Supporting Information

NO-induced Adaptive Aromaticity in Furan, Thiophene and Selenophene

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1. Overview of computational results

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Items	HOMA		ISE (kcal/mol)		$NICS(1)_{zz}$ (ppm)		π-$EDDB_{5MR}$ (*e*)		PBI	
	S_0	T_1	S_0	T_1	S_0	T_1	S_0	T_1	S_0	T_1
Fur.C_2H	0.350	-0.481	-17.4	2.7	-26.4	9.9	2.420	1.453	1.34	1.83
Thi.C_2H	0.894	0.133	-19.3	2.1	-27.7	17.1	2.826	1.221	1.36	1.82
Sel.C_2H	0.851	0.208	-15.5	2.4	-24.5	17.2	2.361	1.226	1.39	1.83
Fur.CHO	0.407	-0.185	-19.6	4.7	-27.0	7.8	2.608	1.546	1.33	1.77
Thi.CHO	0.925	0.263	-21.7	12.3	-28.7	20.7	3.038	1.321	1.33	1.73
Sel.CHO	0.890	0.310	-17.6	25.7	-26.0	23.7	2.580	1.268	1.35	1.72
Fur.CN	0.383	-0.502	-18.5	5.0	-27.0	11.7	2.481	1.381	1.31	1.64
Thi.CN	0.909	0.090	-20.5	4.8	-28.7	21.2	2.918	1.270	1.32	1.62
Sel.CN	0.868	0.167	-16.5	27.1	-25.5	21.4	2.456	1.279	1.34	1.63
Fur.COOH	0.418	-0.363	-19.1	6.2	-26.6	13.8	2.576	1.354	1.28	1.57
Thi.COOH	0.915	0.185	-21.1	7.0	-28.0	26.8	2.993	1.147	1.28	1.53
Sel.COOH	0.876	0.254	-17.1	24.8	-24.9	29.6	2.528	1.102	1.29	1.53
Fur.NO_2	0.450	-0.024	-18.2	3.9	-25.0	9.2	2.506	1.504	1.29	1.71
Thi.NO_2	0.905	0.419	-20.2	6.1	-25.5	23.9	2.897	1.398	1.30	1.69
Sel.NO_2	0.870	0.453	-16.3	7.0	-22.3	28.5	2.498	1.325	1.31	1.69
Fur.NO	0.506	0.410	-20.7	-13.7	-25.7	-21.2	2.732	2.239	1.50	1.63
Thi.NO	0.951	0.907	-22.7	-15.2	-27.1	-21.3	3.145	2.603	1.49	1.64
Sel.NO	0.926	0.897	-18.6	-12.0	-24.6	-18.0	2.736	2.323	1.50	1.69

2. Two-dimension NICS(1)$_{zz}$ scans for **X**.**R** (X = Fur, Thi and Sel; R = C_2H, CHO, CN, COOH and NO_2)

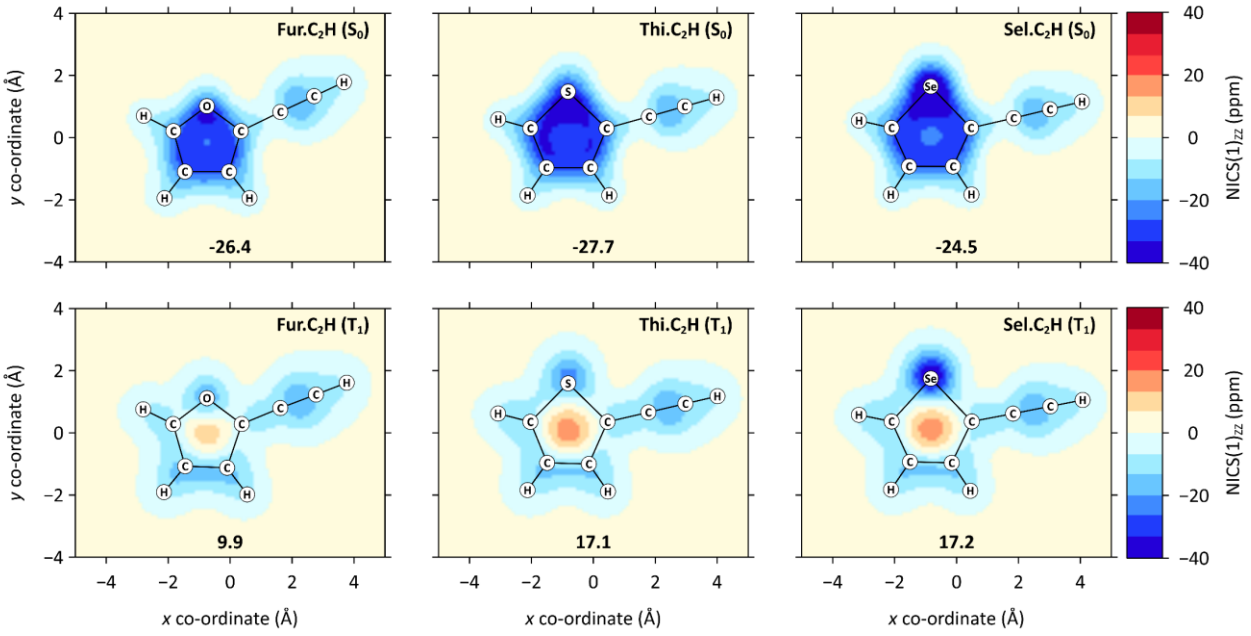


Fig. S1. NICS(1)$_{zz}$ grids for **X.C$_2$H** (X = Fur, Thi and Sel) in S_0 and T_1 states. Each grid covers a 10.1 × 8.1 Å^2 rectangle area parallel to 5MR planes, with 0.1 Å resolution and 8181 (101 x 81) points in total. A fixed colour scale (-40 to 40 p.p.m.) is applied to all grids for easy comparison. NICS(1)$_{zz}$ values were calculated at 1 Å above the centres of these rings.

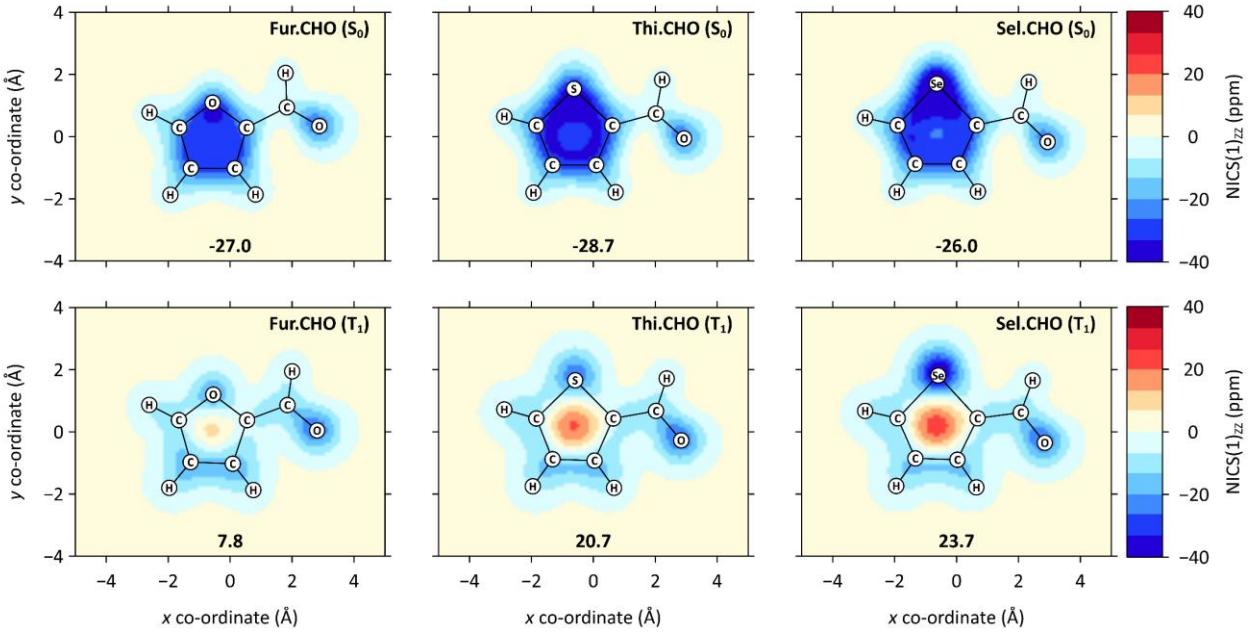


Fig. S2. NICS(1)$_{zz}$ grids for **X.CHO** (X = Fur, Thi and Sel) in S_0 and T_1 states. Each grid covers a 10.1 × 8.1 Å^2 rectangle area parallel to 5MR planes, with 0.1 Å resolution and 8181 (101 x 81) points in total. A fixed colour scale (-40 to 40 p.p.m.) is applied to all grids for easy comparison. NICS(1)$_{zz}$ values were calculated at 1 Å above the centres of these rings.

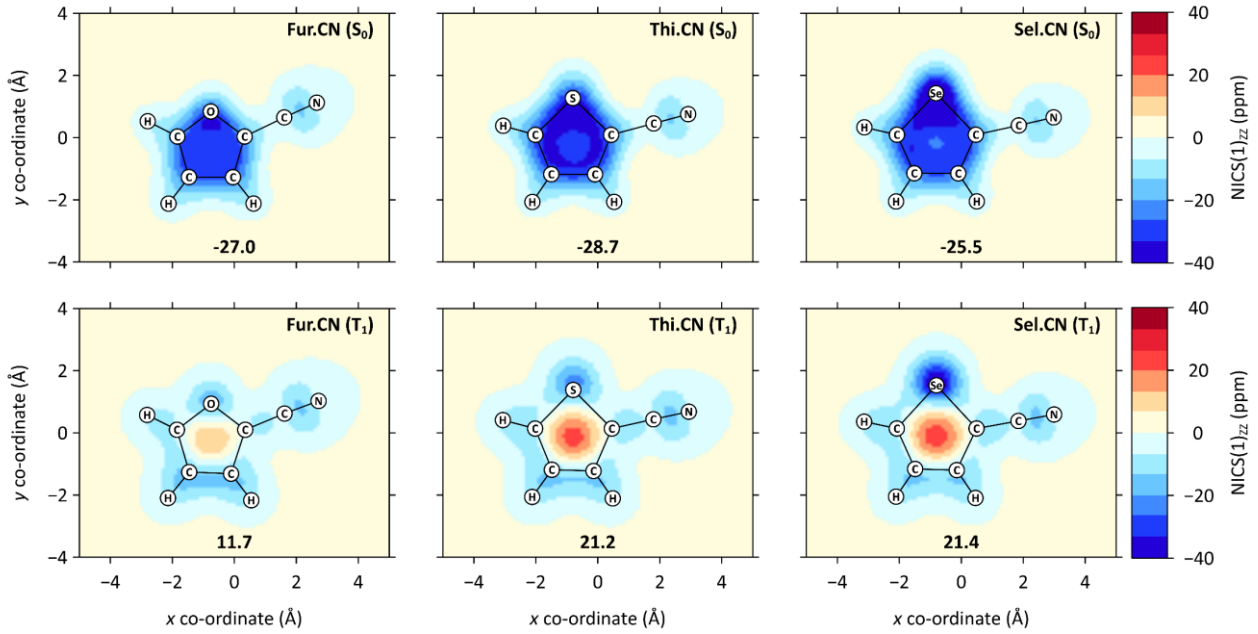


Fig. S3. NICS(1)$_{zz}$ grids for **X.CN** (X = Fur, Thi and Sel) in S_0 and T_1 states. Each grid covers a 10.1 × 8.1 Å^2 rectangle area parallel to 5MR planes, with 0.1 Å resolution and 8181 (101 x 81) points in total. A fixed colour scale (-40 to 40 p.p.m.) is applied to all grids for easy comparison. NICS(1)$_{zz}$ values were calculated at 1 Å above the centres of these rings.

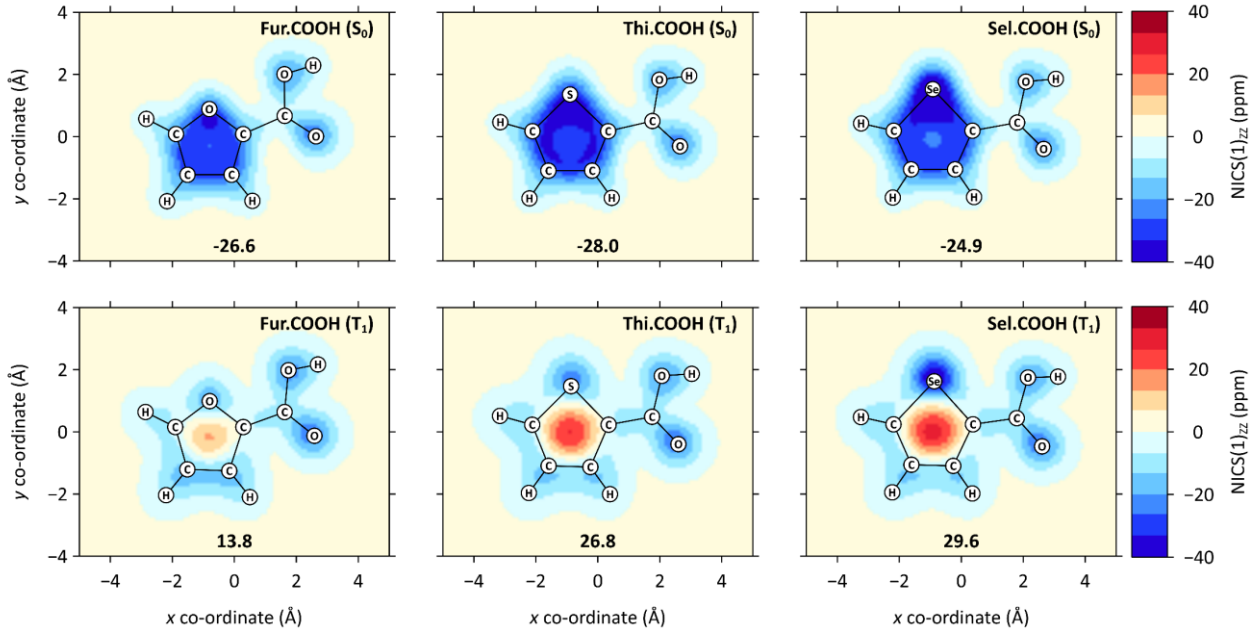


Fig. S4. NICS(1)$_{zz}$ grids for **X.COOH** (X = Fur, Thi and Sel) in S_0 and T_1 states. Each grid covers a 10.1 × 8.1 Å^2 rectangle area parallel to 5MR planes, with 0.1 Å resolution and 8181 (101 x 81) points in total. A fixed colour scale (-40 to 40 p.p.m.) is applied to all grids for easy comparison. NICS(1)$_{zz}$ values were calculated at 1 Å above the centres of these rings.

