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Supplementary Information

Theoretical exploration for the significance of n(S) / n(O) → σ*(C-$C_{(COOMe)}$) anomeric effect.

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Table S1: Selected hyperconjugative interaction energies (E2), corresponding energy gaps ($\Delta E_{d/a}$), % polarization of an orbital and overlap integral (S_{ij}) for methyl 1,3-dioxane-2-carboxylate (2), methyl-1,3-oxathiane-2-carboxylate (3) and methyl 1,3-dithiane-2-carboxylate (4) in axial (n-ax) and equatorial (n-eq) conformation (n=2, 3 and 4).

	donor orbital	acceptor orbital	E(2)	$\Delta E_{d/a}$	% polarization
	$n_{O(ax)}$	$\sigma^*_{C_2-C(ax)}$	7.55-7.69	0.62	50.1%
	$n_{O(eq)}$	$\sigma^*_{C_2-C(ax)}$	1.31-1.2	0.88	50.1%
2-ax	$n_{O(ax)}$	$\sigma^*_{C_2-O}$	10.34-10.5	0.6	67.0%
	$n_{O(eq)}$	$\sigma^*_{C_2-O}$	1.28-1.47	0.86	67.0%
	$\sigma_{O-C(4,6)}$	$\sigma^*_{C_2-C(ax)}$	-	-	-
	$n_{O(ax)}$	$\sigma^*_{C_2-O}$	12.41-12.43	0.61	67.2%
2-eq	$n_{O(eq)}$	$\sigma^*_{C_2-O}$	0.52-0.51	0.88	67.2%
	$\sigma_{O-C(4,6)}$	$\sigma^*_{C_2-C(eq)}$	1.53-1.52	1.13	49.3%
	$n_{O(ax)}$ [$n_{S(ax)}$]	$\sigma^*_{C_2-C(ax)}$	6.62 [3.88]	0.66 [0.58]	49.4%
	$n_{O(eq)}$ [$n_{S(eq)}$]	$\sigma^*_{C_2-C(ax)}$	2.04 [-]	0.89 [-]	49.4%
3-ax	$n_{O(ax)}$ [$n_{S(ax)}$]	$\sigma^*_{C_2-S}$ [$\sigma^*_{C(2)-O}$]	11.99 [4.37]	0.44 [0.55]	46.9% [66.6%]
	$n_{O(eq)}$ [$n_{S(eq)}$]	$\sigma^*_{C_2-S}$ [$\sigma^*_{C(2)-O}$]	2.17 [2.80]	0.67 [0.24]	46.9% [66.6%]
	σ_{O-C_6} [σ_{S-C_4}]	$\sigma^*_{C_2-C(ax)}$	-	-	-
	$n_{O(ax)}$ [$n_{S(ax)}$]	$\sigma^*_{C_2-S}$ [$\sigma^*_{C(2)-O}$]	14.09 [6.48]	0.44 [0.55]	46.8% [66.8%]
3-eq	$n_{O(eq)}$ [$n_{S(eq)}$]	$\sigma^*_{C_2-S}$ [$\sigma^*_{C(2)-O}$]	0.86 [-]	0.68 [-]	46.8% [66.8%]
	σ_{O-C_6} [σ_{S-C_4}]	$\sigma^*_{C_2-C(eq)}$	1.53 [1.13]	1.15 [0.93]	48.7%
	$n_{S(ax)}$	$\sigma^*_{C_2-C(ax)}$	4.54-4.74	0.59	48.4%
4-ax	$n_{S(eq)}$	$\sigma^*_{C_2-C(ax)}$	0.62	0.99	48.4%
	$n_{S(ax)}$	$\sigma^*_{C_2-S}$	4.77-5.07	0.38	44.3%

	$n_{S(eq)}$	$\sigma^{*}_{C_2-S}$	2.13-2.1	0.78	44.3%
	$\sigma_{S-C(4,6)}$	$\sigma^{*}_{C_2-C(ax)}$	-	-	-
	$n_{S(ax)}$	$\sigma^{*}_{C_2-S}$	7.09-6.9	0.38	44.5%
4-eq	$n_{S(eq)}$	$\sigma^{*}_{C_2-S}$	1.13-1.1	0.78	44.5%
	$\sigma_{S-C(4,6)}$	$\sigma^{*}_{C_2-C(eq)}$	1.46-1.51	0.93	48.2%

Molecular electrostatic Calculations (MESP):

The molecular electrostatic potential (MESP)[1-3] calculations have been performed at the B3LYP/6-311+G(d,p)/SMD(Chloroform) and is calculated using charge on the nucleus A (Z_A), its location (R_A) and electron density ρ(r′) using eq S1

$$V(r) = \sum_{A}^{N} \frac{Z_A}{|r - R_A|} - \int \frac{\rho(r')d^3r'}{|r - r'|} \qquad \text{(S1)}$$

The blue regions of MESP surface generally reveal the electron-rich regions, whereas red/orange areas are considered electron-deficient regions. Figure S1 suggest electrostatic repulsion between the ring oxygen and the 2-carbomethoxy substituent.

