1.091610	0.368520	1.977866
60	6	0	-2.464459	0.651212	1.686154
61	6	0	-3.441668	0.039017	2.522691
62	7	0	-0.088479	0.969359	1.214640
63	6	0	-0.291572	1.822945	0.179625
64	6	0	-1.715433	2.147568	-0.219957
65	6	0	-2.785315	1.505717	0.612311
66	8	0	0.654847	2.323851	-0.444811
67	6	0	-4.252401	2.791479	-0.966635
68	6	0	-3.350893	4.031738	-0.827132
69	6	0	-1.925047	3.712451	-0.277394
70	6	0	-1.663806	4.329250	1.057648
71	1	0	-3.845791	-1.269470	4.171914
72	1	0	-1.439590	-1.758901	4.604670
73	1	0	0.319005	-0.686267	3.193418
74	1	0	-4.490825	0.236341	2.331867
75	1	0	0.894721	0.770899	1.466498
76	1	0	-1.789263	1.804393	-1.263953
77	1	0	-5.284328	3.101801	-1.164265
78	1	0	-3.935925	2.192177	-1.827720
79	1	0	-3.836017	4.748768	-0.153927
80	1	0	-3.268280	4.532118	-1.797730
81	1	0	-1.162152	4.067795	-0.979616
82	1	0	-2.474541	4.517106	1.754810
83	1	0	-0.646782	4.411829	1.427452
84	6	0	-4.198819	1.919184	0.294458
85	1	0	-4.840897	1.037452	0.171830
86	1	0	-4.617349	2.478113	1.148298

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^{3}TX-Int2'$_{en}$ E(opt)= -2373.139938 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.851999	0.783271	-0.656373
2	6	0	-5.787778	0.709731	0.561261
3	6	0	-5.289199	-0.352064	1.552426
4	6	0	-5.236915	-1.732410	0.845354
5	6	0	-4.526558	-1.812253	-0.528381
6	6	0	-4.889614	-0.577561	-1.399324
7	6	0	-3.921016	0.123988	2.078804
8	6	0	-6.244324	-0.472060	2.751335
9	6	0	-5.279664	1.900909	-1.617059
10	6	0	-4.986066	-3.097243	-1.266390
11	6	0	-3.403115	1.031673	-0.210022
12	7	0	-3.068777	0.718626	1.052176
13	8	0	-2.564612	1.459929	-1.027701
14	6	0	-3.033951	-1.944041	-0.363601
15	7	0	-2.337757	-2.192659	0.696251
16	6	0	-1.011563	-2.234752	0.254498
17	6	0	-1.001109	-2.029146	-1.135736
18	8	0	-2.293505	-1.843007	-1.535250

19	6	0	0.184262	-2.402811	0.929858
20	6	0	1.382344	-2.411353	0.189897
21	6	0	1.348793	-2.253756	-1.221725
22	6	0	0.140964	-2.038459	-1.908691
23	6	0	2.638504	-2.545526	0.973600
24	6	0	3.953012	-2.596709	0.278819
25	6	0	4.115429	-2.506641	-1.115913
26	6	0	5.102422	-2.721495	1.083652
27	6	0	6.371518	-2.756272	0.528588
28	6	0	6.519332	-2.669469	-0.863491
29	6	0	5.403579	-2.546383	-1.679737
30	8	0	2.596205	-2.595962	2.204347
31	1	0	-6.805232	0.471303	0.223405
32	1	0	-5.837662	1.687542	1.058020
33	1	0	-4.803597	-2.477576	1.520155
34	1	0	-6.277800	-2.032022	0.668868
35	1	0	-3.373664	-0.713387	2.521209
36	1	0	-4.085594	0.871944	2.866429
37	1	0	-7.234842	-0.810556	2.429384
38	1	0	-5.865815	-1.191478	3.486400
39	1	0	-6.366860	0.492780	3.254912
40	1	0	-5.285828	2.869917	-1.107387
41	1	0	-4.586858	1.968144	-2.457996
42	1	0	-6.289119	1.708579	-1.996117
43	1	0	-4.483766	-3.190749	-2.233314
44	1	0	-4.757621	-3.986898	-0.671111
45	1	0	-6.066504	-3.065719	-1.438989
46	1	0	-2.063940	0.754064	1.275199
47	1	0	0.233766	-2.510457	2.005782
48	1	0	0.107044	-1.886964	-2.981763
49	1	0	4.948975	-2.784487	2.155305
50	1	0	7.244903	-2.850700	1.166235
51	1	0	7.508546	-2.695086	-1.311168
52	1	0	5.522476	-2.472787	-2.757153
53	1	0	-5.914609	-0.720795	-1.763936
54	1	0	-4.237060	-0.535759	-2.275616
55	16	0	2.783567	-2.300640	-2.248402
56	6	0	1.742221	5.484430	-1.985199
57	6	0	0.558424	4.920251	-2.486222
58	6	0	-0.029791	3.839967	-1.825182
59	6	0	0.557166	3.320565	-0.673286
60	6	0	1.767672	3.871858	-0.133119
61	6	0	2.330132	4.976188	-0.838439
62	7	0	-0.067007	2.250735	-0.025272
63	6	0	0.375747	1.647397	1.105095
64	6	0	1.739296	2.049442	1.623107
65	6	0	2.315275	3.307331	1.037788
66	8	0	-0.287247	0.771401	1.681244
67	6	0	4.654925	2.567717	1.555126
68	6	0	4.095010	1.238134	2.085137
69	6	0	2.760975	0.864883	1.410021
70	6	0	2.933688	0.553953	-0.039138
71	1	0	2.202276	6.324272	-2.497833

72	1	0	0.096371	5.320054	-3.383521
73	1	0	-0.951217	3.393227	-2.188630
74	1	0	3.245685	5.424736	-0.468855
75	1	0	-0.972448	1.920530	-0.404500
76	1	0	1.625941	2.151101	2.712527
77	1	0	5.569091	2.838960	2.096431
78	1	0	4.925760	2.455026	0.498310
79	1	0	3.936718	1.312798	3.169189
80	1	0	4.817060	0.428014	1.925784
81	1	0	2.328539	-0.003442	1.932606
82	1	0	2.088792	0.548906	-0.717393
83	1	0	3.903500	0.284570	-0.440267
84	6	0	3.613431	3.709326	1.677883
85	1	0	4.019083	4.634146	1.260482
86	1	0	3.437744	3.899029	2.748826

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^{BS}TX-TS2$_{ex}$ E(opt)= -2373.150691 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.913947	0.663471	1.255076
2	6	0	5.932035	1.217827	0.245041
3	6	0	5.545758	0.793051	-1.179475
4	6	0	5.480475	-0.757131	-1.263860
5	6	0	4.716326	-1.520574	-0.152949
6	6	0	4.995256	-0.882363	1.235482
7	6	0	4.209380	1.487752	-1.507408
8	6	0	6.592865	1.273828	-2.197997
9	6	0	5.202444	1.173604	2.673952
10	6	0	5.188352	-2.997995	-0.134022
11	6	0	3.484306	1.076881	0.862926
12	7	0	3.279390	1.529263	-0.383392
13	8	0	2.552860	0.964202	1.685264
14	6	0	3.233861	-1.561546	-0.420743
15	7	0	2.563220	-1.234945	-1.476011
16	6	0	1.226246	-1.489625	-1.145587
17	6	0	1.186102	-2.010896	0.161048
18	8	0	2.467284	-2.067970	0.622446
19	6	0	0.042898	-1.284902	-1.832179
20	6	0	-1.173272	-1.622990	-1.200243
21	6	0	-1.167549	-2.175003	0.109012
22	6	0	0.031040	-2.371807	0.816760
23	6	0	-2.415707	-1.332800	-1.960273
24	6	0	-3.743505	-1.604513	-1.352337
25	6	0	-3.928747	-2.139022	-0.063346
26	6	0	-4.881671	-1.258399	-2.107883
27	6	0	-6.160687	-1.423053	-1.602949
28	6	0	-6.331436	-1.937044	-0.308466
29	6	0	-5.228348	-2.291288	0.455253
30	8	0	-2.348841	-0.820376	-3.081643
31	1	0	6.934538	0.848809	0.499591