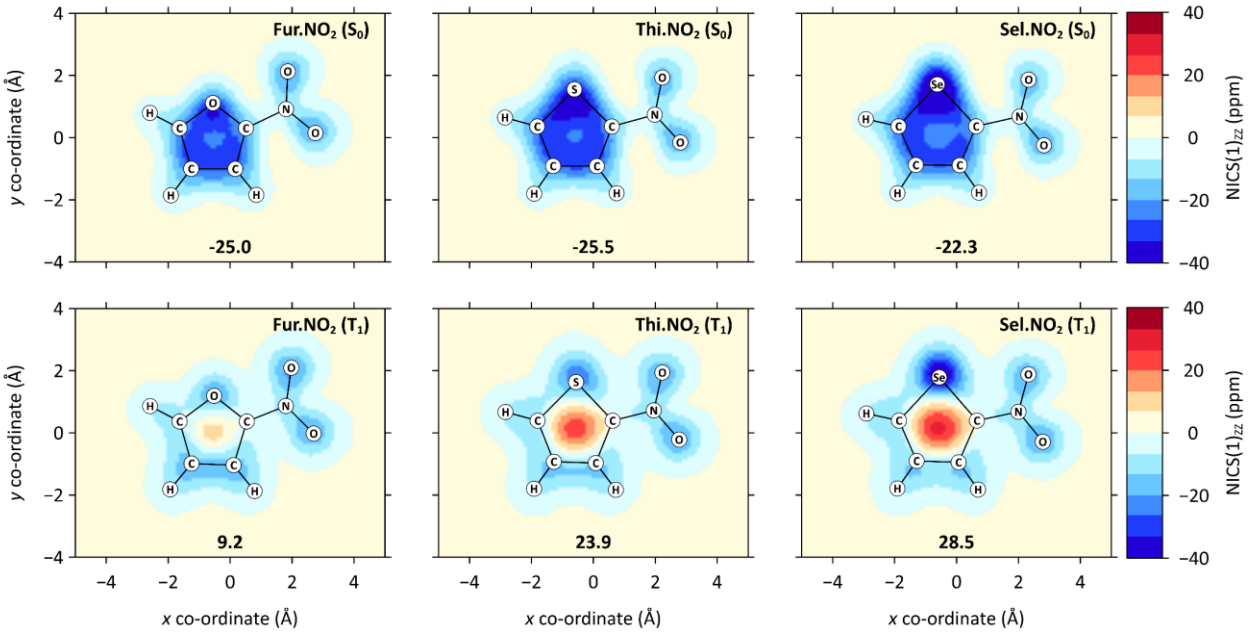


Fig. S5. NICS(1)$_{zz}$ grids for **X.NO$_2$** (X = Fur, Thi and Sel) in S_0 and T_1 states. Each grid covers a 10.1 × 8.1 Å^2 rectangle area parallel to 5MR planes, with 0.1 Å resolution and 8181 (101 x 81) points in total. A fixed colour scale (-40 to 40 p.p.m.) is applied to all grids for easy comparison. NICS(1)$_{zz}$ values were calculated at 1 Å above the centres of these rings.

3. π-AICD plots for **Fur**.**R**, **Thi**.**R** and **Sel**.**R** (R = CHO, NO_2 and NO) in S_0 and T_1 states

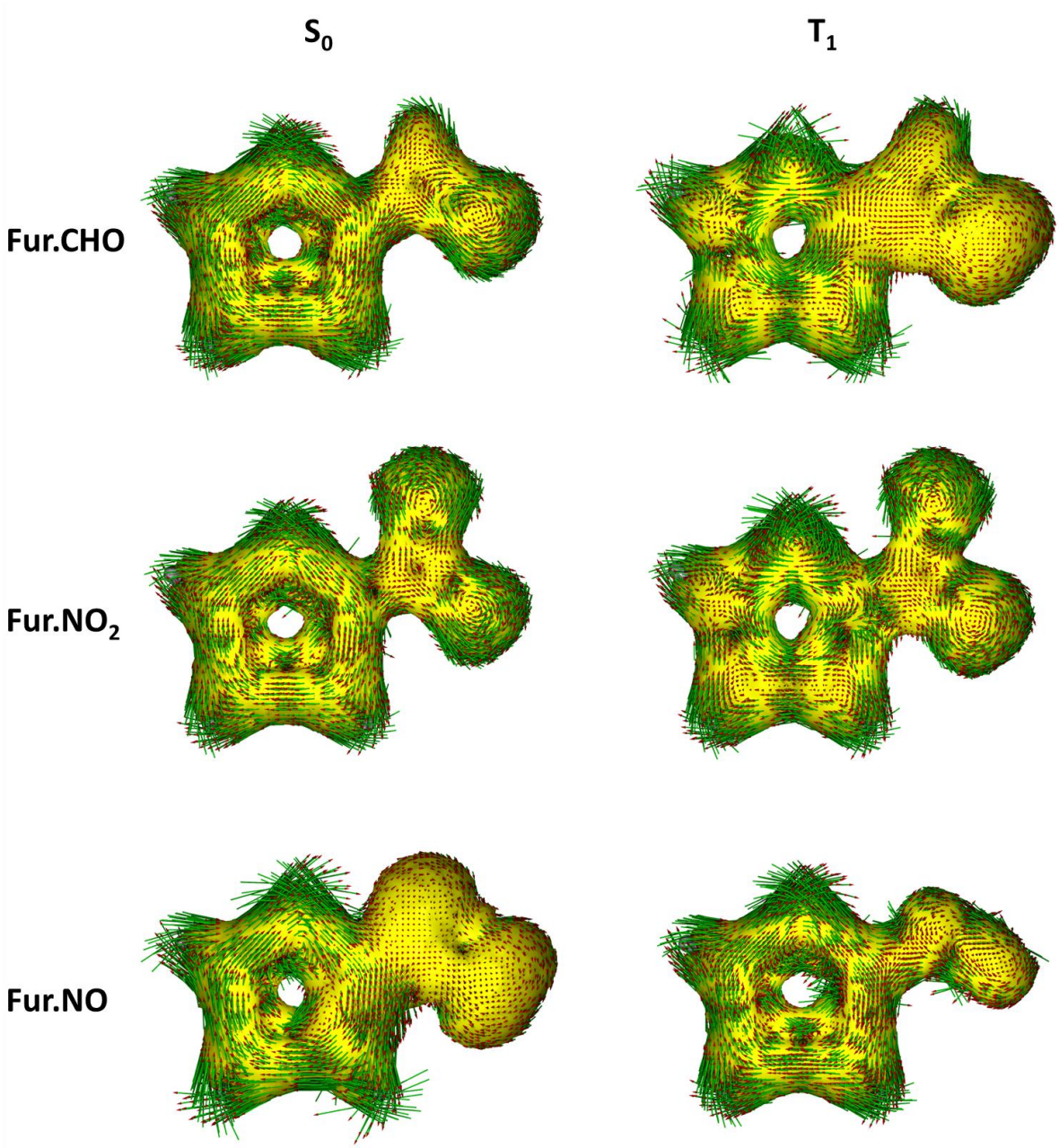


Fig. S6. High resolution of AICD plots for compounds **Fur**.**R** (R = CHO, NO_2 and NO) in S_0 (left column) and T_1 (right column) with 0.03 a.u.

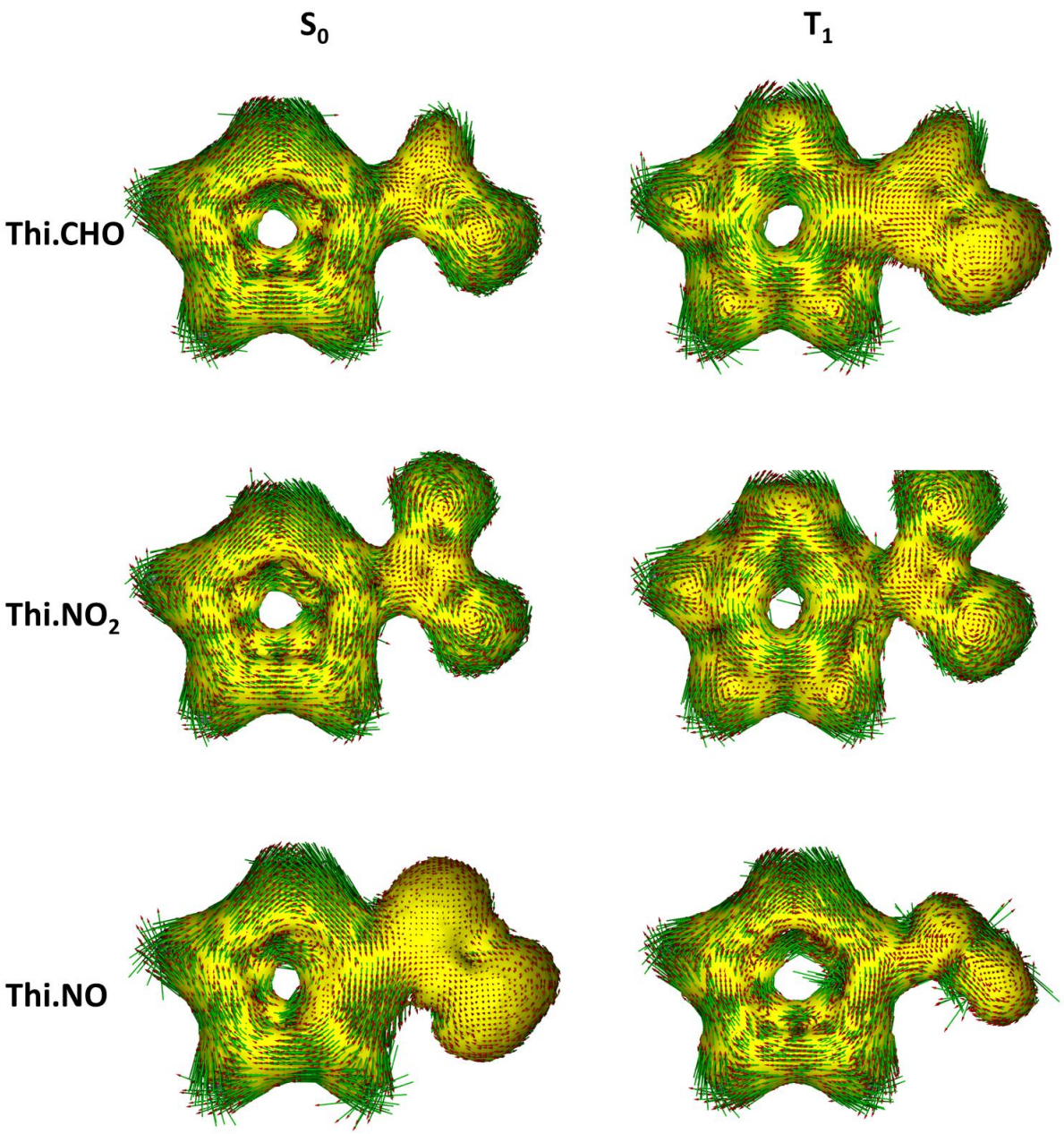


Fig. S7. High resolution of AICD plots for compounds **Thi.R** (R = CHO, NO_2 and NO) in S_0 (left column) and T_1 (right column) with 0.03 a.u.

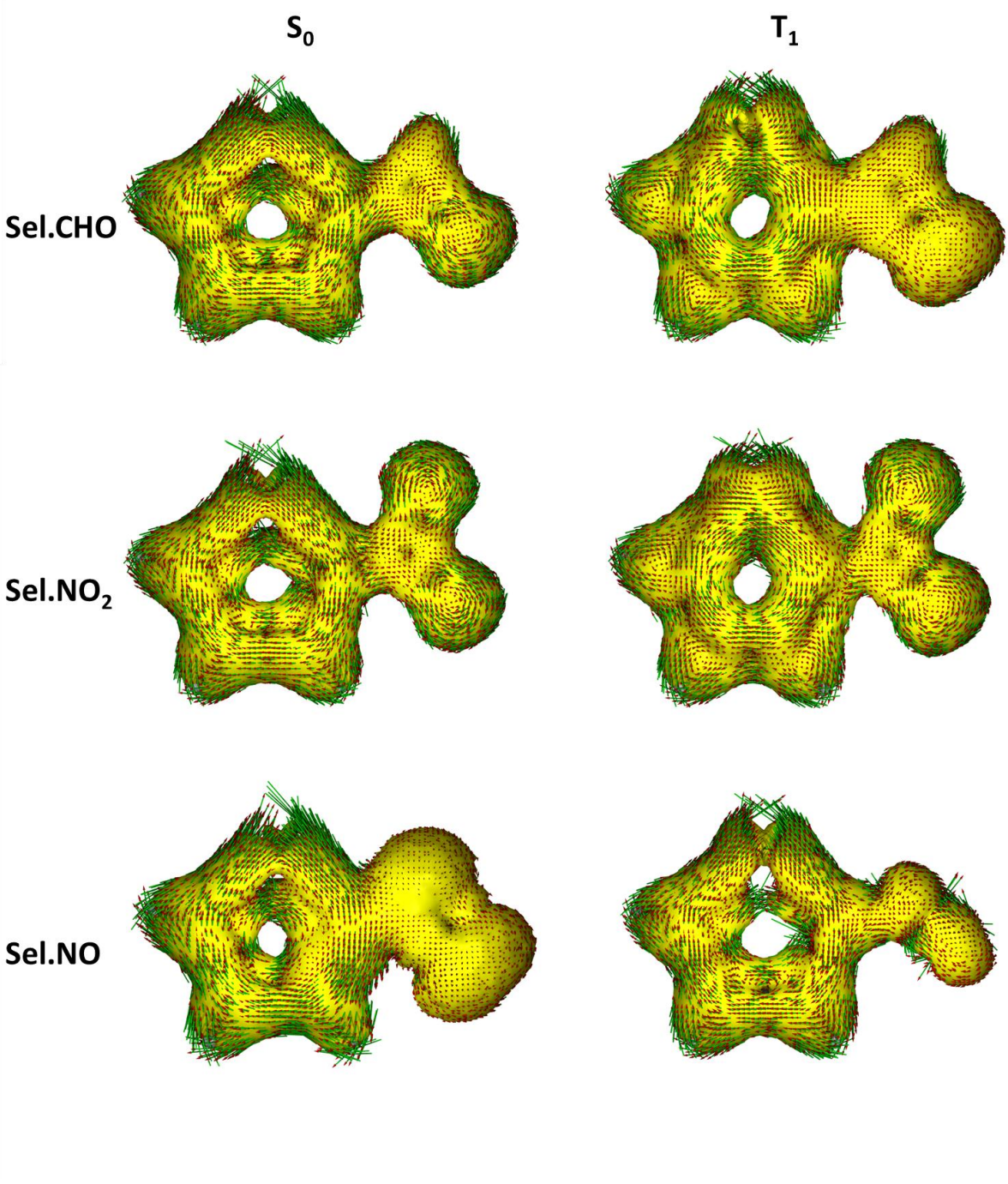


Fig. S8. High resolution of AICD plots for compounds **Sel.R** (R = CHO, NO_2 and NO) in S_0 (left column) and T_1 (right column) with 0.03 a.u.

4. The π-EDDB analysis for **Fur**.**R**, **Thi**.**R** and **Sel**.**R** (R = CHO, NO_2 and NO) in S_0 and T_1 states

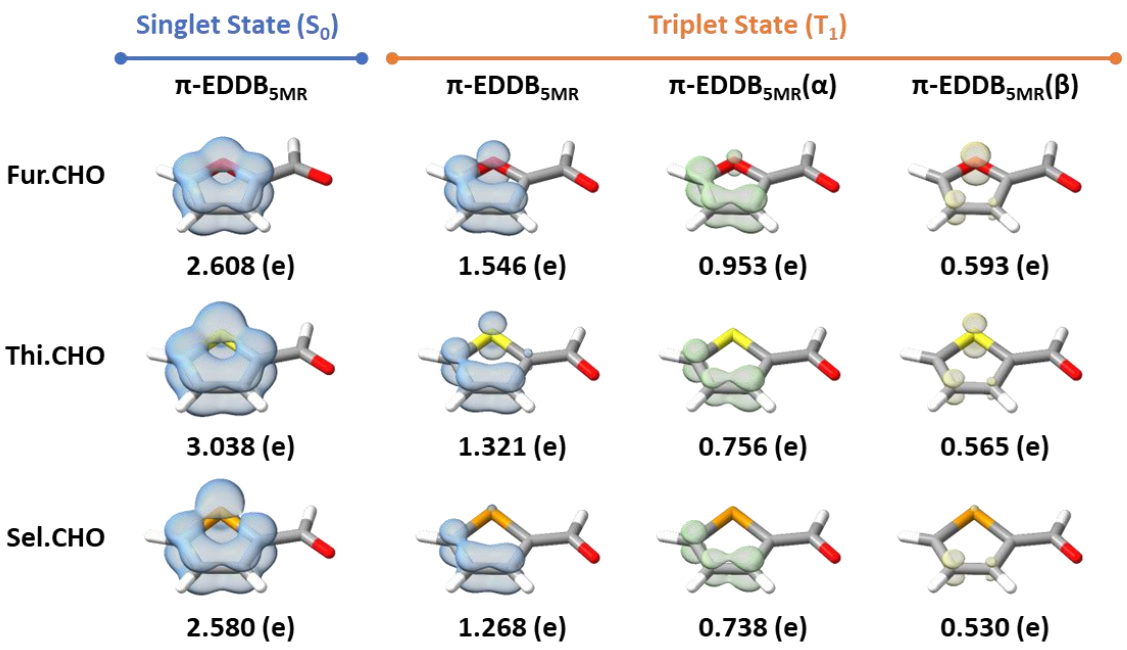


Fig. S9. The EDDB analysis for π-$EDDB_{5MR}$ in S_0 and T_1 states as well as π-$EDDB_{5MR}(\alpha)$ and π-$EDDB_{5MR}(\alpha)$ in T_1 states for **X**.**CHO** (X = Fur, Thi and Sel) with isovalue = 0.01 a.u..