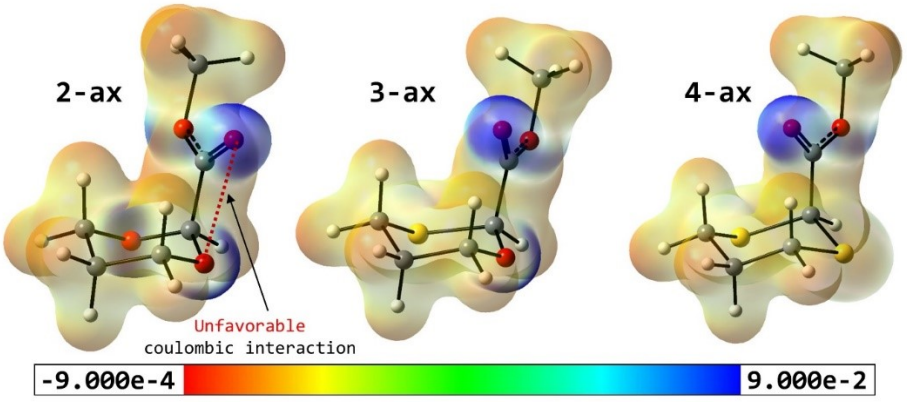


Figure S1: Molecular electrostatic potential (MESP) surface computed at the B3LYP/6-311+G(d,p)/SMD(Chloroform) level of theory showing electrostatic repulsion between the two oxygen atoms in **2**-ax.

Table S2: Comparison of structural parameters in the optimized geometries of 2-ax, 2-eq, 3-ax, 3-eq, 4-ax and 4-eq with those optimized geometries obtained by NBODEL, when switching off the key NBO Interactions.

methyl 1,3-dioxane-2-carboxylate, 2						
bond	**without NBODEL**	**O_{ax} to C-C**	**O_{ax} to C-O**	**O_{eq} to C-C**	**O_{eq} to C-O**	**O-C to C-C**

	ax	eq	ax	eq	ax	eq	ax	eq	ax	eq	ax	eq
Energy	0.0	0.0	6.8	-	9.1	11.4	1.9	-	2.4	0.9	-	2.3
C_2-C	1.54	1.52	1.53	-	1.54	1.52	1.54	-	1.53	1.52	-	1.52
C_2-O_d	1.38	1.38	1.41	-	1.42	1.44	1.39	-	1.38	1.39	-	1.4
C_2-O_a	1.38	1.38	1.38	-	1.36	1.36	1.37	-	1.38	1.38	-	1.38
O-C_2-O	113.3	112.4	113.2	-	111.9	110.9	113.1	-	112.8	112.1	-	112.2

methyl-1,3-oxathiane-2-carboxylate, 3

bond	without NBODEL		O_{ax} to C-C		O_{ax} to C-S		O_{eq} to C-C		O_{eq} to C-S		S_{ax} to C-C	
	ax	eq	ax	eq	ax	eq	ax	eq	ax	eq	ax	eq
Energy	0.00	0.00	6.19	-	7.97	10.09	2.39	-	2.93	0.98	4.33	-
C_2-C	1.52	1.52	1.51	-	1.53	1.52	1.53	-	1.52	1.52	1.52	-
C_2-O	1.38	1.38	1.41	-	1.42	1.43	1.39	-	1.38	1.38	1.38	-
C_2-S	1.83	1.83	1.84	-	1.8	1.8	1.83	-	1.84	1.84	1.86	-
S-C_2-S	114.1	112.5	114.1	-	112.5	110.8	113.9	-	113.9	112.3	114.5	-

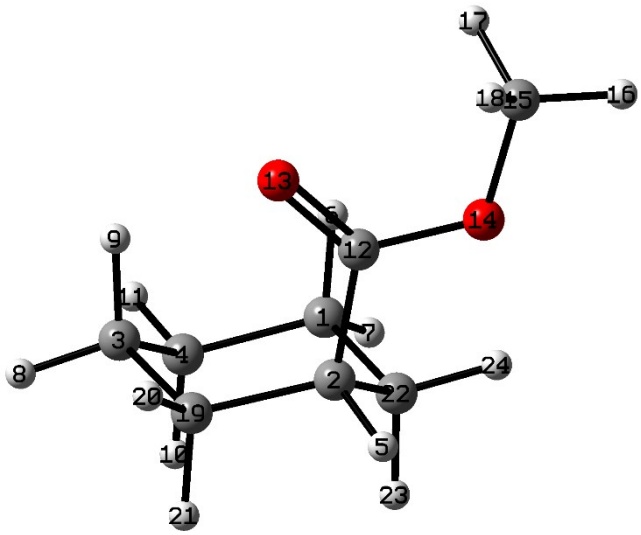
	S_{ax} to C-O		S_{eq} to C-O		S-C to C-C		O-C to C-C	
	ax	eq	ax	eq	ax	eq	ax	eq
	4.41	6.58	1.74	0.79	-	0.00	-	2.08
C_2-C	1.52	1.52	1.52	1.52	-	1.52	-	1.52
C_2-O	1.37	1.37	1.38	1.38	-	1.38	-	1.39
C_2-S	1.86	1.88	1.85	1.84	-	1.83	-	1.83
S-C_2-S	113.5	111.4	113.4	112.1	-	112.5	-	112.3