32	1	0	5.969519	2.313157	0.306332
33	1	0	5.090571	-1.056553	-2.242225
34	1	0	6.517062	-1.113558	-1.215142
35	1	0	3.709243	0.976264	-2.336238
36	1	0	4.412715	2.519237	-1.824642
37	1	0	7.565961	0.808522	-2.008367
38	1	0	6.292844	1.020501	-3.221272
39	1	0	6.723876	2.359769	-2.143666
40	1	0	5.190799	2.268059	2.703758
41	1	0	4.444618	0.809255	3.370354
42	1	0	6.189853	0.834144	3.005201
43	1	0	4.648612	-3.569094	0.626498
44	1	0	5.018245	-3.470680	-1.106522
45	1	0	6.258410	-3.047156	0.090845
46	1	0	2.304404	1.753035	-0.630616
47	1	0	0.013634	-0.853058	-2.824609
48	1	0	0.042836	-2.751589	1.831529
49	1	0	-4.710383	-0.846715	-3.096252
50	1	0	-7.024235	-1.147916	-2.200243
51	1	0	-7.328663	-2.058366	0.104457
52	1	0	-5.362781	-2.685343	1.458528
53	1	0	6.012819	-1.163158	1.534999
54	1	0	4.311274	-1.297960	1.979721
55	16	0	-2.616963	-2.655909	0.982226
56	6	0	-3.100612	0.036869	3.468893
57	6	0	-1.745367	-0.104230	3.797561
58	6	0	-0.764994	0.299027	2.888782
59	6	0	-1.132504	0.838114	1.656789
60	6	0	-2.503974	0.986691	1.285720
61	6	0	-3.470323	0.568888	2.242549
62	7	0	-0.127925	1.238055	0.772293
63	6	0	-0.323660	1.741373	-0.471178
64	6	0	-1.745891	1.901009	-0.982087
65	6	0	-2.834567	1.547559	0.021067
66	8	0	0.629773	2.059138	-1.195994
67	6	0	-4.925640	2.963148	0.186857
68	6	0	-4.185252	4.239718	-0.293564
69	6	0	-1.990387	3.376354	-1.410149
70	6	0	-2.699941	4.061507	-0.268177
71	1	0	-3.866552	-0.276367	4.172366
72	1	0	-1.452660	-0.522104	4.755935
73	1	0	0.291977	0.202594	3.121447
74	1	0	-4.523016	0.657094	2.000325
75	1	0	0.852412	1.153826	1.089818
76	1	0	-4.861421	2.903877	1.279308
77	1	0	-5.991463	3.013327	-0.073799
78	1	0	-4.506599	4.454177	-1.323933
79	1	0	-2.623327	3.396565	-2.304320
80	1	0	-1.040330	3.849125	-1.681118
81	1	0	-4.495670	5.091947	0.323070
82	6	0	-4.271301	1.701206	-0.415332
83	1	0	-4.850928	0.815861	-0.131894
84	1	0	-4.319496	1.750926	-1.510025

85	1	0	-1.792897	1.245656	-1.865419
86	1	0	-2.121547	4.405691	0.584391

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^{BS}TX-TS2$_{en}$ E(opt)= -2373.142314 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.025983	0.801521	0.908305
2	6	0	5.994973	0.877948	-0.284389
3	6	0	5.481719	0.011488	-1.444370
4	6	0	5.333375	-1.458254	-0.969621
5	6	0	4.569778	-1.705133	0.353419
6	6	0	4.988149	-0.659690	1.419346
7	6	0	4.155611	0.634619	-1.924862
8	6	0	6.470532	0.029919	-2.621589
9	6	0	5.473653	1.729165	2.046284
10	6	0	4.904044	-3.125898	0.879908
11	6	0	3.608799	1.209238	0.467788
12	7	0	3.318800	1.140386	-0.842228
13	8	0	2.760910	1.563616	1.309567
14	6	0	3.077419	-1.695300	0.139349
15	7	0	2.391999	-1.902424	-0.937967
16	6	0	1.053950	-1.859309	-0.523677
17	6	0	1.029032	-1.628044	0.864421
18	8	0	2.320393	-1.533818	1.290513
19	6	0	-0.141179	-2.004875	-1.207067
20	6	0	-1.350860	-1.921754	-0.484105
21	6	0	-1.328955	-1.681458	0.915560
22	6	0	-0.118930	-1.529620	1.615451
23	6	0	-2.603290	-2.101818	-1.264114
24	6	0	-3.923283	-1.981233	-0.591240
25	6	0	-4.090630	-1.693614	0.776426
26	6	0	-5.073404	-2.121785	-1.393567
27	6	0	-6.344298	-1.951905	-0.870983
28	6	0	-6.495906	-1.634593	0.487667
29	6	0	-5.382868	-1.510996	1.305622
30	8	0	-2.551736	-2.315919	-2.477900
31	1	0	6.990355	0.540714	0.034080
32	1	0	6.101601	1.918333	-0.617979
33	1	0	4.882928	-2.060779	-1.765080
34	1	0	6.348821	-1.844715	-0.814915
35	1	0	3.574150	-0.104784	-2.486471
36	1	0	4.377396	1.468718	-2.603972
37	1	0	7.429785	-0.412874	-2.333297
38	1	0	6.080200	-0.539266	-3.472992
39	1	0	6.661271	1.054329	-2.958733
40	1	0	5.546463	2.764678	1.698525
41	1	0	4.754098	1.700842	2.866765
42	1	0	6.457650	1.423737	2.418135
43	1	0	4.357988	-3.335609	1.804501
44	1	0	4.633991	-3.884498	0.139042

45	1	0	5.975994	-3.207952	1.086285
46	1	0	2.388133	1.483624	-1.118548
47	1	0	-0.184552	-2.188451	-2.273722
48	1	0	-0.092886	-1.322998	2.678398
49	1	0	-4.918132	-2.357818	-2.440479
50	1	0	-7.216391	-2.057440	-1.508455
51	1	0	-7.486830	-1.485921	0.906736
52	1	0	-5.502041	-1.268811	2.357863
53	1	0	6.001303	-0.915735	1.754065
54	1	0	4.332920	-0.729384	2.291166
55	16	0	-2.767160	-1.550983	1.918687
56	6	0	-2.979308	1.699773	3.312890
57	6	0	-1.639843	1.528283	3.686692
58	6	0	-0.633314	1.637296	2.725951
59	6	0	-0.957422	1.928173	1.400428
60	6	0	-2.310859	2.132188	0.990499
61	6	0	-3.305388	1.984542	1.994912
62	7	0	0.069935	1.986093	0.455157
63	6	0	-0.087800	2.313337	-0.851353
64	6	0	-1.439294	2.880477	-1.281679
65	6	0	-2.589034	2.481458	-0.366684
66	8	0	0.847572	2.223103	-1.656907
67	6	0	-4.735798	1.565214	-1.356311
68	6	0	-4.030845	1.055145	-2.639162
69	6	0	-1.788074	2.388936	-2.697314
70	6	0	-2.541972	1.095681	-2.502328
71	1	0	-3.767635	1.602944	4.053662
72	1	0	-1.379950	1.308869	4.717805
73	1	0	0.412072	1.499587	2.988898
74	1	0	-4.348953	2.095804	1.723032
75	1	0	1.034180	1.778372	0.765663
76	1	0	-1.281190	3.978020	-1.258068
77	1	0	-0.874845	2.269336	-3.288044
78	1	0	-1.978222	0.171944	-2.448261
79	1	0	-2.417005	3.125612	-3.209857
80	6	0	-3.998090	2.805801	-0.810418
81	1	0	-4.337597	1.704537	-3.475002
82	1	0	-4.371958	0.042691	-2.871583
83	1	0	-4.713628	0.777700	-0.595499
84	1	0	-5.791020	1.792667	-1.559017
85	1	0	-3.976269	3.580372	-1.587918
86	1	0	-4.568141	3.235557	0.020856

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^{BS}TX-TS2'$_{en}$ E(opt)= -2373.138092 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.900861	0.794319	-0.605526
2	6	0	-5.826275	0.647901	0.613579
3	6	0	-5.302814	-0.450034	1.551505
4	6	0	-5.230987	-1.794774	0.780917
5	6	0	-4.517529	-1.795033	-0.593070