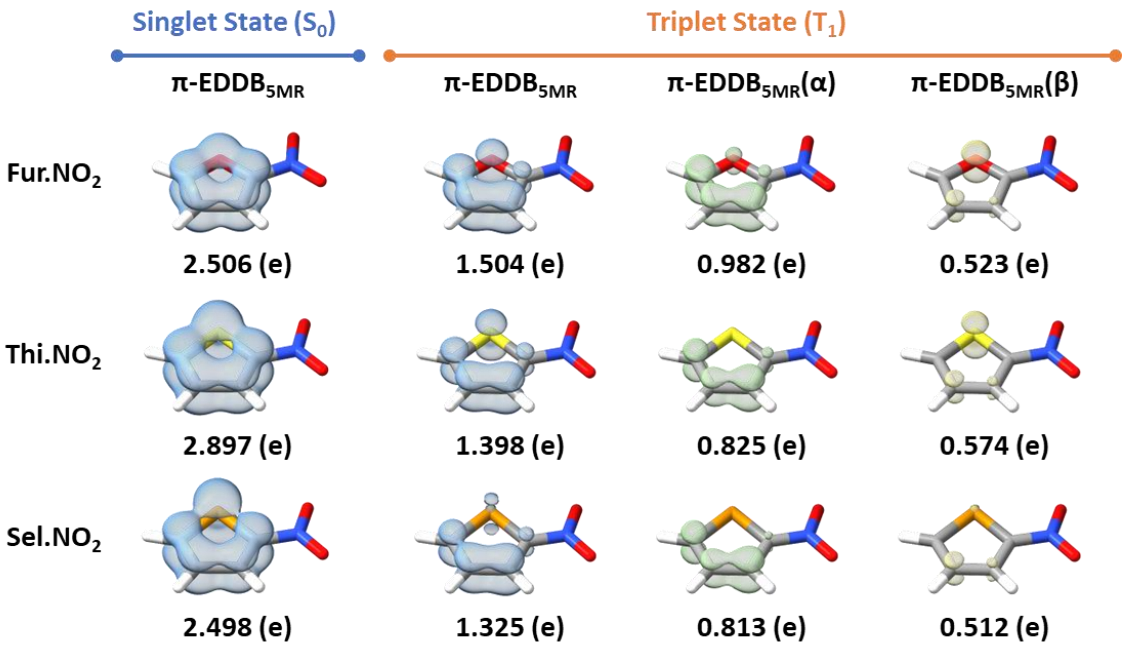


Fig. S10. The EDDB analysis for π-$EDDB_{5MR}$ in S_0 and T_1 states as well as π-$EDDB_{5MR}(\alpha)$ and π-$EDDB_{5MR}(\alpha)$ in T_1 states for **X**.**NO_2** (X = Fur, Thi and Sel) with isovalue = 0.01 a.u..

5. The canonical molecular orbitals of **Fur**.**R**, **Thi**.**R** and **Sel**.**R** (R = CHO, NO_2 and NO) in S_0 and T_1 states

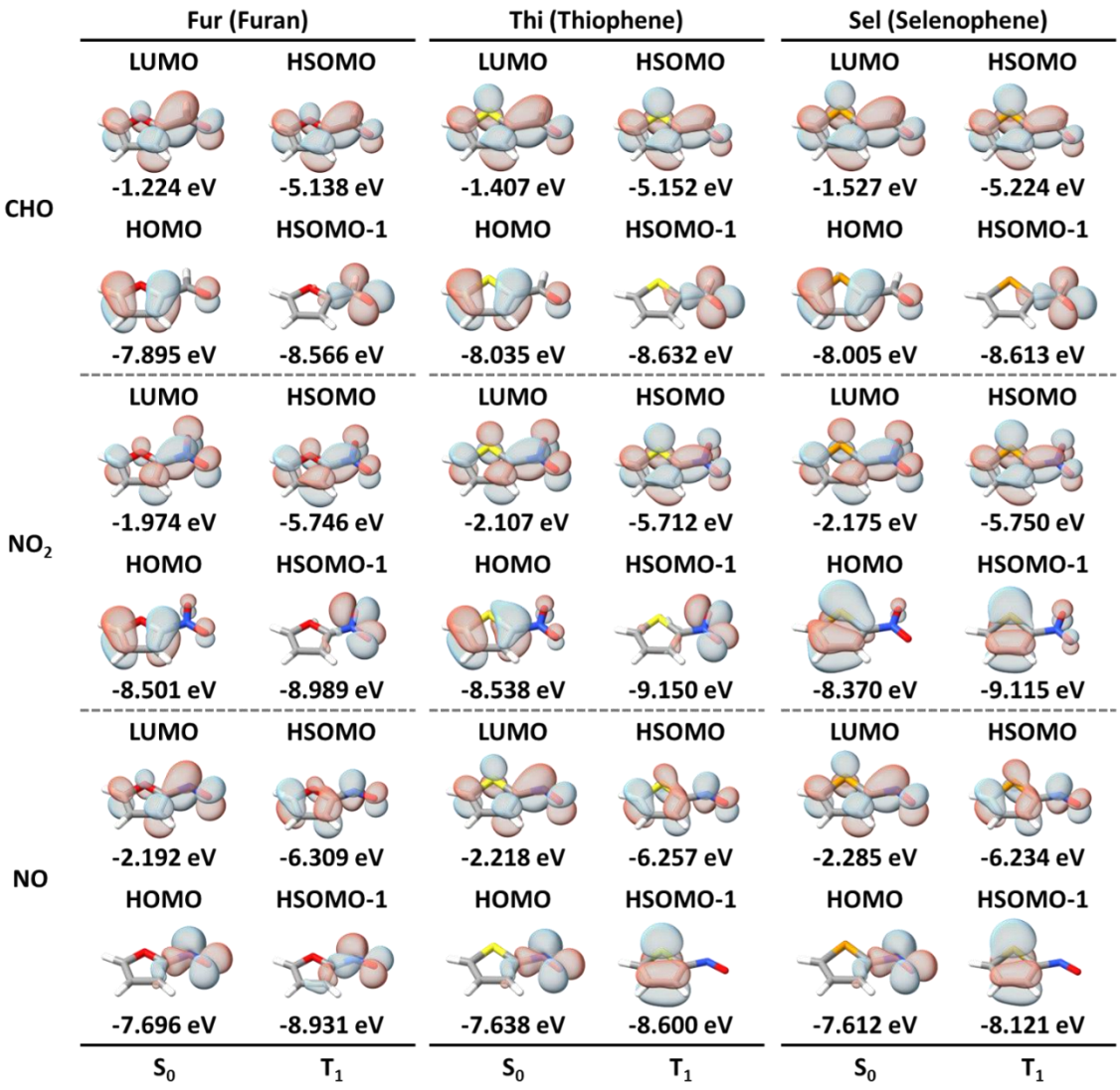


Fig. S11. The frontier molecular orbitals of **Fur**.**R**, **Thi**.**R** and **Sel**.**R** (R = CHO, NO_2 and NO) in ground state (S_0) and triplet state (T_1) without biorthogonalization.

6. The PIO analysis for **Fur**.**NO**, **Thi**.**NO** and **Sel**.**NO** in S_0 state

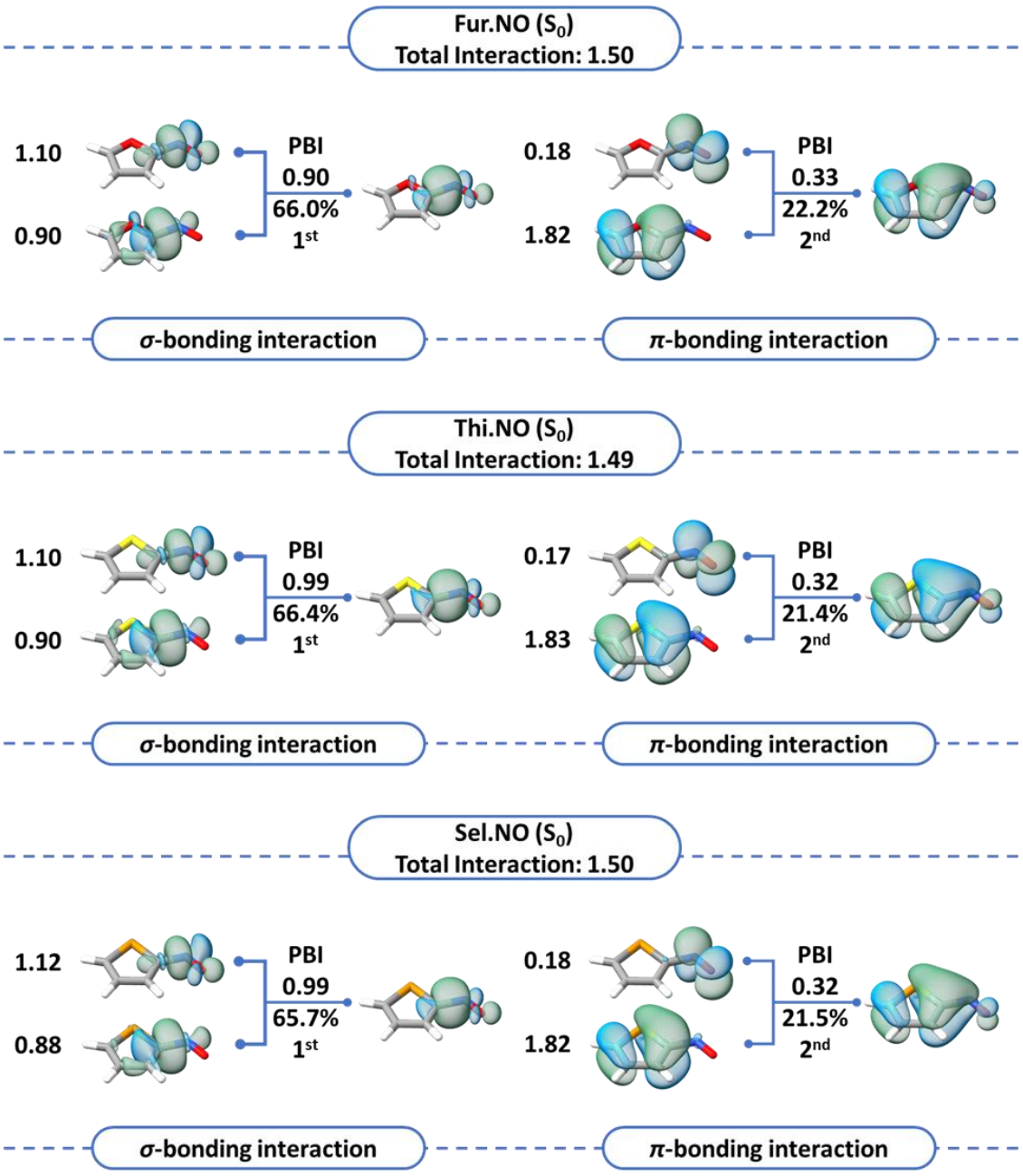
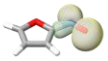
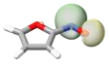
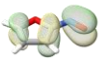
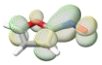
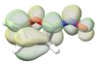


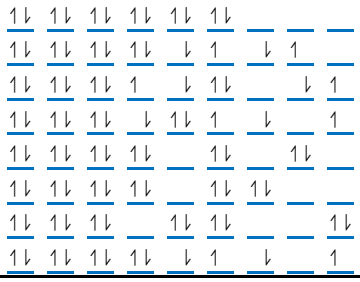
Fig. S12. The PIO analysis for **Fur**.**NO**, **Thi**.**NO** and **Sel**.**NO** in S_0 state. The main contribution of σ and π-bonding were plotted in left and right columns, respectively (isovalue = 0.03 a.u.).

7. The CASSCF computational results for **Fur**.**NO**, **Thi**.**NO** and **Sel**.**NO** in S_0 and T_1 states

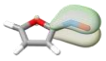
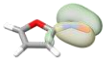
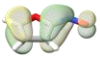
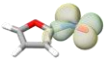
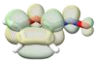
Table S2. The natural orbitals, occupations for natural orbitals, configuration state functions as well as their coefficients and weights for **Fur**.**NO** in S_0 and T_1 states at CASSCF(12*e*,9*o*)/def2-TZVP//MN15/def2-TZVP level of theory.

Fur.**NO** (S_0)

HONO-5	HONO-4	HONO-3	HONO-2	HONO-1	HONO	LUNO	LUNO+1	LUNO+2
								
1.9987	1.9954	1.9938	1.9457	1.9226	1.8643	0.1460	0.0778	0.0557

Configuration State Functions	Coefficients	Weights
	-0.9304	0.8656
	-0.1424	0.0203
	0.0857	0.0074
	-0.0802	0.0064
	0.0764	0.0058
	0.0693	0.0048
	0.0725	0.0053
	0.0505	0.0026

Fur.**NO** (T_1)

HONO-6	HONO-5	HONO-4	HONO-3	HONO-2	HSONO-1	HSONO	LUNO+1	LUNO+2
								
1.9954	1.9645	1.9635	1.9422	1.8999	1.0360	1.0319	0.1030	0.0635

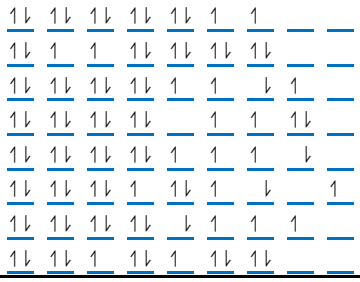
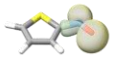
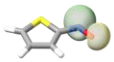
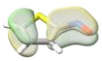
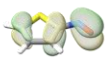
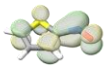
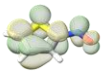
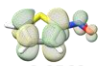
Configuration State Functions	Coefficients	Weights
	0.9295	0.8639
	-0.1549	0.0240
	-0.1393	0.0194
	0.1137	0.0129
	-0.0844	0.0071
	0.0705	0.0050
	-0.0542	0.0029
	0.0517	0.0027

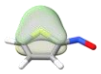
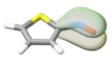
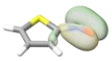
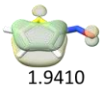
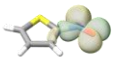
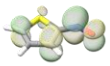
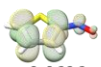
Table S3. The natural orbitals, occupations for natural orbitals, configuration state functions as well as their coefficients and weights for **Thi.NO** in S_0 and T_1 states at CASSCF(12*e*,9*o*)/def2-TZVP//MN15/def2-TZVP level of theory.