methyl 1,3-dithiane-2-carboxylate, 4

bond	without NBODEL		S_{ax} to C-C		S_{ax} to C-S		S_{eq} to C-C		S_{eq} to C-S		S-C to C-C	
	ax	eq	ax	eq	ax	eq	ax	eq	ax	eq	ax	eq
Energy	0.0	0.0	4.8	-	4.1	5.8	1.2	-	2.8	1.6	-	2.1
C_2-C	1.52	1.52	1.51	-	1.52	1.52	1.52	-	1.52	1.52	-	1.52
C_2-S_d	1.81	1.82	1.85	-	1.85	1.86	1.82	-	1.83	1.86	-	1.83
C_2-S_a	1.82	1.83	1.82	-	1.81	1.81	1.82	-	1.82	1.81	-	1.83
S-C_2-S	114.8	113.9	114.8	-	113.5	112.2	114.8	-	114.2	112.2	-	113.8

Table S3: NBO hyperconjugative interactions:

1-ax



Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

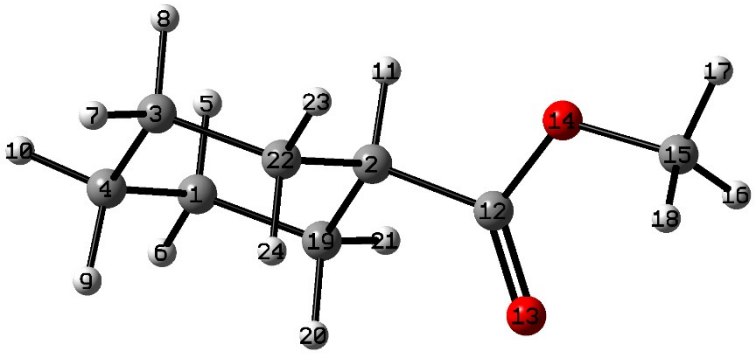
Threshold for printing: 0.50 kcal/mol

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) C 1 - C 4	/ 74. RY*(1) C 3	1.05	1.43	0.035
1. BD (1) C 1 - C 4	/253. RY*(1) C 22	1.00	1.45	0.034
1. BD (1) C 1 - C 4	/283. BD*(1) C 1 - C 22	0.71	0.98	0.024
1. BD (1) C 1 - C 4	/288. BD*(1) C 3 - C 4	0.70	0.99	0.024
1. BD (1) C 1 - C 4	/289. BD*(1) C 3 - H 8	1.68	1.00	0.037
1. BD (1) C 1 - C 4	/304. BD*(1) C 22 - H 24	1.75	1.01	0.038
2. BD (1) C 1 - H 6	/292. BD*(1) C 4 - H 10	2.78	0.88	0.044
2. BD (1) C 1 - H 6	/303. BD*(1) C 22 - H 23	2.83	0.89	0.045
3. BD (1) C 1 - H 7	/287. BD*(1) C 2 - C 22	3.22	0.86	0.047
3. BD (1) C 1 - H 7	/288. BD*(1) C 3 - C 4	2.87	0.88	0.045
4. BD (1) C 1 - C 22	/ 57. RY*(1) C 2	1.39	1.52	0.041
4. BD (1) C 1 - C 22	/ 91. RY*(1) C 4	1.04	1.46	0.035
4. BD (1) C 1 - C 22	/280. BD*(1) C 1 - C 4	0.71	0.99	0.024
4. BD (1) C 1 - C 22	/284. BD*(1) C 2 - H 5	1.56	0.99	0.035
4. BD (1) C 1 - C 22	/287. BD*(1) C 2 - C 22	0.69	0.97	0.023
4. BD (1) C 1 - C 22	/293. BD*(1) C 4 - H 11	1.67	1.01	0.037
5. BD (1) C 2 - H 5	/283. BD*(1) C 1 - C 22	3.00	0.88	0.046
5. BD (1) C 2 - H 5	/291. BD*(1) C 3 - C 19	3.01	0.88	0.046
5. BD (1) C 2 - H 5	/294. BD*(1) C 12 - O 13	2.12	1.09	0.043
5. BD (1) C 2 - H 5	/295. BD*(2) C 12 - O 13	6.63	0.49	0.053
6. BD (1) C 2 - C 12	/160. RY*(1) O 13	1.10	1.43	0.036
6. BD (1) C 2 - C 12	/177. RY*(1) O 14	0.52	1.24	0.023
6. BD (1) C 2 - C 12	/226. RY*(1) C 19	0.77	1.47	0.030
6. BD (1) C 2 - C 12	/253. RY*(1) C 22	0.54	1.50	0.026
6. BD (1) C 2 - C 12	/287. BD*(1) C 2 - C 22	0.64	1.01	0.023
6. BD (1) C 2 - C 12	/294. BD*(1) C 12 - O 13	1.36	1.24	0.037
6. BD (1) C 2 - C 12	/297. BD*(1) O 14 - C 15	4.13	0.89	0.054
6. BD (1) C 2 - C 12	/302. BD*(1) C 19 - H 21	1.40	1.05	0.034
6. BD (1) C 2 - C 12	/303. BD*(1) C 22 - H 23	1.34	1.04	0.034
7. BD (1) C 2 - C 19	/ 74. RY*(1) C 3	0.77	1.44	0.030
7. BD (1) C 2 - C 19	/143. RY*(1) C 12	0.98	1.57	0.035
7. BD (1) C 2 - C 19	/253. RY*(1) C 22	0.75	1.46	0.030
7. BD (1) C 2 - C 19	/284. BD*(1) C 2 - H 5	0.68	1.00	0.023
7. BD (1) C 2 - C 19	/285. BD*(1) C 2 - C 12	0.53	0.97	0.020
7. BD (1) C 2 - C 19	/287. BD*(1) C 2 - C 22	1.08	0.97	0.029
7. BD (1) C 2 - C 19	/289. BD*(1) C 3 - H 8	1.44	1.01	0.034
7. BD (1) C 2 - C 19	/291. BD*(1) C 3 - C 19	0.67	0.99	0.023
7. BD (1) C 2 - C 19	/296. BD*(1) C 12 - O 14	2.77	0.96	0.047
7. BD (1) C 2 - C 19	/304. BD*(1) C 22 - H 24	1.65	1.02	0.037
8. BD (1) C 2 - C 22	/ 40. RY*(1) C 1	0.84	1.46	0.031
8. BD (1) C 2 - C 22	/226. RY*(1) C 19	0.69	1.42	0.028
8. BD (1) C 2 - C 22	/282. BD*(1) C 1 - H 7	1.52	1.00	0.035
8. BD (1) C 2 - C 22	/283. BD*(1) C 1 - C 22	0.58	0.99	0.021
8. BD (1) C 2 - C 22	/284. BD*(1) C 2 - H 5	0.65	0.99	0.023