6	6	0	-4.914844	-0.533399	-1.407257
7	6	0	-3.937959	0.023531	2.088900
8	6	0	-6.246559	-0.641367	2.749924
9	6	0	-5.357409	1.944094	-1.513303
10	6	0	-4.940007	-3.058038	-1.388813
11	6	0	-3.453854	1.049813	-0.158047
12	7	0	-3.103420	0.677810	1.083987
13	8	0	-2.629968	1.532846	-0.959396
14	6	0	-3.022057	-1.896030	-0.429169
15	7	0	-2.326697	-2.230304	0.607927
16	6	0	-0.997139	-2.198464	0.174728
17	6	0	-0.983493	-1.855355	-1.188244
18	8	0	-2.277834	-1.663065	-1.578405
19	6	0	0.198664	-2.414146	0.836560
20	6	0	1.399900	-2.330430	0.106221
21	6	0	1.370110	-2.030459	-1.282214
22	6	0	0.161806	-1.764480	-1.950523
23	6	0	2.654491	-2.543029	0.875188
24	6	0	3.964456	-2.585747	0.171098
25	6	0	4.130044	-2.352361	-1.206791
26	6	0	5.106220	-2.858789	0.949607
27	6	0	6.370976	-2.899121	0.385502
28	6	0	6.522351	-2.665009	-0.989138
29	6	0	5.414161	-2.394157	-1.779541
30	8	0	2.613117	-2.683869	2.098801
31	1	0	-6.841887	0.407439	0.271709
32	1	0	-5.889496	1.600710	1.155415
33	1	0	-4.785528	-2.564020	1.419781
34	1	0	-6.266942	-2.102111	0.589014
35	1	0	-3.373806	-0.824346	2.488480
36	1	0	-4.107261	0.731869	2.911387
37	1	0	-7.233357	-0.982454	2.419366
38	1	0	-5.850058	-1.386769	3.448691
39	1	0	-6.382187	0.297182	3.297917
40	1	0	-5.380801	2.889264	-0.961133
41	1	0	-4.671194	2.063033	-2.353920
42	1	0	-6.364837	1.747455	-1.895504
43	1	0	-4.433032	-3.094247	-2.357341
44	1	0	-4.687979	-3.966409	-0.832812
45	1	0	-6.020490	-3.048650	-1.564100
46	1	0	-2.098089	0.722498	1.303388
47	1	0	0.245622	-2.633572	1.895568
48	1	0	0.129294	-1.509022	-3.003726
49	1	0	4.950842	-3.030154	2.009084
50	1	0	7.238585	-3.110274	1.002747
51	1	0	7.508484	-2.693110	-1.443420
52	1	0	5.535771	-2.209194	-2.843183
53	1	0	-5.939604	-0.684197	-1.769441
54	1	0	-4.271254	-0.438345	-2.285881
55	16	0	2.810200	-1.948394	-2.299520
56	6	0	1.791151	5.362154	-2.025296
57	6	0	0.546815	4.881022	-2.453640
58	6	0	-0.063457	3.827620	-1.770077

59	6	0	0.564601	3.254245	-0.665459
60	6	0	1.834243	3.721023	-0.202953
61	6	0	2.418212	4.795576	-0.924155
62	7	0	-0.076488	2.199499	-0.004960
63	6	0	0.353373	1.594361	1.128879
64	6	0	1.700566	2.005558	1.689185
65	6	0	2.440670	3.075018	0.911072
66	8	0	-0.325143	0.728877	1.701513
67	6	0	4.652062	2.401644	1.957276
68	6	0	3.921098	1.180468	2.536536
69	6	0	2.683998	0.809998	1.695313
70	6	0	3.056686	0.645513	0.247736
71	1	0	2.269141	6.181963	-2.553481
72	1	0	0.052604	5.323771	-3.312980
73	1	0	-1.031703	3.443097	-2.078639
74	1	0	3.381613	5.180589	-0.608656
75	1	0	-0.999268	1.901618	-0.367461
76	1	0	1.495681	2.327361	2.724260
77	1	0	5.418713	2.756369	2.656002
78	1	0	5.167745	2.109184	1.036024
79	1	0	3.602633	1.379273	3.568422
80	1	0	4.599804	0.319667	2.573665
81	1	0	2.213792	-0.086562	2.126156
82	1	0	2.289381	0.648265	-0.517358
83	1	0	4.026676	0.253614	-0.037869
84	6	0	3.682560	3.554653	1.613237
85	1	0	4.213820	4.318799	1.040675
86	1	0	3.366407	4.037619	2.554207

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^{BS}TX-TS2'$_{ex}$ E(opt)= -2373.145249 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.948652	0.150872	1.287379
2	6	0	5.954187	0.940749	0.433261
3	6	0	5.498022	0.962407	-1.033296
4	6	0	5.356341	-0.492332	-1.560046
5	6	0	4.598826	-1.519354	-0.681638
6	6	0	4.958435	-1.323648	0.816499
7	6	0	4.184372	1.766795	-1.081988
8	6	0	6.529408	1.682632	-1.917814
9	6	0	5.311918	0.215137	2.777522
10	6	0	5.002417	-2.953390	-1.114747
11	6	0	3.526484	0.709880	1.101329
12	7	0	3.299562	1.511491	0.049713
13	8	0	2.620322	0.397135	1.899721
14	6	0	3.106811	-1.433810	-0.876507
15	7	0	2.409165	-0.804090	-1.763754
16	6	0	1.076742	-1.108807	-1.456256
17	6	0	1.067598	-1.976901	-0.348207
18	8	0	2.361764	-2.194411	0.017197

19	6	0	-0.124509	-0.695302	-2.004112
20	6	0	-1.327376	-1.173419	-1.438877
21	6	0	-1.290250	-2.070222	-0.337044
22	6	0	-0.072809	-2.482489	0.232160
23	6	0	-2.588097	-0.660766	-2.031161
24	6	0	-3.899969	-1.106098	-1.498366
25	6	0	-4.053613	-1.968629	-0.396257
26	6	0	-5.058235	-0.586070	-2.111628
27	6	0	-6.323813	-0.887107	-1.637111
28	6	0	-6.461633	-1.724597	-0.519390
29	6	0	-5.339977	-2.262180	0.094481
30	8	0	-2.548751	0.173059	-2.943038
31	1	0	6.947177	0.480209	0.522096
32	1	0	6.044259	1.968943	0.806900
33	1	0	4.916388	-0.479706	-2.562663
34	1	0	6.375757	-0.883400	-1.668368
35	1	0	3.631108	1.534886	-1.998057
36	1	0	4.422939	2.838615	-1.098078
37	1	0	7.485867	1.149164	-1.917625
38	1	0	6.181561	1.748699	-2.955093
39	1	0	6.712810	2.700528	-1.557799
40	1	0	5.352413	1.253100	3.123681
41	1	0	4.563508	-0.310211	3.374130
42	1	0	6.293718	-0.239662	2.948301
43	1	0	4.465882	-3.703086	-0.526587
44	1	0	4.774599	-3.116225	-2.172903
45	1	0	6.076728	-3.101226	-0.966446
46	1	0	2.329024	1.835171	-0.073703
47	1	0	-0.176486	-0.003097	-2.835103
48	1	0	-0.034700	-3.133698	1.097399
49	1	0	-4.915310	0.067486	-2.964487
50	1	0	-7.202162	-0.473182	-2.122117
51	1	0	-7.448083	-1.957394	-0.129114
52	1	0	-5.449029	-2.911094	0.958738
53	1	0	5.972750	-1.712680	0.970882
54	1	0	4.285104	-1.915908	1.441145
55	16	0	-2.718114	-2.738092	0.441366
56	6	0	-3.068200	-0.791955	3.544068
57	6	0	-1.715967	-1.079615	3.774950
58	6	0	-0.728771	-0.480395	2.987994
59	6	0	-1.088199	0.399380	1.968924
60	6	0	-2.458637	0.696613	1.697609
61	6	0	-3.432182	0.077535	2.525504
62	7	0	-0.082758	1.007595	1.209619
63	6	0	-0.281994	1.849663	0.163038
64	6	0	-1.704611	2.156751	-0.257116
65	6	0	-2.780238	1.601463	0.653848
66	8	0	0.665585	2.347371	-0.460288
67	6	0	-4.258690	2.757629	-1.019036
68	6	0	-3.301887	3.969638	-1.008684
69	6	0	-1.981906	3.680843	-0.246326
70	6	0	-2.094179	4.010100	1.219290
71	1	0	-3.834908	-1.254837	4.158515

72	1	0	-1.428707	-1.763026	4.568271
73	1	0	0.325215	-0.682816	3.157653
74	1	0	-4.481018	0.286898	2.345787
75	1	0	0.899349	0.808607	1.463891
76	1	0	-1.775815	1.765303	-1.283039
77	1	0	-5.285508	3.081821	-1.219485
78	1	0	-3.977306	2.094813	-1.844447
79	1	0	-3.789626	4.840318	-0.553510
80	1	0	-3.074643	4.247583	-2.043666
81	1	0	-1.152078	4.221203	-0.726435
82	1	0	-2.804988	4.748360	1.579159
83	1	0	-1.295406	3.723682	1.896573
84	6	0	-4.207002	1.941662	0.282500
85	1	0	-4.791360	1.020476	0.152147
86	1	0	-4.687169	2.488669	1.105326