Thi.NO (S_0)

HONO-5	HONO-4	HONO-3	HONO-2	HONO-1	HONO	LUNO	LUNO+1	LUNO+2
								
1.9987	1.9953	1.9933	1.9447	1.9217	1.8697	0.1402	0.0804	0.0560

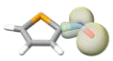
Configuration State Functions	Coefficients	Weights
↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿⇂	0.9312	0.8671
↿⇂ ↿⇂ ↿⇂ ↿⇂ ⇂ ↿ ⇂ ↿	-0.1447	0.0209
↿⇂ ↿⇂ ↿⇂ ⇂ ↿ ↿⇂ ⇂ ↿	-0.0828	0.0069
↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿⇂	-0.0801	0.0064
↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿⇂	-0.0798	0.0064
↿⇂ ↿⇂ ↿⇂ ⇂ ↿⇂ ↿ ⇂ ↿	-0.0748	0.0056
↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿⇂	-0.0688	0.0047
↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿⇂	-0.0544	0.0030

Thi.NO (T_1)

HONO-6	HONO-5	HONO-4	HONO-3	HONO-2	HSONO-1	HSONO	LUNO+1	LUNO+2
								
1.9949	1.9641	1.9633	1.9410	1.8959	1.0362	1.0316	0.1094	0.0636

Configuration State Functions	Coefficients	Weights
↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿ ↿	-0.9271	0.8595
↿⇂ ↿ ↿ ↿⇂ ↿⇂ ↿⇂ ↿⇂	0.1524	0.0232
↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿ ↿ ⇂ ↿	-0.1458	0.0213
↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿ ↿ ↿ ⇂	-0.0889	0.0079
↿⇂ ↿⇂ ↿⇂ ↿ ↿⇂ ↿ ↿ ↿⇂	-0.0848	0.0072
↿⇂ ↿⇂ ↿⇂ ↿ ↿⇂ ↿ ⇂ ↿	0.0717	0.0051
↿⇂ ↿⇂ ↿⇂ ↿⇂ ⇂ ↿ ↿ ↿	-0.0575	0.0033
↿⇂ ↿ ↿ ↿⇂ ↿⇂ ↿⇂ ↿ ⇂	0.0537	0.0029

Table S4. The natural orbitals, occupations for natural orbitals, configuration state functions as well as their coefficients and weights for **Sel**.**NO** in S_0 and T_1 states at CASSCF(12*e*,9*o*)/def2-TZVP//MN15/def2-TZVP level of theory.

	HONO-5	HONO-4	HONO-3	HONO-2	HONO-1	HONO	LUNO	LUNO+1	LUNO+2
									
	1.9987	1.9953	1.9945	1.9435	1.9169	1.8651	0.1446	0.0850	0.0564

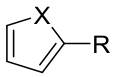
	Configuration State Functions	Coefficients	Weights
Sel.**NO** (S_0)	↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿⇂	0.9289	0.8628
	↿⇂ ↿⇂ ↿⇂ ↿⇂ ⇂ ↿ ⇂ ↿	-0.1591	0.0253
	↿⇂ ↿⇂ ↿⇂ ⇂ ↿⇂ ↿ ⇂ ↿	-0.0870	0.0076
	↿⇂ ↿⇂ ↿⇂ ⇂ ↿ ↿⇂ ⇂ ↿	-0.0839	0.0070
	↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿⇂ ⇂	-0.0793	0.0063
	↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿⇂	-0.0745	0.0056
	↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿⇂ ⇂ ↿⇂	-0.0743	0.0055
	↿⇂ ↿⇂ ↿⇂ ⇂ ↿⇂ ↿ ⇂ ↿	0.0527	0.0028

	HONO-6	HONO-5	HONO-4	HONO-3	HONO-2	HSONO-1	HSONO	LUNO+1	LUNO+2
									
	1.9959	1.9643	1.9637	1.9390	1.8882	1.0357	1.0296	0.1187	0.0648

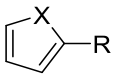
	Configuration State Functions	Coefficients	Weights
Sel.**NO** (T_1)	↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿ ↿	0.9229	0.8517
	↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿ ↿ ⇂ ↿	0.1577	0.0249
	↿⇂ ↿ ↿ ↿⇂ ↿⇂ ↿⇂ ↿⇂	-0.1462	0.0214
	↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿ ↿ ↿ ⇂	0.0973	0.0095
	↿⇂ ↿⇂ ↿⇂ ↿ ↿⇂ ↿ ⇂ ↿	-0.0808	0.0065
	↿⇂ ↿⇂ ↿⇂ ↿⇂ ↿ ↿ ↿⇂	0.0798	0.0064
	↿⇂ ↿⇂ ↿⇂ ↿⇂ ⇂ ↿ ↿ ↿	0.0635	0.0040
	↿⇂ ↿ ↿ ↿⇂ ↿⇂ ↿⇂ ↿ ⇂	-0.0606	0.0037

8. The cartesian coordinates for **X**.**R** in S_0 and T_1 states

Table S5. The optimized cartesian coordinates for **X**.**R** (X = Fur, Thi and Sel; R = C_2H, CHO, CN, COOH, NO_2 and NO) in S_0 and T_1 at level of MN15/def2-TZVP.



S_0



T_1

Fur.C_2H (S_0)

O	-0.74971800	1.01375800	0.00000000
C	0.34800400	0.21081000	0.00000000
C	-0.03668400	-1.09640300	0.00000000
C	-1.46116000	-1.09394600	0.00000000
C	-1.83137200	0.21081000	0.00000000
H	-2.78829800	0.70328200	0.00000000
H	-2.11845700	-1.94681600	0.00000000
H	0.62495000	-1.94590200	0.00000000
C	1.62261000	0.82646700	0.00000000
C	2.71320000	1.33352700	0.00000000

Fur.C_2H (T_1)

O	-0.74790100	1.11642300	0.00000000
C	0.37295000	0.28375100	0.00000000
C	-0.09849300	-1.12315200	0.00000000
C	-1.45260900	-1.07284600	0.00000000
C	-1.84216200	0.28375100	0.00000000
H	-2.80679000	0.75685600	0.00000000
H	-2.13716200	-1.90606600	0.00000000
H	0.55074200	-1.98116200	0.00000000
C	1.62151400	0.79803700	0.00000000
C	2.77368100	1.23211600	0.00000000

Fur.CHO (S_0)

O	-0.56698700	1.09138000	0.00000000
C	0.53130100	0.28889500	0.00000000
C	0.15097100	-1.02009000	0.00000000
C	-1.26898900	-1.01994900	0.00000000
C	-1.64231300	0.28889500	0.00000000
H	-2.60295700	0.77501800	0.00000000
H	-1.92776500	-1.87174900	0.00000000
H	0.82226900	-1.86249600	0.00000000
C	1.83219700	0.94255700	0.00000000
O	2.88135100	0.34057300	0.00000000

Fur.CHO (T_1)

O	-0.54313300	1.19795800	0.00000000
C	0.54707200	0.37668700	0.00000000
C	0.08610900	-1.02559500	0.00000000
C	-1.27585400	-0.97276400	0.00000000
C	-1.65433300	0.37668700	0.00000000
H	-2.61088100	0.86626900	0.00000000
H	-1.96582900	-1.80106500	0.00000000
H	0.75023100	-1.87136600	0.00000000
C	1.85164500	0.86162100	0.00000000
O	2.81127700	0.04474600	0.00000000

Fur.CN (S_0)

O	-0.75880068	0.84013030	0.00000000
C	0.33232364	0.03519060	0.00000000
C	-0.04266752	-1.27277506	0.00000000
C	-1.46583560	-1.27008325	0.00000000
C	-1.83731589	0.03519060	0.00000000
H	-2.79462102	0.52680863	0.00000000
H	-2.12171279	-2.12371271	0.00000000
H	0.62106322	-2.12057088	0.00000000
C	1.61165907	0.64900335	0.00000000
N	2.66176403	1.12468656	0.00000000

Fur.CN (T_1)

O	-0.74829272	0.93547516	0.00000000
C	0.35298987	0.09908545	0.00000000
C	-0.10649024	-1.31404178	0.00000000
C	-1.45596087	-1.26247594	0.00000000
C	-1.85191445	0.09908545	0.00000000
H	-2.81418380	0.57546797	0.00000000
H	-2.14000292	-2.09588094	0.00000000
H	0.54690127	-2.16859921	0.00000000
C	1.61940726	0.62120108	0.00000000
N	2.71936629	1.02586153	0.00000000

Fur.COOH (S_0)

O	-0.80535700	0.88520300	0.00000000
C	0.28578700	0.08203500	0.00000000
C	-0.08943500	-1.22586500	0.00000000
C	-1.51098000	-1.22623100	0.00000000
C	-1.88146800	0.08203500	0.00000000
H	-2.84052800	0.57094400	0.00000000
H	-2.16933900	-2.07816400	0.00000000
H	0.58475300	-2.06578700	0.00000000
C	1.62482900	0.66701100	0.00000000
O	2.63718700	0.00919700	0.00000000

Fur.COOH (T_1)

O	-0.79394700	0.98699200	0.00000000
C	0.29066600	0.15528800	0.00000000
C	-0.16370400	-1.25452400	0.00000000
C	-1.51560600	-1.20573600	0.00000000
C	-1.90653600	0.15528800	0.00000000
H	-2.86553800	0.63847200	0.00000000
H	-2.20234100	-2.03683400	0.00000000
H	0.50241200	-2.09908500	0.00000000
C	1.62252100	0.63686100	0.00000000
O	2.58534100	-0.12704500	0.00000000

Fur.NO_2 (S_0)

O	-0.55388500	1.11156200	0.00000000
C	0.51203600	0.30322600	0.00000000
C	0.16626900	-1.00684200	0.00000000
C	-1.25758300	-1.00326200	0.00000000
C	-1.63315100	0.30322600	0.00000000
H	-2.59041000	0.79459400	0.00000000
H	-1.91302800	-1.85738200	0.00000000
H	0.84610700	-1.84082600	0.00000000

Fur.NO_2 (T_1)

O	-0.51691600	1.19118200	0.00000000
C	0.53799000	0.36445400	0.00000000
C	0.11265800	-1.03943500	0.00000100
C	-1.24855800	-0.98789500	0.00000000
C	-1.63157800	0.36445400	0.00000000
H	-2.58489100	0.85939200	0.00000000
H	-1.93612300	-1.81803500	0.00000100
H	0.79100700	-1.87255600	0.00000000

N	1.80650000	0.91676400	0.00000000
O	1.86262000	2.12887100	0.00000000

Fur.NO (S_0)

O	-0.36384000	1.30821800	0.00000000
C	0.72650000	0.50590500	0.00000000
C	0.35486300	-0.81025900	0.00000000
C	-1.05969400	-0.80770200	0.00000000
C	-1.43325000	0.50590500	0.00000000
H	-2.39520300	0.98952300	0.00000000
H	-1.71999100	-1.65832900	0.00000000
H	1.03094700	-1.64832300	0.00000000
N	1.94704100	1.17588900	0.00000000
O	2.91262800	0.43917300	0.00000000

Thi.C_2H (S_0)

S	-0.81547900	1.47843800	0.00000000
C	0.42789500	0.29963600	0.00000000
C	-0.10183400	-0.96712200	0.00000000
C	-1.51709100	-0.96482100	0.00000000
C	-2.03349200	0.29963600	0.00000000
H	-3.07199700	0.59002400	0.00000000
H	-2.12429000	-1.85820600	0.00000000
H	0.51396500	-1.85451400	0.00000000
C	1.79443800	0.67710400	0.00000000
C	2.95186300	1.00604500	0.00000000

Thi.CHO (S_0)

S	-0.62579600	1.53678400	0.00000000
C	0.61054900	0.35893800	0.00000000
C	0.08966900	-0.91137600	0.00000000
C	-1.32131700	-0.91094000	0.00000000
C	-1.83806900	0.35893800	0.00000000
H	-2.87737400	0.64731000	0.00000000
H	-1.93207500	-1.80196300	0.00000000
H	0.71998500	-1.78918800	0.00000000
C	2.02287800	0.74037000	0.00000000
O	2.93048400	-0.05812500	0.00000000

Thi.CN (S_0)

S	-0.80482624	1.27048678	0.00000000
C	0.42995198	0.08910714	0.00000000
C	-0.08942660	-1.18131909	0.00000000
C	-1.50271636	-1.17785659	0.00000000
C	-2.01610530	0.08910714	0.00000000
H	-3.05441267	0.38048813	0.00000000
H	-2.11105324	-2.06994089	0.00000000
H	0.52859255	-2.06686317	0.00000000
C	1.80186658	0.45476627	0.00000000
N	2.91582862	0.75423632	0.00000000

Thi.COOH (S_0)

S	-0.89576300	1.35521600	0.00000000
C	0.33375600	0.17418800	0.00000000
C	-0.18281300	-1.09472500	0.00000000
C	-1.59551400	-1.09557000	0.00000000
C	-2.10796500	0.17418800	0.00000000
H	-3.14708000	0.46399700	0.00000000
H	-2.20515000	-1.98711800	0.00000000
H	0.44983600	-1.97078700	0.00000000
C	1.76195200	0.50200100	0.00000000
O	2.65337500	-0.30996200	0.00000000

Thi.NO_2 (S_0)

S	-0.60962900	1.55184100	0.00000000
C	0.59735700	0.35722400	0.00000000

N	1.80106100	0.86563200	0.00000000
O	1.97677200	2.09449800	-0.00000100

Fur.NO (T_1)

O	-0.35994200	1.30772000	0.00000000
C	0.72395100	0.49815900	0.00000000
C	0.34471800	-0.82954900	0.00000000
C	-1.07325100	-0.80916000	0.00000000
C	-1.44677500	0.49815900	0.00000000
H	-2.40311800	0.99011300	0.00000000
H	-1.73597200	-1.65818600	0.00000000
H	1.01038400	-1.67483300	0.00000000
N	1.91949800	1.10282200	0.00000000
O	3.02050600	0.57475700	0.00000000

Thi.C_2H (T_1)

S	-0.81301800	1.59110400	0.00000000
C	0.45624800	0.35419200	0.00000000
C	-0.14489200	-1.00214900	0.00000000
C	-1.49269300	-0.96483500	0.00000000
C	-2.03403300	0.35419200	0.00000000
H	-3.07708100	0.62102400	0.00000000
H	-2.12479700	-1.84175700	0.00000000
H	0.47178100	-1.88738100	0.00000000
C	1.77660500	0.65971700	0.00000000
C	2.97310600	0.93799400	0.00000000

Thi.CHO (T_1)

S	-0.58552200	1.65918200	0.00000000
C	0.64107500	0.43028900	0.00000000
C	0.03858200	-0.92555200	0.00000000
C	-1.31701000	-0.88053100	0.00000000
C	-1.84041200	0.43028900	0.00000000
H	-2.87786600	0.71891000	0.00000000
H	-1.95684500	-1.75165200	0.00000000
H	0.66807700	-1.80079400	0.00000000
C	2.02467100	0.67456100	0.00000000
O	2.83735200	-0.27318000	0.00000000

Thi.CN (T_1)

S	-0.79210437	1.38043839	0.00000000
C	0.45192963	0.13802680	0.00000000
C	-0.13838522	-1.22624540	0.00000000
C	-1.48259572	-1.18658713	0.00000000
C	-2.02259982	0.13802680	0.00000000
H	-3.06399361	0.41004746	0.00000000
H	-2.11739750	-2.06112512	0.00000000
H	0.48202788	-2.10838135	0.00000000
C	1.79309494	0.43562023	0.00000000
N	2.93705780	0.68042958	0.00000000

Thi.COOH (T_1)

S	-0.86174300	1.46845500	0.00000000
C	0.34845800	0.22953200	0.00000000
C	-0.23995600	-1.13178400	0.00000000
C	-1.58801300	-1.09291100	0.00000000
C	-2.11789400	0.22953200	0.00000000
H	-3.15650600	0.51330200	0.00000000
H	-2.22556800	-1.96556300	0.00000000
H	0.39369400	-2.00460900	0.00000000
C	1.75152900	0.48411100	0.00000000
O	2.60011700	-0.39636400	0.00000000