8. BD (1) C 2 - C 22	/286. BD*(1) C 2 - C 19	0.99	0.98	0.028
8. BD (1) C 2 - C 22	/294. BD*(1) C 12 - O 13	2.39	1.19	0.048
8. BD (1) C 2 - C 22	/295. BD*(2) C 12 - O 13	1.94	0.60	0.032
8. BD (1) C 2 - C 22	/301. BD*(1) C 19 - H 20	1.69	1.01	0.037
9. BD (1) C 3 - C 4	/ 40. RY*(1) C 1	1.05	1.46	0.035
9. BD (1) C 3 - C 4	/226. RY*(1) C 19	0.90	1.42	0.032
9. BD (1) C 3 - C 4	/280. BD*(1) C 1 - C 4	0.70	0.98	0.023
9. BD (1) C 3 - C 4	/282. BD*(1) C 1 - H 7	1.72	1.00	0.037
9. BD (1) C 3 - C 4	/291. BD*(1) C 3 - C 19	0.67	0.98	0.023
9. BD (1) C 3 - C 4	/301. BD*(1) C 19 - H 20	1.67	1.01	0.037
10. BD (1) C 3 - H 8	/280. BD*(1) C 1 - C 4	2.94	0.88	0.045
10. BD (1) C 3 - H 8	/286. BD*(1) C 2 - C 19	3.22	0.86	0.047
11. BD (1) C 3 - H 9	/226. RY*(1) C 19	0.62	1.30	0.025
11. BD (1) C 3 - H 9	/292. BD*(1) C 4 - H 10	2.86	0.88	0.045
11. BD (1) C 3 - H 9	/302. BD*(1) C 19 - H 21	2.76	0.88	0.044
12. BD (1) C 3 - C 19	/ 58. RY*(2) C 2	1.15	1.48	0.037
12. BD (1) C 3 - C 19	/ 91. RY*(1) C 4	0.99	1.45	0.034
12. BD (1) C 3 - C 19	/284. BD*(1) C 2 - H 5	1.67	0.99	0.036
12. BD (1) C 3 - C 19	/286. BD*(1) C 2 - C 19	0.72	0.97	0.024
12. BD (1) C 3 - C 19	/288. BD*(1) C 3 - C 4	0.66	0.99	0.023
12. BD (1) C 3 - C 19	/293. BD*(1) C 4 - H 11	1.65	1.00	0.036
12. BD (1) C 3 - C 19	/301. BD*(1) C 19 - H 20	0.50	1.01	0.020
13. BD (1) C 4 - H 10	/281. BD*(1) C 1 - H 6	2.88	0.88	0.045
13. BD (1) C 4 - H 10	/290. BD*(1) C 3 - H 9	2.75	0.89	0.044
14. BD (1) C 4 - H 11	/283. BD*(1) C 1 - C 22	2.98	0.87	0.046
14. BD (1) C 4 - H 11	/291. BD*(1) C 3 - C 19	3.03	0.88	0.046
15. BD (1) C 12 - O 13	/143. RY*(1) C 12	1.79	2.07	0.055
15. BD (1) C 12 - O 13	/285. BD*(1) C 2 - C 12	1.49	1.47	0.042
16. BD (2) C 12 - O 13	/284. BD*(1) C 2 - H 5	1.37	0.80	0.029
16. BD (2) C 12 - O 13	/287. BD*(1) C 2 - C 22	1.01	0.77	0.025
16. BD (2) C 12 - O 13	/295. BD*(2) C 12 - O 13	0.68	0.40	0.016
17. BD (1) C 12 - O 14	/ 57. RY*(1) C 2	0.51	1.86	0.027
17. BD (1) C 12 - O 14	/196. RY*(3) C 15	1.50	1.75	0.046
17. BD (1) C 12 - O 14	/286. BD*(1) C 2 - C 19	1.05	1.32	0.033
18. BD (1) O 14 - C 15	/143. RY*(1) C 12	1.42	1.79	0.045
18. BD (1) O 14 - C 15	/285. BD*(1) C 2 - C 12	2.45	1.20	0.049
19. BD (1) C 15 - H 16	/180. RY*(4) O 14	0.53	1.86	0.028
19. BD (1) C 15 - H 16	/296. BD*(1) C 12 - O 14	2.96	0.89	0.047
20. BD (1) C 15 - H 17	/297. BD*(1) O 14 - C 15	0.63	0.78	0.020
21. BD (1) C 15 - H 18	/178. RY*(2) O 14	0.67	1.31	0.026
21. BD (1) C 15 - H 18	/297. BD*(1) O 14 - C 15	0.64	0.78	0.020
22. BD (1) C 19 - H 20	/287. BD*(1) C 2 - C 22	3.11	0.86	0.046
22. BD (1) C 19 - H 20	/288. BD*(1) C 3 - C 4	2.87	0.88	0.045
23. BD (1) C 19 - H 21	/285. BD*(1) C 2 - C 12	3.30	0.86	0.048
23. BD (1) C 19 - H 21	/290. BD*(1) C 3 - H 9	2.78	0.89	0.045
24. BD (1) C 22 - H 23	/281. BD*(1) C 1 - H 6	2.90	0.89	0.045
24. BD (1) C 22 - H 23	/285. BD*(1) C 2 - C 12	3.42	0.86	0.049
25. BD (1) C 22 - H 24	/280. BD*(1) C 1 - C 4	2.78	0.88	0.044
25. BD (1) C 22 - H 24	/286. BD*(1) C 2 - C 19	2.97	0.87	0.045
26. CR (1) C 1	/256. RY*(4) C 22	0.82	11.23	0.086
27. CR (1) C 2	/255. RY*(3) C 22	0.52	11.09	0.068
27. CR (1) C 2	/294. BD*(1) C 12 - O 13	0.73	10.65	0.079
28. CR (1) C 3	/ 94. RY*(4) C 4	0.54	11.06	0.069
28. CR (1) C 3	/229. RY*(4) C 19	0.75	11.33	0.082
29. CR (1) C 4	/ 42. RY*(3) C 1	0.51	11.07	0.067
29. CR (1) C 4	/ 76. RY*(3) C 3	0.54	11.05	0.069
30. CR (1) C 12	/ 59. RY*(3) C 2	0.91	11.27	0.090
30. CR (1) C 12	/297. BD*(1) O 14 - C 15	1.20	10.44	0.100
31. CR (1) O 13	/143. RY*(1) C 12	7.10	19.82	0.337
31. CR (1) O 13	/285. BD*(1) C 2 - C 12	0.69	19.23	0.105
32. CR (1) O 14	/143. RY*(1) C 12	1.27	19.95	0.143
32. CR (1) O 14	/144. RY*(2) C 12	0.86	20.75	0.120
32. CR (1) O 14	/146. RY*(4) C 12	1.00	20.73	0.129
32. CR (1) O 14	/194. RY*(1) C 15	0.58	19.98	0.096
32. CR (1) O 14	/196. RY*(3) C 15	0.61	19.79	0.098
33. CR (1) C 15	/212. RY*(2) H 16	0.54	12.18	0.072
33. CR (1) C 15	/296. BD*(1) C 12 - O 14	0.85	10.46	0.086
33. CR (1) C 15	/297. BD*(1) O 14 - C 15	1.77	10.35	0.121
34. CR (1) C 19	/ 58. RY*(2) C 2	0.68	10.91	0.077
34. CR (1) C 19	/ 76. RY*(3) C 3	0.70	11.05	0.079
35. CR (1) C 22	/ 42. RY*(3) C 1	0.79	11.07	0.084
35. CR (1) C 22	/ 58. RY*(2) C 2	0.59	10.92	0.072
35. CR (1) C 22	/275. RY*(1) H 24	0.54	11.29	0.070
36. LP (1) O 13	/143. RY*(1) C 12	17.42	1.68	0.153