TX-Prod$_{RSR}$ E(opt)= -2373.215338 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.924171	0.651921	1.185767
2	6	0	5.943091	1.164174	0.154790
3	6	0	5.553246	0.684423	-1.251137
4	6	0	5.475527	-0.868291	-1.274617
5	6	0	4.718581	-1.585821	-0.128007
6	6	0	5.011460	-0.892739	1.231190
7	6	0	4.222854	1.377663	-1.604890
8	6	0	6.603327	1.115596	-2.288701
9	6	0	5.207605	1.223227	2.582167
10	6	0	5.184156	-3.062949	-0.055316
11	6	0	3.492846	1.044064	0.773959
12	7	0	3.293250	1.467652	-0.483419
13	8	0	2.557164	0.941914	1.592668
14	6	0	3.232605	-1.623539	-0.374515
15	7	0	2.547145	-1.308847	-1.423539
16	6	0	1.211877	-1.515040	-1.055458
17	6	0	1.188069	-1.997793	0.266415
18	8	0	2.477171	-2.084354	0.697778
19	6	0	0.018955	-1.296335	-1.720378
20	6	0	-1.189216	-1.589969	-1.052896
21	6	0	-1.169425	-2.102761	0.272571
22	6	0	0.039664	-2.307973	0.959119
23	6	0	-2.441697	-1.315395	-1.798649
24	6	0	-3.746131	-1.768422	-1.249517
25	6	0	-3.922353	-2.257653	0.057873
26	6	0	-4.877673	-1.642479	-2.080677
27	6	0	-6.143750	-1.975003	-1.630294
28	6	0	-6.309343	-2.439811	-0.316252
29	6	0	-5.212335	-2.580983	0.520172
30	8	0	-2.407413	-0.706824	-2.872395
31	1	0	6.944941	0.803342	0.423326

32	1	0	5.983105	2.260976	0.171889
33	1	0	5.074084	-1.201624	-2.237291
34	1	0	6.510072	-1.230132	-1.222659
35	1	0	3.718205	0.840174	-2.414358
36	1	0	4.435092	2.394804	-1.960261
37	1	0	7.573205	0.651430	-2.080584
38	1	0	6.300929	0.823164	-3.300810
39	1	0	6.742184	2.201876	-2.278614
40	1	0	5.195438	2.317987	2.564468
41	1	0	4.447215	0.888534	3.290646
42	1	0	6.193955	0.899128	2.931623
43	1	0	4.647175	-3.601836	0.730286
44	1	0	5.005305	-3.572204	-1.007610
45	1	0	6.255498	-3.108634	0.164153
46	1	0	2.316413	1.670613	-0.743888
47	1	0	-0.022280	-0.886330	-2.721576
48	1	0	0.067085	-2.668977	1.980474
49	1	0	-4.715028	-1.258031	-3.081577
50	1	0	-7.002564	-1.871751	-2.286023
51	1	0	-7.298590	-2.695989	0.051879
52	1	0	-5.343394	-2.945738	1.535045
53	1	0	6.032983	-1.158450	1.531095
54	1	0	4.336093	-1.279356	1.998340
55	16	0	-2.613416	-2.469896	1.208744
56	6	0	-3.107294	0.435175	3.508874
57	6	0	-1.767458	0.142914	3.770706
58	6	0	-0.794008	0.446188	2.823671
59	6	0	-1.157772	1.040187	1.607111
60	6	0	-2.504149	1.335951	1.318041
61	6	0	-3.458272	1.026419	2.295392
62	7	0	-0.133450	1.326045	0.689888
63	6	0	-0.301018	1.824389	-0.559544
64	6	0	-1.689311	2.226719	-0.985045
65	6	0	-2.858382	2.062653	0.041717
66	8	0	0.656359	1.991131	-1.328765
67	6	0	-4.782517	2.914697	-1.254154
68	6	0	-4.380087	4.021033	-0.262567
69	6	0	-1.870123	3.776939	-0.958661
70	6	0	-2.955462	3.642947	0.145838
71	1	0	-3.874137	0.207719	4.243211
72	1	0	-1.478239	-0.316976	4.711292
73	1	0	0.255718	0.234909	3.007668
74	1	0	-4.500968	1.263330	2.107968
75	1	0	0.837600	1.147371	0.990204
76	1	0	-1.870199	1.757928	-1.956644
77	1	0	-4.337526	3.109979	-2.237208
78	1	0	-5.864228	2.842020	-1.404039
79	1	0	-5.036018	3.990313	0.617310
80	1	0	-0.973367	4.329219	-0.667027
81	1	0	-2.653154	4.057515	1.110935
82	1	0	-2.232370	4.193780	-1.902633
83	1	0	-4.445404	5.029174	-0.687977
84	6	0	-4.181124	1.632012	-0.646016

85	1	0	-4.004507	0.864537	-1.399185
86	1	0	-4.875333	1.207644	0.084961

TX-Prod$_{SRS}$ E(opt)= -2373.215449 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.903222	1.255371	0.677064
2	6	0	5.851739	1.273261	-0.533980
3	6	0	5.467368	0.166637	-1.527490
4	6	0	5.536578	-1.212910	-0.819555
5	6	0	4.809064	-1.350015	0.539539
6	6	0	5.070748	-0.096810	1.415006
7	6	0	4.064502	0.510205	-2.069328
8	6	0	6.441551	0.135653	-2.716641
9	6	0	5.217658	2.405566	1.643482
10	6	0	5.334215	-2.606327	1.281495
11	6	0	3.442327	1.387436	0.209997
12	7	0	3.160276	1.055425	-1.061216
13	8	0	2.557270	1.760811	1.003581
14	6	0	3.331780	-1.573806	0.342882
15	7	0	2.696031	-2.035219	-0.684511
16	6	0	1.351342	-2.048614	-0.294581
17	6	0	1.270235	-1.585065	1.031495
18	8	0	2.537090	-1.299748	1.446267
19	6	0	0.190972	-2.397329	-0.963111
20	6	0	-1.042041	-2.270937	-0.289708
21	6	0	-1.080332	-1.786862	1.045466
22	6	0	0.095751	-1.442190	1.734226
23	6	0	-2.256025	-2.651543	-1.060224
24	6	0	-3.604218	-2.377429	-0.493538
25	6	0	-3.832109	-1.886073	0.806134
26	6	0	-4.710556	-2.570806	-1.343876
27	6	0	-5.999796	-2.282804	-0.927073
28	6	0	-6.213911	-1.793583	0.370490
29	6	0	-5.143256	-1.598163	1.230746
30	8	0	-2.149214	-3.143113	-2.184505
31	1	0	6.885048	1.135717	-0.188493
32	1	0	5.808874	2.250529	-1.032242
33	1	0	5.184694	-1.995910	-1.498924
34	1	0	6.597300	-1.415186	-0.623262
35	1	0	3.596323	-0.382904	-2.496630
36	1	0	4.164935	1.250411	-2.874418
37	1	0	7.455094	-0.113670	-2.385057
38	1	0	6.136461	-0.613029	-3.456625
39	1	0	6.481857	1.108907	-3.217265
40	1	0	5.143535	3.372263	1.135030
41	1	0	4.510500	2.409488	2.475118
42	1	0	6.235393	2.302785	2.035215
43	1	0	4.816729	-2.737515	2.236660
44	1	0	5.176546	-3.504563	0.676875

45	1	0	6.405871	-2.505644	1.481218
46	1	0	2.182643	1.184690	-1.361189
47	1	0	0.191639	-2.759047	-1.984012
48	1	0	0.075058	-1.049284	2.743248
49	1	0	-4.506121	-2.942954	-2.341705
50	1	0	-6.837996	-2.429545	-1.600903
51	1	0	-7.219548	-1.557772	0.706373
52	1	0	-5.308738	-1.203641	2.229165
53	1	0	6.109084	-0.150731	1.765835
54	1	0	4.429710	-0.116030	2.299896
55	16	0	-2.560175	-1.561413	1.972636
56	6	0	-3.052488	1.923506	3.212400
57	6	0	-1.697606	1.778091	3.522311
58	6	0	-0.749023	1.749216	2.504114
59	6	0	-1.150692	1.872138	1.165466
60	6	0	-2.505114	2.059627	0.837669
61	6	0	-3.438840	2.065474	1.880485
62	7	0	-0.164772	1.778551	0.169183
63	6	0	-0.393402	1.729153	-1.167412
64	6	0	-1.799777	1.988493	-1.646236
65	6	0	-2.927967	2.241890	-0.597590
66	8	0	0.514719	1.504299	-1.979148
67	6	0	-4.567611	3.214974	-2.127374
68	6	0	-4.991832	1.749777	-1.903887
69	6	0	-2.579618	0.766745	-2.212448
70	6	0	-3.769170	1.079359	-1.262807
71	1	0	-3.799173	1.931603	4.000690
72	1	0	-1.378633	1.682138	4.556194
73	1	0	0.308755	1.631996	2.723381
74	1	0	-4.492020	2.180585	1.636990
75	1	0	0.820069	1.708524	0.473028
76	1	0	-1.712278	2.798206	-2.377657
77	1	0	-3.953385	3.295545	-3.032847
78	1	0	-5.415156	3.895499	-2.255364
79	1	0	-5.833893	1.713497	-1.200807
80	1	0	-2.089181	-0.187153	-2.013106
81	1	0	-4.045798	0.259936	-0.602536
82	1	0	-2.801686	0.816066	-3.282259
83	1	0	-5.313067	1.246183	-2.822305
84	6	0	-3.725703	3.536603	-0.878197
85	1	0	-3.065699	4.402121	-1.002997
86	1	0	-4.388398	3.753734	-0.032719