Thi.NO_2 (T_1)

S	-0.55674400	1.63437300	0.00000000
C	0.62366100	0.39122900	0.00000000

C	0.11350700	-0.91791900	0.00000000
C	-1.29990000	-0.91327900	0.00000000
C	-1.81151400	0.35722400	0.00000000
H	-2.85155300	0.64412100	0.00000000
H	-1.91027800	-1.80405800	0.00000000
H	0.75311300	-1.78761100	0.00000000
N	1.98310300	0.73650100	0.00000000
O	2.22624200	1.93142800	0.00000000

C	0.07911800	-0.97150100	0.00000000
C	-1.27515000	-0.92888900	0.00000000
C	-1.79829400	0.39122900	0.00000000
H	-2.83852400	0.67079900	0.00000000
H	-1.91485500	-1.79968100	0.00000000
H	0.72658000	-1.83244400	0.00000000
N	1.95296500	0.72359300	0.00000000
O	2.22850400	1.93821100	0.00000000

Thi.NO (S_0)

S	-0.38368100	1.72181000	0.00000000
C	0.84516800	0.53847700	0.00000000
C	0.33918600	-0.74092900	0.00000000
C	-1.06697400	-0.73648300	0.00000000
C	-1.58395000	0.53847700	0.00000000
H	-2.62529300	0.81981200	0.00000000
H	-1.68031900	-1.62559100	0.00000000
H	0.97373000	-1.61479300	0.00000000
N	2.17705700	0.99210700	0.00000000
O	3.00507600	0.10711200	0.00000000

Thi.NO (T_1)

S	-0.38789400	1.73453400	0.00000000
C	0.84901500	0.53678400	0.00000000
C	0.32672800	-0.75026400	0.00000000
C	-1.08165500	-0.72984900	0.00000000
C	-1.60050900	0.53678400	0.00000000
H	-2.63911500	0.82457900	0.00000000
H	-1.69537900	-1.61902700	0.00000000
H	0.95031600	-1.63123000	0.00000000
N	2.14457000	0.90468400	0.00000000
O	3.13392300	0.19300500	0.00000000

Sel.C_2H (S_0)

Se	-0.83214100	1.64587900	0.00000000
C	0.46435800	0.31261500	0.00000000
C	-0.11348500	-0.92679400	0.00000000
C	-1.53484500	-0.92464900	0.00000000
C	-2.09966200	0.31261500	0.00000000
H	-3.15215300	0.54825400	0.00000000
H	-2.12103900	-1.83340900	0.00000000
H	0.48185300	-1.82944500	0.00000000
C	1.84406800	0.62717900	0.00000000
C	3.01405000	0.91087700	0.00000000

Sel.C_2H (T_1)

Se	-0.83067000	1.74852591	-0.00000000
C	0.49235900	0.36539791	0.00000000
C	-0.15629000	-0.96559909	-0.00000000
C	-1.50464800	-0.93148609	-0.00000000
C	-2.09830800	0.36539891	-0.00000000
H	-3.15375900	0.57865791	-0.00000000
H	-2.11635100	-1.82403309	-0.00000000
H	0.44374300	-1.86342909	0.00000000
C	1.82312500	0.61786591	0.00000000
C	3.02856900	0.85312291	0.00000000

Sel.CHO (S_0)

Se	-0.64086400	1.70053600	0.00000000
C	0.64607800	0.36816000	0.00000000
C	0.07786200	-0.87589100	0.00000000
C	-1.33883000	-0.87535700	0.00000000
C	-1.90173500	0.36816000	0.00000000
H	-2.95441700	0.60383700	0.00000000
H	-1.92981200	-1.78102900	0.00000000
H	0.68948400	-1.76826600	0.00000000
C	2.07653700	0.67591200	0.00000000
O	2.94165100	-0.16866700	0.00000000

Sel.CHO (T_1)

Se	-0.59174000	1.81154500	0.00000000
C	0.67841800	0.43522600	0.00000000
C	0.02696300	-0.89696800	0.00000000
C	-1.32947200	-0.85409400	0.00000000
C	-1.90195200	0.43522600	0.00000000
H	-2.95213500	0.67400300	0.00000000
H	-1.94973700	-1.74056600	0.00000000
H	0.63893200	-1.78572700	0.00000000
C	2.07348400	0.62136100	0.00000000
O	2.84967600	-0.35202800	0.00000000

Sel.CN (S_0)

Se	-0.81683741	1.42852058	0.00000000
C	0.46939010	0.09290927	0.00000000
C	-0.09774452	-1.15106322	0.00000000
C	-1.51703431	-1.14761739	0.00000000
C	-2.07738034	0.09290927	0.00000000
H	-3.12940172	0.33095810	0.00000000
H	-2.10539268	-2.05440876	0.00000000
H	0.50022352	-2.05162389	0.00000000
C	1.85492023	0.39317207	0.00000000
N	2.97991661	0.65071410	0.00000000

Sel.CN (T_1)

Se	-0.80297748	1.52834887	0.00000000
C	0.49147408	0.14022893	0.00000000
C	-0.14646172	-1.19954267	0.00000000
C	-1.49153010	-1.16276332	0.00000000
C	-2.08205596	0.14022893	0.00000000
H	-3.13594870	0.35992431	0.00000000
H	-2.10656569	-2.05254870	0.00000000
H	0.45688637	-2.09458948	0.00000000
C	1.84281378	0.38260211	0.00000000
N	2.99406822	0.59039931	0.00000000

Sel.COOH (S_0)

Se	-0.91827300	1.52460100	0.00000000
C	0.36033700	0.18993200	0.00000000
C	-0.20265700	-1.05309700	0.00000000
C	-1.62142800	-1.05367300	0.00000000
C	-2.18067900	0.18993200	0.00000000
H	-3.23373700	0.42507800	0.00000000
H	-2.21082800	-1.96016800	0.00000000
H	0.41089600	-1.94412100	0.00000000

Sel.COOH (T_1)

Se	-0.87393000	1.62604100	0.00000000
C	0.37659400	0.24223500	0.00000000
C	-0.26033900	-1.09513100	0.00000000
C	-1.60992100	-1.05826500	0.00000000
C	-2.18797400	0.24223500	0.00000000
H	-3.23931300	0.47542000	0.00000000
H	-2.22823600	-1.94591200	0.00000000
H	0.35618400	-1.98139200	0.00000000

C	1.80145700	0.45145600	0.00000000
O	2.65885100	-0.39653600	0.00000000

C	1.78903400	0.44045900	0.00000000
O	2.60693100	-0.46723700	0.00000000

Sel.NO_2 (S_0)

Se	-0.62093300	1.71138400	0.00000000
C	0.63188700	0.36368000	0.00000000
C	0.10304700	-0.88860800	0.00000000
C	-1.31570000	-0.88211300	0.00000000
C	-1.87285300	0.36368000	0.00000000
H	-2.92685700	0.59445400	0.00000000
H	-1.90772600	-1.78637700	0.00000000
H	0.72458700	-1.77226600	0.00000000
N	2.03300300	0.67865300	0.00000000
O	2.32870300	1.86346200	0.00000000

Sel.NO_2 (T_1)

Se	-0.55686000	1.78566200	0.00000000
C	0.65729200	0.39451900	0.00000000
C	0.06650200	-0.94790500	0.00000000
C	-1.28942500	-0.90447300	0.00000000
C	-1.85899600	0.39451900	0.00000000
H	-2.91212700	0.62181000	0.00000000
H	-1.91097000	-1.78958800	0.00000000
H	0.69583500	-1.82328500	0.00000000
N	1.99981500	0.67672700	0.00000000
O	2.32161900	1.88008800	0.00000000

Sel.NO (S_0)

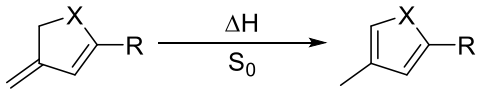
Se	-0.38655500	1.87467600	0.00000000
C	0.89021900	0.53796700	0.00000000
C	0.33802200	-0.71681100	0.00000000
C	-1.07366100	-0.71116900	0.00000000
C	-1.63635600	0.53796700	0.00000000
H	-2.69082600	0.76599900	0.00000000
H	-1.66779600	-1.61460100	0.00000000
H	0.95402600	-1.60514200	0.00000000
N	2.24349700	0.92705200	0.00000000
O	3.02943000	0.00406100	0.00000000

Sel.NO (T_1)

Se	-0.39284000	1.88821700	0.00000000
C	0.89735600	0.53693600	0.00000000
C	0.32429700	-0.72800800	0.00000000
C	-1.08653200	-0.70501900	0.00000000
C	-1.65355200	0.53693600	0.00000000
H	-2.70577000	0.77086700	0.00000000
H	-1.68159900	-1.60833500	0.00000000
H	0.92863300	-1.62353600	0.00000000
N	2.20243100	0.83791200	0.00000000
O	3.16757600	0.09403100	0.00000000

9. The cartesian coordinates for **X**.**R** used in isodesmic equations in S_0 and T_1 states

Table S6. The optimized cartesian coordinates for **X**.**R** (X = Fur, Thi and Sel; R = C_2H, CHO, CN, COOH, NO_2 and NO) used in isodesmic equations in their S_0 states at level of MN15/def2-TZVP.



Fur.C_2H (S_0)				**Fur.C_2H (S_0)**			
O	-0.65007200	0.54269300	0.12227000	O	-0.62194500	0.63670400	0.28957700
C	0.02090600	-0.59533700	0.43991000	C	-0.07854500	-0.53986700	-0.11658500
C	1.35987800	-0.48100700	0.38909100	C	1.26249900	-0.38927200	-0.30051800
C	1.67688600	0.87801700	-0.00526500	C	1.57206800	0.97034200	0.01202800
C	0.32875500	1.54431800	-0.17839600	C	0.38638800	1.53205500	0.36085500
H	0.18549600	2.38098200	0.50691700	H	0.11956700	2.52805500	0.67237500
H	2.06487100	-1.26656300	0.60509900	H	1.94334800	-1.16083900	-0.62113900
C	2.87285400	1.44302000	-0.18352200	C	2.90971600	1.63105200	-0.03465800
H	3.78369400	0.87892500	-0.03384900	H	3.61516900	1.14202700	0.63892700
H	2.97183700	2.47876100	-0.48215200	H	3.33447600	1.59175200	-1.03892900
C	-0.76768100	-1.72976600	0.77613900	H	2.83600700	2.67800700	0.25829400
C	-1.42958800	-2.69134600	1.06105000	C	-0.93841000	-1.65398100	-0.27131200
H	-2.01593100	-3.54281900	1.31333900	C	-1.65626300	-2.60927400	-0.40723400
H	0.16255800	1.89123200	-1.19928500	H	-2.29327500	-3.45293500	-0.52676000
Fur.CHO (S_0)				**Fur.CHO (S_0)**			
O	0.73837700	-0.54657100	1.13842700	O	0.86109800	-0.56073700	1.05878100
C	0.26554700	-0.59840300	-0.13228900	C	0.23638600	-0.60312600	-0.14659500
C	0.72598400	0.36564200	-0.94339300	C	0.60474900	0.47090600	-0.89974000
C	1.62698900	1.19838800	-0.16774100	C	1.51714400	1.22976700	-0.11191600
C	1.62413500	0.57781700	1.21538900	C	1.62523500	0.54535900	1.06193700
H	2.61020000	0.22024400	1.51527500	H	2.19664200	0.73349700	1.95597500
H	0.46193200	0.48333800	-1.98181600	H	0.25492000	0.67894500	-1.89815700
C	2.31358600	2.27245300	-0.56213600	C	2.20903400	2.49938300	-0.48315700
H	2.24317200	2.63392600	-1.57920700	H	2.83146400	2.36354400	-1.36855800
H	2.95959800	2.81508800	0.11603200	H	1.48969400	3.28862100	-0.70555600
C	-0.67450300	-1.69338200	-0.43432200	H	2.84858900	2.84556800	0.32813500
O	-1.16738700	-1.85405700	-1.52411000	C	-0.65813000	-1.72469800	-0.39213600
H	-0.89521000	-2.36289200	0.41538500	O	-1.27301600	-1.87661100	-1.42329300
H	1.24929200	1.26057000	1.97923000	H	-0.73720900	-2.43970300	0.44696600
Fur.CN (S_0)				**Fur.CN (S_0)**			
O	0.73857200	-0.53507200	1.16948400	O	0.88644400	-0.55959300	1.09547000
C	0.26595400	-0.60055700	-0.09764500	C	0.24619400	-0.60989000	-0.09669800
C	0.71997800	0.34896300	-0.92790200	C	0.59319300	0.45477600	-0.86801900
C	1.62382400	1.19327700	-0.16513200	C	1.51813800	1.22511100	-0.09913500
C	1.62583600	0.59344900	1.22530900	C	1.64840500	0.55366300	1.07489500
H	2.61089000	0.23627000	1.52711000	H	2.23123900	0.74593500	1.95995900
H	0.45870700	0.45955400	-1.96728200	H	0.23107900	0.66038900	-1.86206500
C	2.30680100	2.26056400	-0.57955800	C	2.19438400	2.49354000	-0.50055800
H	2.23267600	2.60693900	-1.60157300	H	2.80044900	2.34987100	-1.39599600
H	2.95490300	2.81400600	0.08752900	H	1.46604700	3.27581600	-0.71812700
C	-0.64678700	-1.66141200	-0.38682200	H	2.84739300	2.85315200	0.29369000
N	-1.38380400	-2.51017000	-0.63847600	C	-0.63120900	-1.69966700	-0.33556300
H	1.25000700	1.28379200	1.98105800	N	-1.34931600	-2.57494500	-0.55379500
	0.00000000	0.00000000	0.00000000		0.00000000	0.00000000	0.00000000
Fur.COOH (S_0)				**Fur.COOH (S_0)**			
O	-0.25123200	0.21802800	1.15431800	O	-0.12753900	0.17963900	1.17527400
C	0.07457300	-0.64721700	0.16839600	C	0.05303300	-0.65484100	0.12621800
C	1.16425700	-0.32068800	-0.53969300	C	1.08252300	-0.22374700	-0.65050200
C	1.67885000	0.92414900	0.00286000	C	1.57954900	0.96602100	-0.04091500
C	0.72490000	1.26812200	1.12917000	C	0.79909100	1.14917400	1.05941000

H	1.21911800	1.30055900	2.10111600
H	1.56768400	-0.89268600	-1.35897100
C	2.74631200	1.62316300	-0.38593400
H	3.36310600	1.28462500	-1.20755000
H	3.03036800	2.54610900	0.10315000
C	-0.77039100	-1.84291300	-0.04036100
O	-0.55345500	-2.66511600	-0.89473700
O	-1.79539100	-1.91508900	0.81463400
H	-2.28739600	-2.72474100	0.60186400

H	0.79567600	1.90790100	1.82441900
H	1.43088000	-0.70997200	-1.54731900
C	2.70824600	1.82644600	-0.50353700
H	3.64132900	1.26293900	-0.54595400
H	2.51822600	2.22206400	-1.50221600
H	2.85522500	2.67013400	0.17005400
C	-0.80823300	-1.82452600	-0.03543800
O	-0.70183700	-2.60894900	-0.94714000
O	-1.73100300	-1.94191600	0.93062000

Fur.NO_2 (S_0)

O	-0.71938400	0.67528600	0.15994500
C	-0.07954800	-0.46728700	-0.09667700
C	1.25401000	-0.43132600	-0.14125700
C	1.62578200	0.94918200	0.12427300
C	0.30666000	1.67351400	0.32249100
H	0.20567400	2.10062800	1.32014000
H	1.90447600	-1.26646600	-0.33594000
C	2.84727400	1.47920700	0.18425600
H	3.72642300	0.86943500	0.02638700
H	2.99995600	2.53042100	0.39152100
N	-0.91870800	-1.63441000	-0.30074900
O	-2.11773200	-1.47941200	-0.22263400
O	-0.33684400	-2.67833600	-0.53506000
H	0.13799200	2.45352700	-0.41984300