36. LP (1) O 13	/157. RY*(15) C 12	1.10	3.52	0.056
36. LP (1) O 13	/285. BD*(1) C 2 - C 12	2.23	1.08	0.044
36. LP (1) O 13	/296. BD*(1) C 12 - O 14	1.11	1.07	0.031
37. LP (2) O 13	/144. RY*(2) C 12	2.84	2.05	0.071
37. LP (2) O 13	/146. RY*(4) C 12	1.24	2.04	0.047
37. LP (2) O 13	/285. BD*(1) C 2 - C 12	17.05	0.65	0.096
37. LP (2) O 13	/296. BD*(1) C 12 - O 14	32.00	0.64	0.129
37. LP (2) O 13	/298. BD*(1) C 15 - H 16	0.78	0.67	0.021
38. LP (1) O 14	/143. RY*(1) C 12	2.44	1.54	0.055
38. LP (1) O 14	/146. RY*(4) C 12	2.43	2.33	0.068
38. LP (1) O 14	/194. RY*(1) C 15	2.14	1.58	0.052
38. LP (1) O 14	/294. BD*(1) C 12 - O 13	7.62	1.17	0.085
38. LP (1) O 14	/298. BD*(1) C 15 - H 16	2.28	0.96	0.042
38. LP (1) O 14	/299. BD*(1) C 15 - H 17	0.51	0.95	0.020
38. LP (1) O 14	/300. BD*(1) C 15 - H 18	0.58	0.95	0.021
39. LP (2) O 14	/145. RY*(3) C 12	2.51	1.92	0.065
39. LP (2) O 14	/195. RY*(2) C 15	1.74	1.61	0.050
39. LP (2) O 14	/295. BD*(2) C 12 - O 13	47.58	0.34	0.113
39. LP (2) O 14	/299. BD*(1) C 15 - H 17	4.60	0.72	0.054
39. LP (2) O 14	/300. BD*(1) C 15 - H 18	4.51	0.72	0.053
295. BD*(2) C 12 - O 13	/145. RY*(3) C 12	1.64	1.58	0.135
295. BD*(2) C 12 - O 13	/161. RY*(2) O 13	1.44	0.55	0.075
295. BD*(2) C 12 - O 13	/284. BD*(1) C 2 - H 5	0.98	0.40	0.051
295. BD*(2) C 12 - O 13	/287. BD*(1) C 2 - C 22	0.82	0.37	0.044