TX-Prod'$_{RSS}$ E(opt)= -2373.215866 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.931704	0.375258	1.260941
2	6	0	5.924815	1.077425	0.320233
3	6	0	5.487051	0.895623	-1.140699
4	6	0	5.399150	-0.618786	-1.475432

5	6	0	4.648796	-1.541590	-0.483130
6	6	0	4.982886	-1.146842	0.981171
7	6	0	4.149171	1.643561	-1.304833
8	6	0	6.506759	1.529722	-2.101343
9	6	0	5.279498	0.637046	2.732947
10	6	0	5.084204	-3.010873	-0.722897
11	6	0	3.497407	0.868010	0.996446
12	7	0	3.255352	1.505858	-0.159251
13	8	0	2.595973	0.647848	1.829751
14	6	0	3.159501	-1.508886	-0.710442
15	7	0	2.474176	-1.034925	-1.698317
16	6	0	1.138769	-1.294452	-1.366142
17	6	0	1.114456	-1.974675	-0.134002
18	8	0	2.403851	-2.124461	0.280333
19	6	0	-0.053914	-0.978894	-1.991265
20	6	0	-1.264132	-1.364369	-1.374659
21	6	0	-1.243614	-2.064851	-0.138390
22	6	0	-0.034264	-2.381058	0.505172
23	6	0	-2.514968	-0.966407	-2.068863
24	6	0	-3.835315	-1.309075	-1.481164
25	6	0	-4.005221	-1.968337	-0.248799
26	6	0	-4.982811	-0.888499	-2.184024
27	6	0	-6.254557	-1.090020	-1.675455
28	6	0	-6.409165	-1.725726	-0.433701
29	6	0	-5.298614	-2.163875	0.272005
30	8	0	-2.462698	-0.308227	-3.112393
31	1	0	6.929333	0.661955	0.476443
32	1	0	5.980930	2.147466	0.558614
33	1	0	4.981638	-0.750938	-2.478944
34	1	0	6.431239	-0.989728	-1.511400
35	1	0	3.617116	1.279701	-2.189888
36	1	0	4.354802	2.711912	-1.454627
37	1	0	7.479062	1.031568	-2.024609
38	1	0	6.170154	1.451481	-3.141460
39	1	0	6.654326	2.590626	-1.873095
40	1	0	5.289832	1.711160	2.945029
41	1	0	4.539572	0.171808	3.387180
42	1	0	6.271193	0.234067	2.965551
43	1	0	4.551114	-3.688899	-0.050359
44	1	0	4.875654	-3.312276	-1.754229
45	1	0	6.158379	-3.118520	-0.542214
46	1	0	2.276880	1.781011	-0.331728
47	1	0	-0.094921	-0.428956	-2.923040
48	1	0	-0.009009	-2.881307	1.465856
49	1	0	-4.824979	-0.387787	-3.132526
50	1	0	-7.124914	-0.752750	-2.229295
51	1	0	-7.400897	-1.878355	-0.017980
52	1	0	-5.421239	-2.654323	1.233426
53	1	0	6.004262	-1.486941	1.193650
54	1	0	4.316121	-1.671584	1.669939
55	16	0	-2.683733	-2.576621	0.731507
56	6	0	-3.012483	-0.407901	3.702892
57	6	0	-1.661826	-0.715863	3.876241

58	6	0	-0.705663	-0.185661	3.011761
59	6	0	-1.103245	0.661730	1.970511
60	6	0	-2.460362	0.992491	1.787990
61	6	0	-3.399196	0.439864	2.662883
62	7	0	-0.117175	1.176151	1.110629
63	6	0	-0.338667	1.830444	-0.060917
64	6	0	-1.769752	2.070409	-0.476445
65	6	0	-2.805352	1.963887	0.694564
66	8	0	0.595758	2.202953	-0.783997
67	6	0	-4.339739	2.549208	-1.247644
68	6	0	-3.410875	3.780628	-1.375896
69	6	0	-2.133582	3.584630	-0.541087
70	6	0	-2.503035	3.479350	0.961313
71	1	0	-3.760187	-0.822991	4.372082
72	1	0	-1.348995	-1.372071	4.683432
73	1	0	0.349612	-0.417003	3.127316
74	1	0	-4.449627	0.678997	2.529602
75	1	0	0.869138	0.999697	1.361272
76	1	0	-1.934381	1.490570	-1.388034
77	1	0	-5.378160	2.815602	-1.470847
78	1	0	-4.046100	1.817769	-2.007377
79	1	0	-3.914743	4.692974	-1.031031
80	1	0	-3.158678	3.937058	-2.431008
81	1	0	-1.332940	4.270306	-0.828713
82	1	0	-3.332764	4.090388	1.333786
83	1	0	-1.635343	3.611715	1.614324
84	6	0	-4.241566	1.865634	0.135315
85	1	0	-4.550320	0.820429	0.047081
86	1	0	-4.925503	2.337940	0.851801

TX-Prod'$_{SRR}$ E(opt)= -2373.206808 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.894600	1.151484	-0.426425
2	6	0	-5.827817	0.897855	0.768901
3	6	0	-5.375212	-0.349756	1.541929
4	6	0	-5.387221	-1.577310	0.592366
5	6	0	-4.671713	-1.430084	-0.772663
6	6	0	-4.995165	-0.048840	-1.402694
7	6	0	-3.983873	-0.039372	2.130014
8	6	0	-6.330116	-0.646521	2.709699
9	6	0	-5.275554	2.442648	-1.163030
10	6	0	-5.159202	-2.547345	-1.731887
11	6	0	-3.433928	1.252248	0.040339
12	7	0	-3.111414	0.701496	1.222218
13	8	0	-2.579760	1.782648	-0.695957
14	6	0	-3.185157	-1.633904	-0.627607
15	7	0	-2.521300	-2.184242	0.335520
16	6	0	-1.186081	-2.137535	-0.077375
17	6	0	-1.136651	-1.551256	-1.354722

18	8	0	-2.415165	-1.233906	-1.711670
19	6	0	-0.011439	-2.524799	0.541906
20	6	0	1.205125	-2.349530	-0.146591
21	6	0	1.211379	-1.783909	-1.450168
22	6	0	0.024316	-1.357948	-2.072302
23	6	0	2.437019	-2.747522	0.585203
24	6	0	3.773571	-2.478540	-0.009781
25	6	0	3.976112	-1.970402	-1.305875
26	6	0	4.898647	-2.718146	0.803373
27	6	0	6.182914	-2.465119	0.349935
28	6	0	6.371695	-1.968395	-0.948475
29	6	0	5.280729	-1.724356	-1.770725
30	8	0	2.355711	-3.255174	1.704618
31	1	0	-6.856767	0.771856	0.406219
32	1	0	-5.829585	1.768801	1.437318
33	1	0	-4.991892	-2.453871	1.115409
34	1	0	-6.439946	-1.790017	0.366380
35	1	0	-3.472178	-0.967940	2.401089
36	1	0	-4.110225	0.552831	3.046494
37	1	0	-7.335545	-0.878617	2.342763
38	1	0	-5.980518	-1.503408	3.296764
39	1	0	-6.408743	0.214391	3.382134
40	1	0	-5.239891	3.301765	-0.485257
41	1	0	-4.581545	2.633271	-1.983823
42	1	0	-6.292756	2.364746	-1.561710
43	1	0	-4.650638	-2.478488	-2.698019
44	1	0	-4.959758	-3.535491	-1.305991
45	1	0	-6.236667	-2.454413	-1.901386
46	1	0	-2.110064	0.696323	1.466509
47	1	0	0.009309	-2.947787	1.538341
48	1	0	0.021103	-0.896403	-3.053227
49	1	0	4.713321	-3.103644	1.799865
50	1	0	7.036841	-2.649950	0.994051
51	1	0	7.373389	-1.764591	-1.315510
52	1	0	5.429959	-1.326769	-2.770614
53	1	0	-6.029058	-0.087250	-1.768193
54	1	0	-4.351464	0.127359	-2.268510
55	16	0	2.671470	-1.583642	-2.423898
56	6	0	2.404268	4.609658	-2.121805
57	6	0	1.059203	4.396028	-2.426073
58	6	0	0.302087	3.512228	-1.660070
59	6	0	0.895792	2.837295	-0.586352
60	6	0	2.253655	3.036751	-0.263856
61	6	0	2.986186	3.931943	-1.047875
62	7	0	0.100457	1.944158	0.153741
63	6	0	0.435928	1.355472	1.329263
64	6	0	1.810209	1.647282	1.886416
65	6	0	2.836007	2.215471	0.857334
66	8	0	-0.357677	0.626915	1.943255
67	6	0	4.743530	1.807241	2.507107
68	6	0	3.839428	0.647384	2.991007
69	6	0	2.714621	0.386632	1.979914
70	6	0	3.183844	0.721048	0.534512