Fur.NO_2 (S_0)

O	-0.63643300	0.66676600	0.27819900
C	-0.08927200	-0.48678900	-0.11513600
C	1.24895800	-0.38720100	-0.29866600
C	1.56912000	0.96966700	0.01268600
C	0.38447900	1.54857800	0.35293900
H	0.12578600	2.54783900	0.65985600
H	1.90475000	-1.18123800	-0.61323200
C	2.91351300	1.61619400	-0.02606100
H	3.60703000	1.12043500	0.65409900
H	3.34306700	1.56855100	-1.02734700
H	2.84786000	2.66414800	0.26353200
N	-0.96111000	-1.61086300	-0.27785500
O	-2.14318400	-1.45382500	-0.04980500
O	-0.42791700	-2.64732600	-0.63710100

Fur.NO (S_0)

O	-0.62340400	0.65927000	-0.63763800
C	-0.05981300	-0.49295900	-0.22970500
C	1.19832700	-0.39590000	0.23182000
C	1.57364300	1.00037300	0.13944200
C	0.35286600	1.69039100	-0.44036400
H	0.55616200	2.16041100	-1.40332900
H	1.79679200	-1.21401400	0.59680200
C	2.73083400	1.57057000	0.48305000
H	3.54127800	0.98115700	0.89005700
H	2.89665100	2.63385800	0.36713200
N	-0.90505100	-1.63181900	-0.35900000
O	-0.38395800	-2.65651300	0.01109800
H	-0.06646200	2.43629600	0.23590500

Fur.NO (S_0)

O	-0.60192300	0.71301000	-0.46624000
C	-0.07805900	-0.50730300	-0.21294700
C	1.25146500	-0.40657900	0.08899400
C	1.57014800	0.97416100	0.01675200
C	0.39852700	1.59219900	-0.32467500
H	0.15577400	2.62869500	-0.49225900
H	1.89913900	-1.23373600	0.32949100
C	2.89207900	1.62409600	0.25836000
H	3.24637000	1.42910800	1.27121500
H	3.64709100	1.24747100	-0.43267400
H	2.82395300	2.70343600	0.12727900
N	-0.97825300	-1.56385100	-0.31202500
O	-0.48897300	-2.65199000	-0.08095800

Thi.C_2H (S_0)

S	-0.27013900	1.44569600	0.22932600
C	-0.77154900	-0.22288800	0.06789800
C	0.23942000	-1.10681900	-0.02071000
C	1.56287200	-0.51983300	0.03152100
C	1.48074700	0.98544300	0.20450200
H	1.94328400	1.29852500	1.13987000
H	0.07909100	-2.17079400	-0.12800300
C	2.71204200	-1.19658100	-0.05800500
H	2.71402200	-2.27239300	-0.17633100
H	3.67161500	-0.69737900	-0.01548300
C	-2.15909700	-0.52042300	0.03835900
C	-3.34093100	-0.74300100	0.01612500
H	-4.38512100	-0.94649000	-0.00412300
H	1.97635100	1.50614100	-0.61372700

Thi.C_2H (S_0)

S	-0.86883500	0.66808900	0.92239100
C	-0.19241000	-0.56262200	-0.05880100
C	1.09161000	-0.24508600	-0.42047700
C	1.52947000	1.00208000	0.10029000
C	0.55083400	1.59537100	0.84836500
H	0.60975700	2.54402300	1.36005300
H	1.69754100	-0.89094500	-1.04116600
C	2.88818200	1.58268600	-0.14414100
H	2.99699800	2.54499000	0.35478900
H	3.67128200	0.91898000	0.22660800
H	3.06498900	1.73273000	-1.21064800
C	-0.93646200	-1.72026500	-0.39986100
C	-1.57503900	-2.69965300	-0.68456900
H	-2.13711600	-3.56655200	-0.93791100

Thi.CHO (S_0)

S	0.71801800	-0.75828500	1.55861200
C	0.20813800	-0.70258500	-0.10769000
C	0.72397800	0.30301600	-0.83282800
C	1.62058800	1.17176600	-0.09735400
C	1.75469900	0.71500800	1.34474300

Thi.CHO (S_0)

S	0.90657700	-0.76786200	1.46615200
C	0.20305200	-0.69029500	-0.08829900
C	0.63279300	0.41608800	-0.77438200
C	1.54196600	1.20926500	-0.03210600
C	1.76949100	0.66446400	1.20735900

H	2.78579100	0.46066900	1.58649900
H	0.48292300	0.44290500	-1.87842100
C	2.24989000	2.23423700	-0.60904500
H	2.11356900	2.50989400	-1.64661100
H	2.91033100	2.84957300	-0.01150200
C	-0.72838600	-1.72017600	-0.62583400
O	-1.11984700	-1.73793300	-1.76751900
H	-1.05963900	-2.48201800	0.10353500
H	1.42166000	1.48609400	2.03813800

Thi.CN (S_0)

S	0.30672800	1.45386100	0.19928100
C	0.78313100	-0.22037600	0.06895600
C	-0.22457200	-1.10585100	-0.00506100
C	-1.54339600	-0.50418300	0.03398800
C	-1.44800700	0.99920300	0.21368300
H	-1.96050800	1.53160200	-0.58591500
H	-0.07016800	-2.17188000	-0.09760400
C	-2.69225100	-1.17694400	-0.07233000
H	-2.69516900	-2.25284300	-0.18858400
H	-3.65095200	-0.67535500	-0.04594000
C	2.16832300	-0.55237900	0.03904100
N	3.29255700	-0.80671100	0.01578300
H	-1.88086900	1.30752600	1.16474600

Thi.COOH (S_0)

S	-0.54547600	0.33127800	1.52786200
C	-0.03068700	-0.69169600	0.21693600
C	1.06734300	-0.28816600	-0.43884300
C	1.64102100	0.94433500	0.06427500
C	0.83219300	1.47530300	1.23369700
H	1.43838100	1.54052800	2.13647200
H	1.47951500	-0.84387000	-1.27054700
C	2.73215900	1.53747900	-0.42893000
H	3.26480900	1.10620500	-1.26650000
H	3.11780300	2.45966600	-0.01328300
C	-0.76457000	-1.92306900	-0.14101600
O	-0.45763400	-2.66967500	-1.03573800
O	-1.82937600	-2.12674500	0.65013300
H	-2.25895900	-2.94688500	0.35836200

Thi.NO_2 (S_0)

S	0.03640300	1.53464000	0.17366000
C	-0.45418100	-0.12040600	0.05207100
C	0.49289000	-1.05969200	-0.02178000
C	1.82900700	-0.49801700	0.01265900
C	1.77820400	1.01088700	0.18587600
H	2.22347300	1.30856500	1.13462300
H	0.27380200	-2.11392400	-0.10961000
C	2.95509300	-1.20802100	-0.09372000
H	2.92317200	-2.28386000	-0.20495500
H	3.92908800	-0.73630300	-0.07246800
N	-1.87422600	-0.40896800	0.02102600
O	-2.61617400	0.55476400	0.07703600
O	-2.22044700	-1.57163100	-0.05843000
H	2.30827000	1.52268000	-0.61575900

Thi.NO (S_0)

S	-1.07857300	0.80324200	-0.59733700
C	-0.13647600	-0.59704100	-0.17782000
C	1.14673100	-0.37862300	0.15717500
C	1.51881300	1.01882100	0.10706400
C	0.39749300	1.85271500	-0.48515500

H	2.41590300	1.05714100	1.97791400
H	0.29460800	0.63473200	-1.77867200
C	2.16953100	2.47270000	-0.53477400
H	2.75313600	2.28669500	-1.43774400
H	1.40907100	3.21438000	-0.78407600
H	2.83233500	2.90582800	0.21336200
C	-0.73034700	-1.71741200	-0.54866300
O	-1.25386600	-1.70651200	-1.63894600
H	-0.93765200	-2.52849800	0.17556100

Thi.CN (S_0)

S	0.92532200	-0.78949800	1.45880000
C	0.19535500	-0.69380600	-0.08295400
C	0.61291900	0.41760900	-0.76777600
C	1.53802100	1.20226700	-0.03103100
C	1.78529800	0.64615500	1.19483400
H	2.44515100	1.02819000	1.95900200
H	0.26537800	0.65758600	-1.76301400
C	2.15569300	2.46897800	-0.53710400
H	2.72207900	2.28985900	-1.45230300
H	1.39125000	3.21343200	-0.76488100
H	2.83297900	2.89501500	0.20170800
C	-0.72117700	-1.68216000	-0.52944100
N	-1.46582600	-2.48547000	-0.89178200

Thi.COOH (S_0)

S	-0.37101100	0.30262500	1.57108900
C	-0.03637100	-0.67202200	0.21275300
C	1.01096200	-0.17882400	-0.51668600
C	1.55453300	1.01047700	0.03234800
C	0.88280500	1.37014200	1.17203600
H	1.08155000	2.22969900	1.79487200
H	1.36435000	-0.66819400	-1.41459400
C	2.70553600	1.76569900	-0.55727300
H	3.59883900	1.14112300	-0.60907600
H	2.47870900	2.09637300	-1.57214500
H	2.94269100	2.64558600	0.03965900
C	-0.79208000	-1.88427700	-0.11208400
O	-0.57977900	-2.59367200	-1.06437300
O	-1.77140200	-2.13679400	0.77734100

Thi.NO_2 (S_0)

S	-1.02594200	0.86152500	0.40056700
C	-0.17875200	-0.51847700	-0.10775100
C	1.15916300	-0.31732100	-0.26848500
C	1.51869500	1.02161300	0.03490300
C	0.41885700	1.75101300	0.40835200
H	0.40462000	2.79293300	0.69167800
H	1.83443400	-1.09803000	-0.58756600
C	2.91373100	1.55924800	-0.04417500
H	3.58207700	1.01394400	0.62381000
H	3.31263400	1.46611200	-1.05533300
H	2.94114900	2.61166800	0.23483200
N	-0.88050000	-1.75259500	-0.32786000
O	-2.08452900	-1.74390200	-0.13369900
O	-0.22898800	-2.71279400	-0.69316100

Thi.NO (S_0)

S	-0.98630000	0.85997500	-0.56005000
C	-0.14273400	-0.58210000	-0.21796300
C	1.18316600	-0.35706000	0.06427200
C	1.51453000	1.01342500	0.00007100
C	0.41387900	1.77332600	-0.33127500

H	0.66087700	2.18440900	-1.48985000
H	1.81034400	-1.17052500	0.47599700
C	2.68864000	1.51439500	0.52373500
H	3.46024400	0.86122900	0.90981300
H	2.90302700	2.57481100	0.48796600
N	-0.83023300	-1.84869500	-0.14741100
O	-0.11027900	-2.80480300	0.00264800
H	0.17725600	2.73118700	0.11844500

Sel.C_2H (S_0)

Se	0.27359600	-1.21676700	0.09973300
C	0.70131800	0.63112600	0.06586800
C	-0.37141400	1.44072400	0.04314400
C	-1.67513800	0.80302300	0.03729200
C	-1.59845000	-0.69239700	0.26181300
H	-1.93298300	-0.94715300	1.26651000
H	-0.27435700	2.51806000	-0.00554500
C	-2.82759100	1.45625200	-0.14291200
H	-2.84215200	2.53091100	-0.27267900
H	-3.77772200	0.93787000	-0.16425100
C	2.06061800	1.02754500	0.03792300
C	3.22597500	1.32741900	0.01423800
H	4.25413600	1.60040400	-0.00658000
H	-2.19777700	-1.24438600	-0.45863200

Sel.CHO (S_0)

Se	-0.00947300	-1.35780400	0.11386000
C	0.80885700	0.34395600	0.04790900
C	-0.04541300	1.37823000	0.02368400
C	-1.45903600	1.05061600	0.04220400
C	-1.71387300	-0.41973300	0.30195200
H	-2.06595400	-0.57464000	1.32097800
H	0.30967700	2.39967700	-0.04463500
C	-2.43361900	1.94510100	-0.15113400
H	-2.20189800	2.99139400	-0.30349700
H	-3.47730700	1.65765400	-0.16202600
C	2.27745600	0.47482200	-0.00950900
O	2.84685300	1.53910500	-0.03891200
H	2.84536800	-0.47390400	-0.02448700
H	-2.44132400	-0.84054900	-0.38815700

Sel.CN (S_0)

Se	0.50717200	-0.68699900	1.72238800
C	0.15732200	-0.71146200	-0.13740300
C	0.78201500	0.24402900	-0.84334900
C	1.62169100	1.15541400	-0.08569800
C	1.80549900	0.72441100	1.35347300
H	2.80055700	0.30876600	1.50604000
H	0.64495400	0.35841000	-1.91105400
C	2.17360200	2.25653500	-0.60318800
H	2.03698900	2.50728400	-1.64727200
H	2.77132500	2.92980000	-0.00235100
C	-0.73563900	-1.67569000	-0.67947300
N	-1.46420500	-2.46731500	-1.09559700
H	1.65627400	1.54642300	2.04958600

Sel.COOH (S_0)

Se	0.12733800	-1.32878000	0.09778700
C	-0.48893500	0.45216200	0.04623800
C	0.46963800	1.38738200	0.01917700
C	1.83967400	0.90693800	0.02429800
C	1.93374400	-0.59116300	0.23070800
H	2.57641800	-1.06444600	-0.50833900

H	0.38883600	2.84663400	-0.44707700
H	1.86773400	-1.15872000	0.30409000
C	2.88069000	1.57062400	0.25752700
H	3.21723600	1.32980200	1.26695100
H	3.61009900	1.15485600	-0.43910400
H	2.88772100	2.65432900	0.14801800
N	-0.87429000	-1.78244500	-0.26335500
O	-0.22322800	-2.77393000	-0.01179100

Sel.C_2H (S_0)

Se	-0.99907700	0.72703800	1.01078700
C	-0.21750600	-0.57848100	-0.05717500
C	1.05827500	-0.22748400	-0.39652900
C	1.51217900	1.02324800	0.11955000
C	0.57932600	1.66531000	0.87602400
H	0.70001500	2.62027500	1.36529800
H	1.67597200	-0.86434300	-1.01718400
C	2.88504000	1.55926800	-0.15608100
H	3.03236500	2.52417400	0.32761000
H	3.65291800	0.87516600	0.20992700
H	3.04669700	1.68847900	-1.22788600
C	-0.92170500	-1.75041100	-0.42315300
C	-1.53613600	-2.74125100	-0.72454900
H	-2.07756100	-3.61716200	-0.99171800

Sel.CHO (S_0)

Se	0.92129500	-0.84880500	1.61139000
C	0.18816100	-0.71464200	-0.08448300
C	0.63920500	0.39788800	-0.73564800
C	1.55294000	1.20365900	-0.00165000
C	1.81931900	0.71023100	1.24504700
H	2.48014300	1.15170300	1.97618900
H	0.30816600	0.62757400	-1.74117500
C	2.15551100	2.46263300	-0.54928600
H	2.72393800	2.25925400	-1.45833800
H	1.38014700	3.18705500	-0.80398500
H	2.82636600	2.92393300	0.17432300
C	-0.75044800	-1.71086500	-0.59954500
O	-1.24863900	-1.65568800	-1.70037300
H	-0.98950500	-2.54321600	0.09022000

Sel.CN (S_0)