1-eq



Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

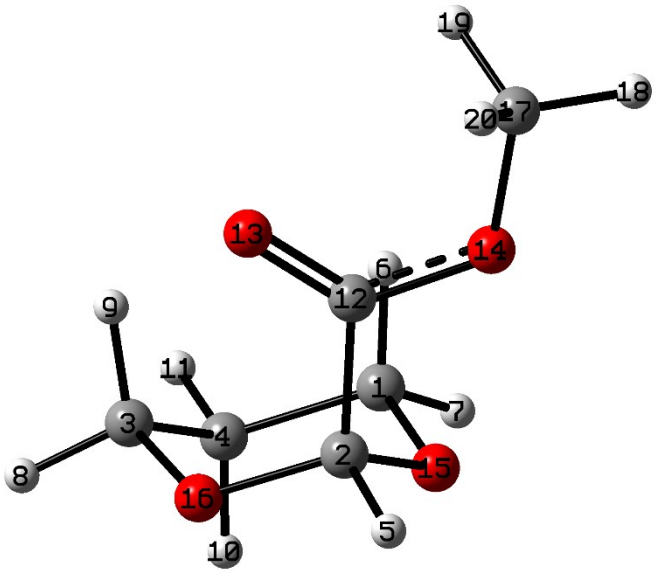
Threshold for printing: 0.50 kcal/mol

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) C 1 - C 4	/ 74. RY*(1) C 3	0.97	1.43	0.033
1. BD (1) C 1 - C 4	/226. RY*(1) C 19	1.01	1.43	0.034
1. BD (1) C 1 - C 4	/283. BD*(1) C 1 - C 19	0.71	0.99	0.024
1. BD (1) C 1 - C 4	/288. BD*(1) C 3 - C 4	0.71	0.99	0.024
1. BD (1) C 1 - C 4	/289. BD*(1) C 3 - H 7	1.71	1.00	0.037
1. BD (1) C 1 - C 4	/302. BD*(1) C 19 - H 21	1.69	1.00	0.037
2. BD (1) C 1 - H 5	/292. BD*(1) C 4 - H 9	2.80	0.88	0.044
2. BD (1) C 1 - H 5	/301. BD*(1) C 19 - H 20	2.84	0.89	0.045
3. BD (1) C 1 - H 6	/286. BD*(1) C 2 - C 19	2.98	0.87	0.045
3. BD (1) C 1 - H 6	/288. BD*(1) C 3 - C 4	2.92	0.88	0.045
4. BD (1) C 1 - C 19	/ 57. RY*(1) C 2	0.59	1.43	0.026
4. BD (1) C 1 - C 19	/ 91. RY*(1) C 4	0.98	1.45	0.034
4. BD (1) C 1 - C 19	/280. BD*(1) C 1 - C 4	0.70	0.99	0.024
4. BD (1) C 1 - C 19	/285. BD*(1) C 2 - C 12	2.04	0.98	0.040
4. BD (1) C 1 - C 19	/286. BD*(1) C 2 - C 19	0.88	0.98	0.026
4. BD (1) C 1 - C 19	/293. BD*(1) C 4 - H 10	1.65	1.00	0.036
5. BD (1) C 2 - H 11	/294. BD*(1) C 12 - O 13	4.03	1.08	0.059
5. BD (1) C 2 - H 11	/295. BD*(2) C 12 - O 13	2.55	0.50	0.033
5. BD (1) C 2 - H 11	/296. BD*(1) C 12 - O 14	0.71	0.85	0.022
5. BD (1) C 2 - H 11	/301. BD*(1) C 19 - H 20	2.73	0.90	0.044
5. BD (1) C 2 - H 11	/304. BD*(1) C 22 - H 24	2.74	0.89	0.044