71	1	0	2.999650	5.296992	-2.715325
72	1	0	0.595095	4.918635	-3.257577
73	1	0	-0.748568	3.337486	-1.874533
74	1	0	4.035141	4.098988	-0.824925
75	1	0	-0.872879	1.811524	-0.166977
76	1	0	1.668245	2.211287	2.817662
77	1	0	5.246522	2.290067	3.351296
78	1	0	5.539866	1.380783	1.887768
79	1	0	3.393956	0.871057	3.968408
80	1	0	4.443806	-0.258263	3.119104
81	1	0	2.206541	-0.561788	2.161026
82	1	0	2.494646	0.324457	-0.212137
83	1	0	4.205810	0.477307	0.234488
84	6	0	3.988646	2.860872	1.656724
85	1	0	4.707826	3.344006	0.987655
86	1	0	3.567957	3.655583	2.285491

OX E(opt)= -1377.650441 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.071251	1.325901	-0.453847
2	6	0	4.956904	0.182948	-0.980649
3	6	0	4.246869	-1.170184	-0.821344
4	6	0	3.943300	-1.410609	0.679587
5	6	0	3.181078	-0.285110	1.418885
6	6	0	3.787727	1.094458	1.054662
7	6	0	2.980973	-1.140668	-1.706813
8	6	0	5.142203	-2.318229	-1.315222
9	6	0	4.756950	2.685458	-0.637156
10	6	0	3.298570	-0.500217	2.950159
11	6	0	2.726562	1.346556	-1.200961
12	7	0	2.278265	0.140540	-1.664018
13	8	0	2.054819	2.365580	-1.319697
14	6	0	1.708676	-0.365493	1.103873
15	7	0	1.010180	-1.412994	0.805622
16	6	0	-0.295665	-0.937752	0.649308
17	6	0	-0.295623	0.450893	0.897755
18	8	0	0.983223	0.809116	1.212530
19	6	0	-1.476398	-1.571962	0.299212
20	6	0	-2.642660	-0.793343	0.203651
21	6	0	-2.594443	0.598795	0.460634
22	6	0	-1.411513	1.258500	0.815701
23	6	0	-3.919967	-1.434465	-0.173399
24	6	0	-5.072591	-0.514713	-0.245765
25	6	0	-4.910976	0.851556	0.029931
26	8	0	-3.704458	1.394504	0.374780
27	6	0	-6.350324	-0.986867	-0.592507
28	6	0	-7.429745	-0.119868	-0.660775
29	6	0	-7.245017	1.245129	-0.380884
30	6	0	-5.992679	1.736634	-0.035974

31	8	0	-4.014209	-2.637561	-0.409639
32	1	0	5.908166	0.176285	-0.431759
33	1	0	5.200953	0.355216	-2.037328
34	1	0	3.405186	-2.355229	0.805533
35	1	0	4.910170	-1.522811	1.186913
36	1	0	2.289229	-1.928158	-1.389852
37	1	0	3.276341	-1.349240	-2.745024
38	1	0	6.049902	-2.392059	-0.707269
39	1	0	4.619718	-3.279801	-1.255890
40	1	0	5.447189	-2.161477	-2.355450
41	1	0	4.996674	2.860398	-1.690778
42	1	0	4.098565	3.491773	-0.308522
43	1	0	5.688951	2.721695	-0.062864
44	1	0	2.751622	0.276287	3.494123
45	1	0	2.888891	-1.474105	3.233603
46	1	0	4.348512	-0.460159	3.257739
47	1	0	1.375207	0.194810	-2.118263
48	1	0	-1.538636	-2.634765	0.095913
49	1	0	-1.393764	2.325876	0.994005
50	1	0	-6.448845	-2.047200	-0.801045
51	1	0	-8.413979	-0.490414	-0.929057
52	1	0	-8.088031	1.927770	-0.433769
53	1	0	-5.826734	2.785716	0.183428
54	1	0	4.749082	1.171313	1.578305
55	1	0	3.150744	1.898249	1.433927

SeX E(opt)= -3701.352077 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.571980	-1.202293	-0.602190
2	6	0	-5.452413	-0.009398	-1.014375
3	6	0	-4.739829	1.318687	-0.715747
4	6	0	-4.442645	1.404984	0.803086
5	6	0	-3.686980	0.208018	1.427980
6	6	0	-4.295383	-1.125757	0.923352
7	6	0	-3.470278	1.375447	-1.594335
8	6	0	-5.630288	2.513358	-1.094513
9	6	0	-5.259590	-2.534393	-0.925782
10	6	0	-3.810800	0.267658	2.972648
11	6	0	-3.223180	-1.150715	-1.340677
12	7	0	-2.770184	0.094674	-1.677849
13	8	0	-2.552607	-2.154290	-1.557262
14	6	0	-2.213024	0.315322	1.129199
15	7	0	-1.510458	1.386616	0.943022
16	6	0	-0.206139	0.923709	0.742666
17	6	0	-0.211241	-0.478225	0.844822
18	8	0	-1.491680	-0.866446	1.117881
19	6	0	0.978233	1.583976	0.465207
20	6	0	2.156763	0.829381	0.288658
21	6	0	2.107282	-0.584792	0.396640

22	6	0	0.909177	-1.263406	0.678797
23	6	0	3.385205	1.626953	-0.009759
24	6	0	4.713795	0.976597	-0.212539
25	6	0	4.963160	-0.406298	-0.165698
26	6	0	5.799218	1.838750	-0.473088
27	6	0	7.079943	1.352535	-0.679148
28	6	0	7.310950	-0.028937	-0.629546
29	6	0	6.261393	-0.900648	-0.375043
30	8	0	3.300432	2.852876	-0.089409
31	1	0	-6.406155	-0.055666	-0.471710
32	1	0	-5.692074	-0.073060	-2.084107
33	1	0	-3.902451	2.330204	1.026387
34	1	0	-5.411541	1.468283	1.314982
35	1	0	-2.778234	2.125263	-1.196858
36	1	0	-3.760717	1.688246	-2.607446
37	1	0	-6.540522	2.527687	-0.486040
38	1	0	-5.105807	3.462496	-0.935805
39	1	0	-5.930944	2.463688	-2.146563
40	1	0	-5.493773	-2.601169	-1.992977
41	1	0	-4.604841	-3.371635	-0.676885
42	1	0	-6.194941	-2.626076	-0.363194
43	1	0	-3.268619	-0.561641	3.437723
44	1	0	-3.399663	1.206564	3.354804
45	1	0	-4.862316	0.200199	3.269897
46	1	0	-1.864370	0.084443	-2.129816
47	1	0	1.031867	2.662078	0.377183
48	1	0	0.859340	-2.344106	0.751070
49	1	0	5.588776	2.901767	-0.505810
50	1	0	7.898297	2.037560	-0.877691
51	1	0	8.309778	-0.424670	-0.789198
52	1	0	6.444855	-1.970942	-0.337309
53	1	0	-5.259427	-1.252139	1.432210
54	1	0	-3.662357	-1.965790	1.222136
55	34	0	3.623914	-1.707082	0.168984

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^{3}OX-TS1$_{ex}$ E(opt)= -2050.155513 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.846681	0.641586	1.244977
2	6	0	5.892687	1.085303	0.209507
3	6	0	5.486547	0.602869	-1.190735
4	6	0	5.348998	-0.944090	-1.188990
5	6	0	4.540967	-1.606217	-0.044956
6	6	0	4.839503	-0.905716	1.309138
7	6	0	4.183928	1.338777	-1.561030
8	6	0	6.555708	0.977557	-2.230636
9	6	0	5.164564	1.209675	2.635152
10	6	0	4.946386	-3.099939	0.062044
11	6	0	3.441181	1.106889	0.828310
12	7	0	3.253325	1.484051	-0.445671