Se	0.93237400	-0.87709300	1.59013400
C	0.17475900	-0.71506800	-0.09426000
C	0.61875100	0.40387400	-0.73803800
C	1.54838700	1.19646900	-0.00317300
C	1.83044900	0.68613200	1.22853600
H	2.50314800	1.11301100	1.95732900
H	0.28311600	0.66173000	-1.73424700
C	2.14339000	2.45975100	-0.54852400
H	2.69644200	2.26516000	-1.46893200
H	1.36550700	3.18881000	-0.78144900
H	2.82720400	2.91116100	0.16883000
C	-0.74616300	-1.67085300	-0.59300200
N	-1.49492400	-2.45492800	-0.98914700

Sel.COOH (S_0)

Se	-0.46083100	0.33965500	1.71214600
C	-0.05870600	-0.68414700	0.22670700
C	0.98746700	-0.16612400	-0.47655200
C	1.54619400	1.02892500	0.06039800
C	0.91936300	1.44215100	1.20076200
H	1.17015200	2.31880200	1.77985200

H	0.22687200	2.44183700	-0.03478500
C	2.90337900	1.69975500	-0.13864500
H	2.78354300	2.76878600	-0.25935100
H	3.91130600	1.30494600	-0.15558100
C	-1.92519600	0.78632600	0.00498600
O	-2.37520200	1.90416600	-0.02113300
O	-2.69897500	-0.31230500	-0.00313300
H	-3.62411700	-0.02025600	-0.03436800

Sel.NO_2 (S_0)

Se	0.06062800	-1.34141300	0.08158600
C	-0.48638900	0.45091500	0.05820600
C	0.45754300	1.39420400	0.03345500
C	1.81510000	0.87908600	0.02360600
C	1.87685000	-0.62045800	0.24203900
H	2.52806400	-1.11004800	-0.47837500
H	0.22159600	2.44880100	-0.01306400
C	2.89265800	1.64650800	-0.16287000
H	2.79666800	2.71742900	-0.28658600
H	3.88986600	1.22665700	-0.19649000
N	-1.90446700	0.74008300	0.01836300
O	-2.64446100	-0.22768400	-0.02044600
O	-2.25718900	1.90353600	0.02285700
H	2.23451300	-0.84485400	1.24603000

Sel.NO (S_0)

Se	-1.23787100	0.86849600	-0.49868800
C	-0.15243200	-0.63040500	-0.14456000
C	1.13765900	-0.37320800	0.12634700
C	1.50550800	1.02859500	0.09726300
C	0.42638500	1.89634800	-0.51333500
H	0.66381800	2.11831600	-1.55338100
H	1.82768200	-1.15634100	0.41398100
C	2.66613200	1.50345100	0.56183400
H	3.42114100	0.83487200	0.95503000
H	2.88884400	2.56283500	0.55860600
N	-0.79470100	-1.90277000	-0.05587800
O	-0.03588800	-2.84084400	-0.08626600
H	0.29158800	2.83177900	0.02431500

H	1.34833400	-0.64901700	-1.37649800
C	2.70126400	1.74575000	-0.57210300
H	3.57918700	1.09979900	-0.62780700
H	2.45894500	2.05587600	-1.59004700
H	2.97016400	2.63433200	-0.00226700
C	-0.78501100	-1.90220900	-0.13800900
O	-0.54593300	-2.59007900	-1.09986000
O	-1.77604000	-2.19055800	0.72922900

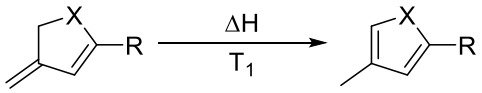
Sel.NO_2 (S_0)

Se	-1.17015900	0.92618600	0.44086200
C	-0.19877700	-0.53594300	-0.10958500
C	1.12918400	-0.29728900	-0.25843400
C	1.50016500	1.04513700	0.04418100
C	0.44069200	1.81980200	0.42330200
H	0.48982000	2.86355200	0.69701500
H	1.81703500	-1.06872900	-0.57701400
C	2.91204900	1.53983600	-0.04905500
H	3.56852300	0.97610400	0.61571000
H	3.29893200	1.42907600	-1.06331200
H	2.97468300	2.59208000	0.22476600
N	-0.85157100	-1.79418900	-0.34423300
O	-2.05801300	-1.82970400	-0.16056100
O	-0.16591300	-2.73098100	-0.70752700

Sel.NO (S_0)

Se	-1.12910800	0.90944000	-0.59801100
C	-0.15475900	-0.61393000	-0.21747000
C	1.15865600	-0.34216500	0.05710400
C	1.49494400	1.03321700	-0.00646800
C	0.43012700	1.83409100	-0.33376800
H	0.46012300	2.90877100	-0.43704100
H	1.85922100	-1.13078800	0.29927300
C	2.87646800	1.55255200	0.25840700
H	3.20301200	1.29542900	1.26727200
H	3.59589800	1.12050100	-0.43894600
H	2.91354900	2.63629900	0.15583600
N	-0.83275000	-1.84741500	-0.24712800
O	-0.13804000	-2.80728600	0.01125000

Table S7. The optimized cartesian coordinates for **X**.**R** (X = Fur, Thi and Sel; R = C_2H, CHO, CN, COOH, NO_2 and NO) used in isodesmic equations in their T_1 states at level of MN15/def2-TZVP.



Fur.C_2H (T_1)			**Fur.C_2H (T_1)**		
O	-0.65520100	0.56234000	0.11645500	O	-0.71581300	0.73149900	0.06038000
C	-0.06943200	-0.61971500	0.44810500	C	-0.15316800	-0.53598900	-0.12543300
C	1.38015000	-0.44966000	0.37997700	C	1.31262500	-0.38968700	-0.17229100
C	1.65332600	0.82563400	0.01011900	C	1.59107700	0.92386700	-0.01817100
C	0.34020000	1.53117200	-0.17501000	C	0.34255700	1.60388100	0.12376100
H	0.22314000	2.38253900	0.50429300	H	0.10897000	2.64364300	0.26601700
H	2.09010400	-1.23259800	0.59536200	H	2.00155900	-1.20697800	-0.30665800
C	2.90295900	1.45759000	-0.18799000	C	2.92042700	1.59552900	0.00766900
H	3.82501300	0.91561200	-0.04462500	H	3.72289300	0.87138700	-0.11995200
H	2.96146000	2.49339500	-0.48621700	H	2.99593700	2.33875700	-0.78853300
C	-0.81804700	-1.72190500	0.77458200	H	3.07369800	2.11781100	0.95411300
C	-1.45516000	-2.71990100	1.06965300	C	-0.94245100	-1.63120700	-0.22907600
H	-2.01451600	-3.58669700	1.32601300	C	-1.63331400	-2.64299200	-0.32653300
H	0.20046400	1.89330400	-1.19937100	H	-2.23419800	-3.51569700	-0.41036900
Fur.CHO (T_1)				**Fur.CHO (T_1)**			
O	0.74561100	-0.54239700	1.14950800	O	0.70274900	-0.47277500	1.20846100
C	0.22730000	-0.67196000	-0.08066900	C	0.23112700	-0.66384500	-0.06336400
C	0.74525500	0.38711400	-0.93572700	C	0.72373600	0.41716400	-0.92311400
C	1.58770800	1.15807500	-0.19271100	C	1.48034800	1.23039800	-0.14070200
C	1.61893100	0.58032900	1.19434200	C	1.46225300	0.67670700	1.16691200
H	2.61578500	0.24028700	1.48872200	H	1.92010300	0.98838200	2.08852500
H	0.47662500	0.49844000	-1.97348900	H	0.49448000	0.49775500	-1.97198000
C	2.32491400	2.29115700	-0.57044200	C	2.21012500	2.47250100	-0.52237100
H	2.27116700	2.67073700	-1.57924300	H	2.07078100	2.69054600	-1.57905500
H	2.95929100	2.80661200	0.13500000	H	1.85370700	3.32616500	0.05641600
C	-0.67221800	-1.70611700	-0.40096400	H	3.27917000	2.37028700	-0.32880600
O	-1.14681300	-1.81749300	-1.54377300	C	-0.58436600	-1.74680700	-0.39419900
H	-0.92736000	-2.40249000	0.41181400	O	-0.99287800	-1.88027100	-1.57528000
H	1.25551600	1.27986600	1.95235600	H	-0.84473700	-2.45549300	0.40124100
Fur.CN (T_1)				**Fur.CN (T_1)**			
O	0.74304700	-0.53375400	1.17072000	O	0.70260100	-0.46950500	1.23069100
C	0.22068900	-0.67206900	-0.06724100	C	0.23919200	-0.66254600	-0.06275000
C	0.74259400	0.38249700	-0.92999500	C	0.73654100	0.41761500	-0.93030600
C	1.58158200	1.15176200	-0.19521700	C	1.48046200	1.23010200	-0.15275500
C	1.61556500	0.58892000	1.19554100	C	1.45945600	0.68410000	1.17682300
H	2.61540300	0.25477800	1.49058400	H	1.91453600	1.01025100	2.09385300
H	0.48441800	0.50102700	-1.97007200	H	0.52295300	0.50510600	-1.98229900
C	2.32969300	2.29173700	-0.58032900	C	2.21109500	2.46972700	-0.53043700
H	2.28044600	2.66843800	-1.59000600	H	2.08369400	2.68921500	-1.58837500
H	2.96260500	2.80526500	0.12696400	H	1.84926700	3.32206300	0.04803600
C	-0.66406000	-1.69879800	-0.34831800	H	3.27792800	2.36721400	-0.32212500
N	-1.41186800	-2.55026900	-0.62333500	C	-0.55721200	-1.74314600	-0.35076100
H	1.25744200	1.30006900	1.94680000	N	-1.23807200	-2.65203800	-0.63553300
Fur.COOH (T_1)				**Fur.COOH (T_1)**			
O	-0.24518000	0.22014200	1.14876600	O	-0.30531700	0.30580900	1.10572300
C	0.01111100	-0.68529400	0.19424600	C	0.00617600	-0.65908800	0.18069400
C	1.19946900	-0.29229800	-0.54686100	C	1.19603600	-0.25969700	-0.57849200
C	1.65746200	0.87226700	-0.01940800	C	1.58054100	0.94104500	-0.09616600
C	0.73538400	1.25062000	1.10401500	C	0.65337000	1.29103400	0.94441100
H	1.24320500	1.29633400	2.07235300	H	0.58261500	2.14875800	1.58796100
H	1.60835200	-0.86056900	-1.36644900	H	1.63607600	-0.85276000	-1.36227000
C	2.77621400	1.65095800	-0.38908900	C	2.72747200	1.79372300	-0.51036400
H	3.41519200	1.34489300	-1.20280700	H	3.28798800	1.32369600	-1.31567400
H	3.01545400	2.56541800	0.13212300	H	2.37998500	2.77054900	-0.85269100

C	-0.80104200	-1.83600400	-0.00722300
O	-0.56964600	-2.66498900	-0.87825300
O	-1.84956700	-1.94137800	0.84040000
H	-2.31103300	-2.75794600	0.59532300

Fur.NO_2 (T_1)

O	-0.71481900	0.67192600	0.15911200
C	-0.16030400	-0.49681400	-0.09948400
C	1.28366000	-0.41039800	-0.13814200
C	1.60513400	0.89121300	0.11332100
C	0.32003400	1.64440900	0.31607100
H	0.23338800	2.08010800	1.31408600
H	1.93004900	-1.24843800	-0.33324800
C	2.86990200	1.49550300	0.18666600
H	3.76596500	0.91416900	0.03390700
H	2.97358500	2.54936300	0.39635900
N	-0.94510100	-1.60177000	-0.29303700
O	-2.17532600	-1.49058600	-0.22271400
O	-0.31588800	-2.65738800	-0.53169500
H	0.16575000	2.43266700	-0.42434900

Fur.NO (T_1)

O	-0.61907400	0.65513600	-0.63691800
C	-0.06672400	-0.51124000	-0.22989500
C	1.22345800	-0.38567200	0.24023300
C	1.57731200	0.99372300	0.14237400
C	0.35800700	1.68260800	-0.43810900
H	0.56684600	2.15360400	-1.39974500
H	1.83172100	-1.19485700	0.60831300
C	2.73365700	1.59140500	0.48192700
H	3.55585700	1.02083800	0.89123700
H	2.87693900	2.65644000	0.35689100
N	-0.82019900	-1.59901900	-0.33338800
O	-0.55258000	-2.75186600	-0.03707400
H	-0.05735200	2.43002200	0.23942000

Thi.C_2H (T_1)

S	-1.06856600	0.76691900	0.10479600
C	-0.18705500	-0.66668300	0.47242300
C	1.24952500	-0.41151000	0.35555400
C	1.58694800	0.85397000	-0.00497300
C	0.39929900	1.75461500	-0.21547900
H	0.42473500	2.61128900	0.46287700
H	1.96884900	-1.19553400	0.54895300
C	2.89437900	1.35798300	-0.18642400
H	3.75530100	0.72339900	-0.03888300
H	3.06006700	2.38486600	-0.47548800
C	-0.79042300	-1.85437700	0.82003700
C	-1.31864600	-2.90801800	1.12818800
H	-1.77980800	-3.82734900	1.39706700
H	0.36985600	2.14154000	-1.23730400

Thi.CHO (T_1)

S	0.70036900	-0.72827200	1.54614800
C	0.15445900	-0.75994000	-0.06689800
C	0.74552600	0.32524700	-0.83535900
C	1.59532900	1.12910100	-0.13017900
C	1.74205400	0.71663000	1.31075700
H	2.77658100	0.46369700	1.55438500
H	0.50101700	0.44616200	-1.88110300
C	2.29668500	2.24024400	-0.61956900
H	2.19634000	2.54173700	-1.65145800
H	2.94903700	2.81639700	0.01969700

H	3.40397100	1.96714100	0.32892300
C	-0.76083500	-1.84493500	0.03951300
O	-0.48105200	-2.70707800	-0.78824800
O	-1.81327600	-1.94702500	0.88154800

Fur.NO_2 (T_1)

O	-0.03096100	1.27940800	0.06844500
C	0.41957300	0.01992200	0.05464400
C	-0.58986000	-0.89111400	0.01664700
C	-1.78976900	-0.11065600	-0.00911900
C	-1.38980300	1.18636800	0.02301900
H	-1.92675300	2.11886000	0.01245400
H	-0.48335600	-1.96238900	-0.00203400
C	-3.19121600	-0.61929400	-0.06741400
H	-3.35435300	-1.21701500	-0.96517200
H	-3.41537000	-1.25087500	0.79324300
H	-3.90301800	0.20516100	-0.07646300
N	1.78712100	-0.14749500	0.17196200
O	2.65039100	0.73173000	-0.23381000
O	2.32633600	-1.31913000	0.05351400

Fur.NO (T_1)

O	-0.60369600	0.70433000	-0.46437700
C	-0.07009200	-0.51074400	-0.20952000
C	1.27218600	-0.40368000	0.09369300
C	1.57306000	0.98416900	0.01599500
C	0.40678200	1.60004400	-0.32317300
H	0.15428500	2.63262600	-0.49264500
H	1.93047100	-1.22100700	0.33529600
C	2.89362700	1.63691100	0.25583700
H	3.24917500	1.44240500	1.26861200
H	3.64866700	1.26038800	-0.43561300
H	2.82280700	2.71601300	0.12398500
N	-0.90164000	-1.55741500	-0.29265700
O	-0.63829300	-2.73532100	-0.10512100

Thi.C_2H (T_1)

S	-1.11451000	0.96317400	0.21542600
C	-0.25287400	-0.55902500	-0.10377400
C	1.19685300	-0.32212300	-0.18957300
C	1.53594900	0.96909700	-0.01033900
C	0.39096200	1.81636700	0.22424300
H	0.41937800	2.88028900	0.39338900
H	1.88765500	-1.13077400	-0.37907700
C	2.91906600	1.52812800	-0.03849100
H	3.65340400	0.74676100	-0.22732000
H	3.01246000	2.28860100	-0.81718000
H	3.16036200	2.00974600	0.91188700
C	-0.90487000	-1.74324900	-0.23899600
C	-1.49965600	-2.80920800	-0.36003700
H	-2.01338100	-3.73395900	-0.46523700