6. BD (1) C 2 - C 12	/160. RY*(1) O 13	1.21	1.39	0.037
6. BD (1) C 2 - C 12	/177. RY*(1) O 14	0.67	1.26	0.026
6. BD (1) C 2 - C 12	/182. RY*(6) O 14	0.56	2.01	0.030
6. BD (1) C 2 - C 12	/227. RY*(2) C 19	0.79	1.44	0.030
6. BD (1) C 2 - C 12	/254. RY*(2) C 22	0.63	1.64	0.029
6. BD (1) C 2 - C 12	/283. BD*(1) C 1 - C 19	1.77	1.04	0.038
6. BD (1) C 2 - C 12	/286. BD*(1) C 2 - C 19	0.55	1.03	0.021
6. BD (1) C 2 - C 12	/287. BD*(1) C 2 - C 22	0.67	1.01	0.023
6. BD (1) C 2 - C 12	/291. BD*(1) C 3 - C 22	1.89	1.04	0.040
6. BD (1) C 2 - C 12	/294. BD*(1) C 12 - O 13	1.56	1.24	0.039
6. BD (1) C 2 - C 12	/297. BD*(1) O 14 - C 15	4.19	0.90	0.055
7. BD (1) C 2 - C 19	/ 40. RY*(1) C 1	1.05	1.44	0.035
7. BD (1) C 2 - C 19	/143. RY*(1) C 12	1.12	1.55	0.037
7. BD (1) C 2 - C 19	/253. RY*(1) C 22	0.97	1.45	0.034
7. BD (1) C 2 - C 19	/282. BD*(1) C 1 - H 6	1.50	1.01	0.035
7. BD (1) C 2 - C 19	/283. BD*(1) C 1 - C 19	0.67	0.99	0.023
7. BD (1) C 2 - C 19	/284. BD*(1) C 2 - H 11	0.59	1.00	0.022
7. BD (1) C 2 - C 19	/285. BD*(1) C 2 - C 12	0.64	0.98	0.023
7. BD (1) C 2 - C 19	/287. BD*(1) C 2 - C 22	1.14	0.96	0.030
7. BD (1) C 2 - C 19	/295. BD*(2) C 12 - O 13	0.78	0.61	0.020
7. BD (1) C 2 - C 19	/296. BD*(1) C 12 - O 14	2.35	0.96	0.043
7. BD (1) C 2 - C 19	/303. BD*(1) C 22 - H 23	1.59	1.01	0.036
8. BD (1) C 2 - C 22	/ 74. RY*(1) C 3	1.04	1.43	0.035
8. BD (1) C 2 - C 22	/147. RY*(5) C 12	1.06	1.53	0.036
8. BD (1) C 2 - C 22	/226. RY*(1) C 19	1.08	1.43	0.035
8. BD (1) C 2 - C 22	/284. BD*(1) C 2 - H 11	0.55	0.99	0.021
8. BD (1) C 2 - C 22	/285. BD*(1) C 2 - C 12	0.57	0.98	0.021
8. BD (1) C 2 - C 22	/286. BD*(1) C 2 - C 19	1.03	0.98	0.028
8. BD (1) C 2 - C 22	/289. BD*(1) C 3 - H 7	1.52	1.00	0.035
8. BD (1) C 2 - C 22	/291. BD*(1) C 3 - C 22	0.57	0.98	0.021
8. BD (1) C 2 - C 22	/294. BD*(1) C 12 - O 13	1.27	1.18	0.035
8. BD (1) C 2 - C 22	/295. BD*(2) C 12 - O 13	3.76	0.60	0.044
8. BD (1) C 2 - C 22	/302. BD*(1) C 19 - H 21	1.73	1.00	0.037
9. BD (1) C 3 - C 4	/ 40. RY*(1) C 1	0.97	1.43	0.033
9. BD (1) C 3 - C 4	/253. RY*(1) C 22	1.06	1.45	0.035
9. BD (1) C 3 - C 4	/280. BD*(1) C 1 - C 4	0.70	0.99	0.024
9. BD (1) C 3 - C 4	/282. BD*(1) C 1 - H 6	1.70	1.00	0.037
9. BD (1) C 3 - C 4	/291. BD*(1) C 3 - C 22	0.71	0.99	0.024
9. BD (1) C 3 - C 4	/303. BD*(1) C 22 - H 23	1.68	1.01	0.037
10. BD (1) C 3 - H 7	/280. BD*(1) C 1 - C 4	2.90	0.88	0.045