13	8	0	2.510252	1.096917	1.658403
14	6	0	3.060813	-1.599343	-0.330863
15	7	0	2.417752	-1.293800	-1.408677
16	6	0	1.068351	-1.505795	-1.098608
17	6	0	0.990737	-1.982167	0.226148
18	8	0	2.261662	-2.046293	0.715442
19	6	0	-0.095558	-1.300828	-1.822060
20	6	0	-1.320502	-1.611539	-1.203009
21	6	0	-1.343650	-2.124912	0.117245
22	6	0	-0.182598	-2.312953	0.872120
23	6	0	-2.588791	-1.352412	-1.909375
24	6	0	-3.797731	-1.794565	-1.191213
25	6	0	-3.703375	-2.293593	0.116451
26	6	0	-5.071201	-1.672714	-1.775323
27	6	0	-6.210299	-2.032349	-1.071068
28	6	0	-6.093167	-2.514500	0.244492
29	6	0	-4.846176	-2.644807	0.843011
30	8	0	-2.638351	-0.790951	-3.006787
31	1	0	6.874631	0.679363	0.487364
32	1	0	5.987007	2.179023	0.211003
33	1	0	4.952011	-1.279746	-2.152613
34	1	0	6.367414	-1.345026	-1.110418
35	1	0	3.661954	0.806555	-2.362569
36	1	0	4.435416	2.341254	-1.932727
37	1	0	7.505692	0.477996	-2.012851
38	1	0	6.244685	0.683027	-3.239513
39	1	0	6.737852	2.057506	-2.235223
40	1	0	5.211687	2.303268	2.606852
41	1	0	4.389544	0.924195	3.349149
42	1	0	6.132961	0.835850	2.985050
43	1	0	4.376734	-3.602255	0.848689
44	1	0	4.761095	-3.619179	-0.883628
45	1	0	6.011858	-3.183889	0.298339
46	1	0	2.283786	1.706538	-0.715901
47	1	0	-0.101210	-0.890966	-2.824431
48	1	0	-0.231907	-2.661075	1.895006
49	1	0	-5.118705	-1.278440	-2.785040
50	1	0	-7.189884	-1.937232	-1.528938
51	1	0	-6.983594	-2.787365	0.803177
52	1	0	-4.727764	-3.006146	1.858405
53	1	0	5.835873	-1.225918	1.639097
54	1	0	4.123965	-1.239685	2.065044
55	6	0	-3.164243	0.015974	3.322176
56	6	0	-1.819456	0.011873	3.722487
57	6	0	-0.823808	0.451158	2.841859
58	6	0	-1.159383	0.895125	1.564905
59	6	0	-2.531937	0.913916	1.125076
60	6	0	-3.514024	0.456724	2.056377
61	7	0	-0.150873	1.326527	0.708252
62	6	0	-0.345895	1.663118	-0.612973
63	6	0	-1.714631	1.722765	-1.068678
64	6	0	-2.835792	1.368693	-0.175369
65	8	0	0.622653	1.926612	-1.355160

66	6	0	-4.976907	2.768075	-0.120104
67	6	0	-4.323893	4.095056	-0.557030
68	6	0	-1.825943	4.198087	-0.908025
69	6	0	-2.907594	4.211941	-0.084423
70	1	0	-3.935548	-0.331132	4.003538
71	1	0	-1.544180	-0.333122	4.714438
72	1	0	0.222943	0.447250	3.132397
73	1	0	-4.554184	0.436236	1.752523
74	1	0	0.823095	1.293840	1.048161
75	1	0	-4.988211	2.712310	0.975388
76	1	0	-6.023750	2.752575	-0.449957
77	1	0	-4.360324	4.178329	-1.650683
78	1	0	-1.940805	4.246727	-1.986685
79	1	0	-0.816000	4.302168	-0.528254
80	1	0	-4.919676	4.925544	-0.151521
81	6	0	-4.244366	1.525293	-0.677844
82	1	0	-4.836375	0.639937	-0.421745
83	1	0	-4.232032	1.569365	-1.773267
84	1	0	-1.863915	1.715082	-2.141396
85	1	0	-2.752391	4.228245	0.993363
86	8	0	-2.508460	-2.450105	0.754113

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^{3}OX-TS1$_{en}$ E(opt)= -2050.147386 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.911042	-1.037145	-0.689113
2	6	0	5.866645	-0.776186	0.488106
3	6	0	5.337415	0.369705	1.362537
4	6	0	5.217874	1.653182	0.502226
5	6	0	4.434518	1.530400	-0.826497
6	6	0	4.836367	0.234064	-1.570957
7	6	0	3.992792	-0.090105	1.967130
8	6	0	6.302779	0.665187	2.522107
9	6	0	5.398550	-2.217030	-1.541540
10	6	0	4.763611	2.750620	-1.728128
11	6	0	3.505848	-1.360913	-0.157401
12	7	0	3.167462	-0.878093	1.054812
13	8	0	2.707974	-2.021765	-0.845197
14	6	0	2.948515	1.615183	-0.580227
15	7	0	2.323449	2.313479	0.312058
16	6	0	0.967594	2.167467	-0.003779
17	6	0	0.864936	1.331209	-1.135483
18	8	0	2.131987	0.993334	-1.511757
19	6	0	-0.182213	2.699823	0.559001
20	6	0	-1.419878	2.358273	-0.016183
21	6	0	-1.470880	1.473619	-1.120740
22	6	0	-0.322576	0.951879	-1.723537
23	6	0	-2.670755	2.914314	0.542080
24	6	0	-3.907660	2.394461	-0.081361
25	6	0	-3.839329	1.470805	-1.135675

26	6	0	-5.171562	2.755481	0.415657
27	6	0	-6.325982	2.204086	-0.120433
28	6	0	-6.232019	1.272096	-1.169156
29	6	0	-4.995214	0.901749	-1.681753
30	8	0	-2.686035	3.723211	1.467016
31	1	0	6.863952	-0.528762	0.100668
32	1	0	5.974856	-1.687183	1.091035
33	1	0	4.789587	2.464835	1.098871
34	1	0	6.238880	1.956536	0.237236
35	1	0	3.413073	0.781748	2.291692
36	1	0	4.193053	-0.701980	2.856671
37	1	0	7.269929	1.014428	2.145304
38	1	0	5.899703	1.441637	3.182305
39	1	0	6.480782	-0.232229	3.124128
40	1	0	5.483147	-3.125183	-0.936513
41	1	0	4.696285	-2.420981	-2.351862
42	1	0	6.383875	-1.994066	-1.964858
43	1	0	4.206304	2.699764	-2.668880
44	1	0	4.501274	3.683334	-1.220824
45	1	0	5.832784	2.767703	-1.962955
46	1	0	2.293144	-1.253026	1.450528
47	1	0	-0.168096	3.368600	1.411680
48	1	0	-0.394947	0.272689	-2.561200
49	1	0	-5.198986	3.466636	1.234917
50	1	0	-7.298992	2.484353	0.270359
51	1	0	-7.133797	0.831044	-1.583535
52	1	0	-4.889566	0.171509	-2.476355
53	1	0	5.837704	0.396167	-1.989321
54	1	0	4.161850	0.057683	-2.413116
55	6	0	-3.059765	-2.640601	-2.702199
56	6	0	-1.733764	-2.481047	-3.129344
57	6	0	-0.706201	-2.362293	-2.184948
58	6	0	-0.991023	-2.386700	-0.821268
59	6	0	-2.339965	-2.577097	-0.351155
60	6	0	-3.355292	-2.695761	-1.348423
61	7	0	0.044251	-2.211114	0.092236
62	6	0	-0.097393	-2.301539	1.461220
63	6	0	-1.431234	-2.534108	1.955365
64	6	0	-2.588089	-2.643026	1.038192
65	8	0	0.889847	-2.144508	2.211001
66	6	0	-4.866402	-1.616221	1.588501
67	6	0	-4.272301	-0.470108	2.428397
68	6	0	-1.766124	-0.158978	2.693648
69	6	0	-2.904617	-0.098858	1.953018
70	1	0	-3.858528	-2.736697	-3.432144
71	1	0	-1.497108	-2.453995	-4.188520
72	1	0	0.327838	-2.241269	-2.496649
73	1	0	-4.383171	-2.840835	-1.035392
74	1	0	1.009972	-2.135048	-0.264249
75	1	0	-5.868121	-1.869539	1.958174
76	1	0	-4.986025	-1.270833	0.554918
77	1	0	-4.933706	0.403823	2.341405
78	1	0	-1.790301	-0.408002	3.750314

79	1	0	-0.815193	0.175555	2.295503
80	1	0	-4.241610	-0.752140	3.488419
81	6	0	-3.962090	-2.872780	1.610455
82	1	0	-3.868302	-3.216409	2.648211
83	1	0	-4.469373	-3.679540	1.064473
84	1	0	-1.520820	-2.836144	2.990827
85	1	0	-2.825306	0.180597	0.910871
86	8	0	-2.653664	1.054310	-1.668052

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^{3}SeX-TS1$_{ex}$ E(opt)= -4373.857076 hartree