Thi.CHO (T_1)

S	0.89771800	-0.75549400	1.51286500
C	0.19406900	-0.71363500	-0.07023300
C	0.64327800	0.40927000	-0.77305900
C	1.53715400	1.20477000	-0.02658400
C	1.76211500	0.69135200	1.22511800
H	2.40015300	1.10238100	1.99177900
H	0.32848800	0.63081500	-1.78368900
C	2.16652800	2.46294200	-0.54149800
H	2.76009000	2.26519400	-1.43576400
H	1.40628000	3.19861200	-0.80972200

C	-0.75451500	-1.72349200	-0.57302700
O	-1.13157500	-1.71948600	-1.74921400
H	-1.11391500	-2.48568000	0.13899500
H	1.42432300	1.50981800	1.99154500

Thi.CN (T_1)

S	0.72666500	-0.76912000	1.52394200
C	0.15096000	-0.76934800	-0.08746800
C	0.72497600	0.34235300	-0.84392500
C	1.57550800	1.12916900	-0.13535500
C	1.75065400	0.68850300	1.29204600
H	2.79320100	0.44237800	1.50955000
H	0.47415300	0.50085000	-1.88324600
C	2.26933900	2.26583900	-0.60943000
H	2.15434700	2.59484400	-1.63098500
H	2.92618000	2.82621600	0.03828300
C	-0.74084800	-1.71911100	-0.56506200
N	-1.48902100	-2.51176700	-0.97453300
H	1.44143900	1.46879400	1.99227900

Thi.COOH (T_1)

S	-0.51947100	0.31220700	1.49923300
C	-0.07836300	-0.73725600	0.23935100
C	1.10715600	-0.26315500	-0.45585000
C	1.61902800	0.90255000	0.02887000
C	0.83644100	1.45135300	1.19162000
H	1.45394900	1.53426100	2.08985900
H	1.51540900	-0.82279300	-1.28567400
C	2.75309300	1.59072200	-0.44450800
H	3.32154800	1.20599400	-1.27774200
H	3.07719200	2.51333400	0.01310700
C	-0.78876200	-1.93191000	-0.08775400
O	-0.48234400	-2.69410300	-0.99005600
O	-1.86338700	-2.15491000	0.71125400
H	-2.26887800	-2.98093300	0.40681900

Thi.NO_2 (T_1)

S	-1.11489200	0.81814100	0.20431200
C	-0.22185100	-0.57545000	-0.11306500
C	1.20656900	-0.37549400	-0.12808000
C	1.55902300	0.92342300	0.12164500
C	0.37160800	1.82164200	0.35000600
H	0.39921400	2.27864600	1.34197700
H	1.88228600	-1.19466400	-0.32050300
C	2.85886800	1.44050400	0.17594900
H	3.71248800	0.79995700	0.01283200
H	3.03562600	2.48581800	0.38107500
N	-0.87897000	-1.76491200	-0.32873900
O	-2.12100000	-1.74397100	-0.27617600
O	-0.18496400	-2.76859100	-0.55929500
H	0.33202900	2.62891500	-0.38508800

Thi.NO (T_1)

S	-1.01905900	0.77381400	-0.79064400
C	-0.13772000	-0.63076200	-0.22354500
C	1.15089000	-0.36174600	0.20878800
C	1.51698400	1.00853000	0.11055200
C	0.39211700	1.85835800	-0.45224300
H	0.69720500	2.34706000	-1.37667100
H	1.80490100	-1.13611600	0.58385900
C	2.71326100	1.52259400	0.46679800
H	3.49301400	0.88733200	0.86479700
H	2.92840000	2.57807200	0.36632100

H	2.82014600	2.90864800	0.20740600
C	-0.68444700	-1.70137300	-0.49682400
O	-1.23850100	-1.70303200	-1.69199100
H	-0.98647400	-2.54973900	0.11487900

Thi.CN (T_1)

S	0.40081400	1.49298300	0.18092100
C	0.85147600	-0.20566100	-0.01209300
C	-0.32918100	-1.07429500	-0.10637400
C	-1.48132700	-0.39961100	0.05307500
C	-1.26898500	1.02139800	0.26454900
H	-2.03466300	1.74669100	0.48445300
H	-0.23895600	-2.13746600	-0.27229500
C	-2.85500600	-0.97564700	0.03403600
H	-2.82794700	-2.05141300	-0.12855400
H	-3.36640700	-0.77734900	0.97887000
H	-3.45317000	-0.51657900	-0.75646800
C	2.16702100	-0.61176500	-0.03501500
N	3.28299500	-0.95734600	-0.06423600

Thi.COOH (T_1)

S	-0.32236500	0.21113200	1.71655500
C	-0.06755600	-0.68558000	0.23685500
C	1.01174900	-0.12784800	-0.57796200
C	1.57841100	0.95560900	-0.01597100
C	0.97053400	1.29309200	1.25868900
H	1.25166900	2.11600700	1.89491400
H	1.28225600	-0.57857800	-1.52142300
C	2.69852800	1.76495800	-0.57307400
H	3.54789000	1.77138800	0.11417400
H	3.02871200	1.36864200	-1.53142600
H	2.39093600	2.80418100	-0.71155000
C	-0.83435800	-1.83508200	-0.12716200
O	-0.66666300	-2.47003300	-1.15710300
O	-1.77870000	-2.16242800	0.78687300

Thi.NO_2 (T_1)

S	-0.02813300	-1.54319600	-0.07999800
C	0.49449500	0.08666600	0.02413800
C	-0.54787400	0.99390100	0.02613500
C	-1.79883100	0.33776000	-0.05957000
C	-1.65643300	-1.02359100	-0.12232400
H	-2.44516600	-1.75641700	-0.19242800
H	-0.40123300	2.06242700	0.08638400
C	-3.11529000	1.05058600	-0.07917600
H	-3.94052300	0.34336600	-0.14817000
H	-3.25090700	1.64430500	0.82607000
H	-3.17802600	1.73049000	-0.93016800
N	1.80941000	0.37877700	0.09421200
O	2.79607300	-0.44813800	0.09405400
O	2.34338400	1.55081000	0.17553900

Thi.NO (T_1)

S	-0.99046600	0.86767800	-0.58523500
C	-0.14348400	-0.58602700	-0.22091800
C	1.19147400	-0.34952800	0.07253800
C	1.51373000	1.02497700	-0.00294700
C	0.42734600	1.78644200	-0.34770800
H	0.40103100	2.85773400	-0.47299200
H	1.88070900	-1.14226900	0.32566200
C	2.87978200	1.57828000	0.26275000
H	3.20619600	1.34266800	1.27697800
H	3.61354700	1.15399700	-0.42448600

N	-0.72038600	-1.82035000	-0.23655800
O	-0.30199900	-2.91225800	0.10530400
H	0.09025900	2.62659400	0.25851000

Sel.C_2H (T_1)

Se	-1.21016100	0.81986900	0.05574600
C	-0.21349700	-0.69744200	0.46779900
C	1.21247700	-0.39248300	0.36216900
C	1.56500500	0.87066100	0.00255100
C	0.42246300	1.81781100	-0.24736900
H	0.45740400	2.67324400	0.42990500
H	1.94277200	-1.16442500	0.56867500
C	2.88959800	1.34125700	-0.14816500
H	3.73043800	0.68601400	0.02402300
H	3.08780300	2.36233200	-0.43764900
C	-0.77471700	-1.90324400	0.81424100
C	-1.27268200	-2.97249300	1.12145300
H	-1.70597700	-3.90548900	1.38950200
H	0.43353400	2.19549700	-1.27153500

Sel.CHO (T_1)

Se	0.70934300	-0.81703000	1.66780300
C	0.14485300	-0.79737500	-0.08375800
C	0.74223900	0.31404300	-0.80364500
C	1.58756700	1.13075700	-0.10389400
C	1.78589900	0.75869400	1.34161900
H	2.82986400	0.52934900	1.56169000
H	0.50141900	0.45358300	-1.84904700
C	2.25718600	2.24874500	-0.62030900
H	2.13089300	2.53538300	-1.65377900
H	2.91050700	2.84538200	-0.00091800
C	-0.75125100	-1.74564800	-0.63795000
O	-1.11133800	-1.70557900	-1.81801600
H	-1.11930700	-2.53426700	0.04153500
H	1.46384100	1.55612600	2.01339000

Sel.CN (T_1)

Se	0.68168600	-0.82616900	1.65196800
C	0.12540600	-0.79628200	-0.11027900
C	0.73850700	0.32046500	-0.82336500
C	1.57879600	1.12086000	-0.11431400
C	1.76697600	0.74384800	1.32916200
H	2.81027900	0.51123000	1.55128800
H	0.51776300	0.48273100	-1.87001200
C	2.26707700	2.24718800	-0.62068600
H	2.15339600	2.54408500	-1.65237800
H	2.91817300	2.83143100	0.01171200
C	-0.75443400	-1.72636300	-0.64023400
N	-1.49411000	-2.50833500	-1.08562400
H	1.44804500	1.54491700	1.99886500

Sel.COOH (T_1)

Se	-0.62114300	0.34227300	1.60585800
C	-0.10573100	-0.75569200	0.23159200
C	1.08553200	-0.25343400	-0.42680800
C	1.61610200	0.90750300	0.05624000
C	0.87668800	1.50900500	1.22132800
H	1.50980000	1.58318500	2.10789100
H	1.50356700	-0.80362100	-1.25954100
C	2.76195700	1.55951600	-0.43716800
H	3.31116700	1.14993800	-1.27174500
H	3.11502000	2.47879400	0.00581400
C	-0.79727000	-1.94847900	-0.13265700

H	2.89140400	2.66111700	0.14545600
N	-0.78921400	-1.76741900	-0.24435200
O	-0.34471700	-2.87893400	-0.01443800

Sel.C_2H (T_1)

Se	-0.94394100	0.61018900	1.28194400
C	-0.25321500	-0.60963000	-0.03050200
C	1.07731200	-0.17980600	-0.47853400
C	1.54550600	0.94715100	0.09401700
C	0.65510800	1.54817500	1.05889800
H	0.86172600	2.44904900	1.61358800
H	1.61575100	-0.75409900	-1.21981300
C	2.86841800	1.57495400	-0.20142300
H	2.73724600	2.59416600	-0.57238000
H	3.47592200	1.63845700	0.70440000
H	3.41679200	1.00202500	-0.94753400
C	-0.94735200	-1.70032100	-0.44517300
C	-1.58425700	-2.68229600	-0.81159600
H	-2.13421500	-3.53418600	-1.13097000

Sel.CHO (T_1)

Se	0.93195200	-0.83123500	1.60842600
C	0.14907600	-0.74301500	-0.12437200
C	0.64121600	0.41067500	-0.74955400
C	1.56440700	1.20511200	0.01985900
C	1.86005400	0.74132100	1.28461500
H	2.51669000	1.17441200	2.01898900
H	0.33524300	0.67460700	-1.75213200
C	2.15228200	2.44979700	-0.53774800
H	2.69260500	2.22280400	-1.46052100
H	1.35480300	3.14650000	-0.80907400
H	2.82809300	2.93393500	0.16362300
C	-0.75779400	-1.71728600	-0.60527700
O	-1.27081100	-1.66987300	-1.72603400
H	-0.99121700	-2.54704100	0.09189100

Sel.CN (T_1)

Se	0.92474800	-0.87046400	1.56646400
C	0.12989800	-0.74087300	-0.14643800
C	0.62362400	0.43112000	-0.76520800
C	1.55732300	1.20269700	0.00575800
C	1.86484400	0.71531700	1.25591400
H	2.53101900	1.12546700	1.99455100
H	0.31709600	0.72821100	-1.75778200
C	2.14742000	2.45636200	-0.53616900
H	2.68247900	2.24841100	-1.46619800
H	1.35583500	3.16908300	-0.78093200
H	2.83309300	2.91810300	0.17090300
C	-0.76721500	-1.69971400	-0.59498400
N	-1.51772500	-2.51556300	-0.95182500

Sel.COOH (T_1)

Se	-0.45248300	0.31184100	1.67477800
C	-0.05492500	-0.74828000	0.15856800
C	1.02469900	-0.16603000	-0.51981100
C	1.54962900	1.03830800	0.06571900
C	0.92852700	1.47223400	1.21998000
H	1.16118300	2.34056100	1.81191000
H	1.42676600	-0.60364200	-1.42272800
C	2.69433600	1.75802900	-0.55183300
H	3.56083900	1.09496600	-0.61732600
H	2.44483100	2.04744400	-1.57592100
H	2.96804000	2.64677000	0.01258800

O	-0.47374400	-2.69437900	-1.04226000
O	-1.88579800	-2.19480800	0.64505600
H	-2.28000900	-3.01787200	0.31887300

Sel.NO_2 (T_1)

Se	-1.25104800	0.85700400	0.21775400
C	-0.23071300	-0.60813200	-0.12850600
C	1.18598900	-0.36211400	-0.12922600
C	1.54449700	0.93739000	0.13105800
C	0.39184400	1.87821400	0.37184400
H	0.43888700	2.32449200	1.36685600
H	1.87836700	-1.16789000	-0.32452100
C	2.85300800	1.42453700	0.18511100
H	3.69253200	0.76679000	0.01552400
H	3.05298400	2.46458800	0.39665000
N	-0.85467400	-1.81080700	-0.35856600
O	-2.10025500	-1.81982300	-0.31431900
O	-0.14027300	-2.79828500	-0.59295100
H	0.37488500	2.68800000	-0.35985600

Sel.NO (T_1)

Se	-1.15530400	0.80977300	-0.83471400
C	-0.15174100	-0.67567900	-0.21456500
C	1.13195800	-0.35365900	0.19932700
C	1.49880700	1.01620600	0.09942800
C	0.40780100	1.91429900	-0.45258200
H	0.72843200	2.39977900	-1.37218100
H	1.80566000	-1.11248100	0.57499100
C	2.70756600	1.50297000	0.45794700
H	3.47476800	0.84873200	0.84996900
H	2.94422700	2.55456600	0.36484900
N	-0.68370100	-1.88415500	-0.20251600
O	-0.22979300	-2.95947000	0.14688600
H	0.12918600	2.68024600	0.26842700

C	-0.78841800	-1.91695300	-0.14871200
O	-0.60690800	-2.66157400	-1.09990300
O	-1.78277700	-2.16154700	0.76590700

Sel.NO_2 (T_1)

Se	-1.25943600	0.95935300	0.19823900
C	-0.21353100	-0.56045000	-0.10628700
C	1.20986100	-0.32870500	-0.17775700
C	1.53336600	0.97518900	-0.00742000
C	0.39732600	1.84838600	0.20740700
H	0.46885500	2.91338100	0.36088600
H	1.89632300	-1.14341500	-0.35038100
C	2.91602100	1.53106100	-0.02749200
H	3.65264800	0.74908500	-0.19916300
H	3.01257000	2.28440100	-0.81265700
H	3.14172600	2.02566800	0.92000700
N	-0.84401800	-1.77497300	-0.24041800
O	-2.08714300	-1.76648300	-0.14644500
O	-0.13792000	-2.77756100	-0.44240600

Sel.NO (T_1)

Se	-1.13849800	0.91905800	-0.60115800
C	-0.15596300	-0.62248300	-0.21687000
C	1.17195800	-0.33476500	0.05940900
C	1.49368900	1.04346100	-0.00780700
C	0.43783700	1.84845400	-0.33346600
H	0.46342900	2.92227700	-0.43766500
H	1.88165500	-1.11395200	0.30271400
C	2.87583300	1.56144300	0.25735000
H	3.20151000	1.30301000	1.26635900
H	3.59448700	1.12804200	-0.44025500
H	2.91322500	2.64515900	0.15485400
N	-0.74171700	-1.82695100	-0.22826400
O	-0.26010700	-2.92403700	-0.00488800