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.094902	0.566743	1.240326
2	6	0	6.132781	1.097595	0.237916
3	6	0	5.727000	0.716515	-1.193578
4	6	0	5.603036	-0.827766	-1.307893
5	6	0	4.806232	-1.580907	-0.213335
6	6	0	5.107783	-0.981011	1.187917
7	6	0	4.416899	1.466890	-1.503432
8	6	0	6.789412	1.177583	-2.205253
9	6	0	5.410942	1.032674	2.668297
10	6	0	5.219621	-3.075798	-0.221111
11	6	0	3.682283	1.046766	0.862989
12	7	0	3.488338	1.517789	-0.378519
13	8	0	2.752570	0.963835	1.690110
14	6	0	3.324205	-1.557290	-0.486792
15	7	0	2.671428	-1.176103	-1.534788
16	6	0	1.323520	-1.383483	-1.214411
17	6	0	1.257749	-1.938297	0.075306
18	8	0	2.533506	-2.059878	0.540366
19	6	0	0.152155	-1.102573	-1.895560
20	6	0	-1.082850	-1.405100	-1.281251
21	6	0	-1.100545	-2.008783	0.003539
22	6	0	0.082722	-2.273408	0.710716
23	6	0	-2.297064	-1.000750	-2.045110
24	6	0	-3.672348	-1.288659	-1.546076
25	6	0	-3.986148	-1.880032	-0.309038
26	6	0	-4.737623	-0.888257	-2.379511
27	6	0	-6.060061	-1.051664	-1.999851
28	6	0	-6.356079	-1.622240	-0.754046
29	6	0	-5.327054	-2.032103	0.083236
30	8	0	-2.165039	-0.384913	-3.107049
31	1	0	7.119855	0.682796	0.482587
32	1	0	6.215701	2.189145	0.320186
33	1	0	5.204180	-1.093238	-2.292432
34	1	0	6.625099	-1.224772	-1.264022
35	1	0	3.897335	0.993551	-2.342621
36	1	0	4.659034	2.497035	-1.797769
37	1	0	7.744727	0.672354	-2.027502
38	1	0	6.477948	0.955905	-3.232460

39	1	0	6.961391	2.256591	-2.130066
40	1	0	5.447462	2.125746	2.721584
41	1	0	4.640163	0.687154	3.360047
42	1	0	6.383649	0.643218	2.987915
43	1	0	4.655509	-3.639115	0.527423
44	1	0	5.033217	-3.523144	-1.202605
45	1	0	6.286359	-3.171845	0.004665
46	1	0	2.514891	1.745987	-0.630376
47	1	0	0.150771	-0.624220	-2.866214
48	1	0	0.074903	-2.690428	1.711046
49	1	0	-4.476712	-0.433668	-3.328433
50	1	0	-6.860712	-0.733896	-2.660565
51	1	0	-7.387668	-1.747160	-0.437849
52	1	0	-5.558771	-2.474584	1.048200
53	1	0	6.111179	-1.312027	1.484331
54	1	0	4.403725	-1.380817	1.922133
55	6	0	-3.007614	0.271645	3.436752
56	6	0	-1.663441	0.107646	3.800455
57	6	0	-0.645582	0.460761	2.904321
58	6	0	-0.958488	0.975951	1.649839
59	6	0	-2.331356	1.136885	1.238088
60	6	0	-3.335766	0.768651	2.186106
61	7	0	0.071975	1.344221	0.788453
62	6	0	-0.114355	1.772526	-0.506979
63	6	0	-1.478602	1.951313	-0.939771
64	6	0	-2.614955	1.644966	-0.045380
65	8	0	0.861694	2.010628	-1.248968
66	6	0	-4.664735	3.177853	0.060236
67	6	0	-3.921086	4.468193	-0.338784
68	6	0	-1.417933	4.442795	-0.666919
69	6	0	-2.504125	4.478715	0.147272
70	1	0	-3.796099	-0.003863	4.131005
71	1	0	-1.404067	-0.288549	4.777424
72	1	0	0.400782	0.345700	3.173053
73	1	0	-4.378630	0.861447	1.905082
74	1	0	1.044761	1.234313	1.113100
75	1	0	-4.683995	3.095950	1.153841
76	1	0	-5.709017	3.241523	-0.272056
77	1	0	-3.941949	4.582022	-1.430152
78	1	0	-1.517717	4.539804	-1.743790
79	1	0	-0.407335	4.462254	-0.275090
80	1	0	-4.463920	5.326304	0.083509
81	6	0	-4.015465	1.903522	-0.529275
82	1	0	-4.658649	1.048421	-0.291126
83	1	0	-4.009709	1.976578	-1.623158
84	1	0	-1.635882	2.014890	-2.009070
85	1	0	-2.359378	4.437789	1.225886
86	34	0	-2.685714	-2.497714	0.915967

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^{3}SeX-TS1$_{en}$ E(opt)= -4373.853268 hartree

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-5.206301	0.972641	-0.585297
2	6	0	-6.159396	0.618707	0.569767
3	6	0	-5.605017	-0.563967	1.376803
4	6	0	-5.446086	-1.790219	0.442070
5	6	0	-4.663689	-1.567330	-0.874371
6	6	0	-5.102387	-0.241108	-1.542251
7	6	0	-4.277419	-0.104760	2.017261
8	6	0	-6.568578	-0.954237	2.509568
9	6	0	-5.716063	2.192030	-1.365752
10	6	0	-4.952114	-2.741919	-1.846932
11	6	0	-3.807852	1.290751	-0.031163
12	7	0	-3.466845	0.751669	1.155519
13	8	0	-3.016214	1.995992	-0.681673
14	6	0	-3.176872	-1.614885	-0.626047
15	7	0	-2.529160	-2.309588	0.253530
16	6	0	-1.179200	-2.090582	-0.044794
17	6	0	-1.104409	-1.225503	-1.150422
18	8	0	-2.381405	-0.934733	-1.534425
19	6	0	-0.010677	-2.575582	0.518293
20	6	0	1.228545	-2.168680	-0.021808
21	6	0	1.255631	-1.256415	-1.108468
22	6	0	0.075548	-0.783327	-1.704344
23	6	0	2.436384	-2.759795	0.629335
24	6	0	3.818632	-2.349680	0.233324
25	6	0	4.140222	-1.426592	-0.778657
26	6	0	4.874190	-2.913630	0.978834
27	6	0	6.196202	-2.573439	0.739266
28	6	0	6.500323	-1.649336	-0.270428
29	6	0	5.481175	-1.083049	-1.023291
30	8	0	2.292703	-3.594630	1.522094
31	1	0	-7.149080	0.371231	0.163213
32	1	0	-6.291826	1.488801	1.225925
33	1	0	-4.996356	-2.623108	0.991788
34	1	0	-6.457269	-2.106159	0.155013
35	1	0	-3.677007	-0.977641	2.297871
36	1	0	-4.499713	0.452236	2.937196
37	1	0	-7.524303	-1.304646	2.105619
38	1	0	-6.148859	-1.758709	3.124270
39	1	0	-6.773229	-0.100046	3.163770
40	1	0	-5.824382	3.058600	-0.705918
41	1	0	-5.014111	2.461274	-2.157101
42	1	0	-6.693920	1.974275	-1.808667
43	1	0	-4.393649	-2.619274	-2.780267
44	1	0	-4.663322	-3.694632	-1.393833
45	1	0	-6.019538	-2.777910	-2.087465
46	1	0	-2.591813	1.106254	1.568961
47	1	0	-0.013074	-3.264583	1.353820
48	1	0	0.091606	-0.083486	-2.530382
49	1	0	4.606220	-3.619969	1.756468
50	1	0	6.990021	-3.018904	1.330728
51	1	0	7.531494	-1.370827	-0.467378

52	1	0	5.719504	-0.364086	-1.802445
53	1	0	-6.100283	-0.404706	-1.968266
54	1	0	-4.434517	0.002125	-2.372886
55	6	0	2.683726	3.194883	-2.451281
56	6	0	1.387962	2.906866	-2.901611
57	6	0	0.382403	2.590263	-1.977871
58	6	0	0.660551	2.549205	-0.613281
59	6	0	1.981726	2.846146	-0.119345
60	6	0	2.973377	3.167863	-1.095619
61	7	0	-0.352263	2.204622	0.277085
62	6	0	-0.222492	2.222590	1.650999
63	6	0	1.085949	2.530447	2.170029
64	6	0	2.226758	2.809336	1.270619
65	8	0	-1.196867	1.943967	2.381979
66	6	0	4.574470	1.899599	1.704050
67	6	0	4.092359	0.642225	2.452231
68	6	0	1.621708	0.151015	2.763158
69	6	0	2.736679	0.216732	1.988258
70	1	0	3.464395	3.444239	-3.163987
71	1	0	1.154743	2.936370	-3.961494
72	1	0	-0.632029	2.380965	-2.306677
73	1	0	3.977823	3.405358	-0.763393
74	1	0	-1.311351	2.098225	-0.088515
75	1	0	5.567728	2.191426	2.068271
76	1	0	4.681621	1.658968	0.639815
77	1	0	4.808045	-0.171680	2.266735
78	1	0	1.665580	0.328461	3.833775
79	1	0	0.681365	-0.218070	2.370571
80	1	0	4.082313	0.827174	3.533896
81	6	0	3.584489	3.079763	1.863032
82	1	0	3.476753	3.304451	2.931467
83	1	0	4.027846	3.974042	1.404697
84	1	0	1.146390	2.769930	3.223904
85	1	0	2.639957	0.015197	0.929636
86	34	0	2.851342	-0.537206	-1.846725