10. BD (1) C 3 - H 7	/287. BD*(1) C 2 - C 22	3.06	0.85	0.046
11. BD (1) C 3 - H 8	/292. BD*(1) C 4 - H 9	2.79	0.88	0.044
11. BD (1) C 3 - H 8	/304. BD*(1) C 22 - H 24	2.90	0.88	0.045
12. BD (1) C 3 - C 22	/ 58. RY*(2) C 2	0.74	1.52	0.030
12. BD (1) C 3 - C 22	/ 91. RY*(1) C 4	1.01	1.45	0.034
12. BD (1) C 3 - C 22	/285. BD*(1) C 2 - C 12	1.83	0.98	0.038
12. BD (1) C 3 - C 22	/287. BD*(1) C 2 - C 22	0.80	0.96	0.025
12. BD (1) C 3 - C 22	/288. BD*(1) C 3 - C 4	0.71	0.99	0.024
12. BD (1) C 3 - C 22	/293. BD*(1) C 4 - H 10	1.63	1.01	0.036
12. BD (1) C 3 - C 22	/303. BD*(1) C 22 - H 23	0.50	1.01	0.020
13. BD (1) C 4 - H 9	/281. BD*(1) C 1 - H 5	2.85	0.88	0.045
13. BD (1) C 4 - H 9	/290. BD*(1) C 3 - H 8	2.86	0.88	0.045
14. BD (1) C 4 - H 10	/283. BD*(1) C 1 - C 19	2.99	0.88	0.046
14. BD (1) C 4 - H 10	/291. BD*(1) C 3 - C 22	3.02	0.88	0.046
15. BD (1) C 12 - O 13	/ 57. RY*(1) C 2	0.62	1.93	0.031
15. BD (1) C 12 - O 13	/143. RY*(1) C 12	1.78	2.04	0.054
15. BD (1) C 12 - O 13	/285. BD*(1) C 2 - C 12	1.68	1.48	0.045
16. BD (2) C 12 - O 13	/284. BD*(1) C 2 - H 11	0.63	0.80	0.020
16. BD (2) C 12 - O 13	/287. BD*(1) C 2 - C 22	1.15	0.77	0.027
16. BD (2) C 12 - O 13	/295. BD*(2) C 12 - O 13	0.74	0.41	0.016
17. BD (1) C 12 - O 14	/ 57. RY*(1) C 2	0.80	1.77	0.034
17. BD (1) C 12 - O 14	/196. RY*(3) C 15	1.51	1.76	0.046
17. BD (1) C 12 - O 14	/286. BD*(1) C 2 - C 19	0.91	1.32	0.031
18. BD (1) O 14 - C 15	/143. RY*(1) C 12	1.39	1.78	0.045
18. BD (1) O 14 - C 15	/285. BD*(1) C 2 - C 12	2.42	1.21	0.049
19. BD (1) C 15 - H 16	/178. RY*(2) O 14	0.66	1.27	0.026
19. BD (1) C 15 - H 16	/297. BD*(1) O 14 - C 15	0.63	0.78	0.020
20. BD (1) C 15 - H 17	/180. RY*(4) O 14	0.57	1.80	0.029
20. BD (1) C 15 - H 17	/296. BD*(1) C 12 - O 14	2.87	0.89	0.046
21. BD (1) C 15 - H 18	/178. RY*(2) O 14	0.61	1.27	0.025
21. BD (1) C 15 - H 18	/297. BD*(1) O 14 - C 15	0.66	0.78	0.020
22. BD (1) C 19 - H 20	/ 59. RY*(3) C 2	0.50	1.45	0.024
22. BD (1) C 19 - H 20	/281. BD*(1) C 1 - H 5	2.76	0.88	0.044
22. BD (1) C 19 - H 20	/284. BD*(1) C 2 - H 11	3.00	0.88	0.046

23. BD (1) C 19 - H 21	/280. BD*(1) C 1 - C 4	2.91	0.88	0.045
23. BD (1) C 19 - H 21	/287. BD*(1) C 2 - C 22	3.16	0.85	0.046
24. BD (1) C 22 - H 23	/286. BD*(1) C 2 - C 19	2.96	0.88	0.045
24. BD (1) C 22 - H 23	/288. BD*(1) C 3 - C 4	2.86	0.89	0.045
25. BD (1) C 22 - H 24	/ 57. RY*(1) C 2	0.67	1.33	0.027
25. BD (1) C 22 - H 24	/284. BD*(1) C 2 - H 11	2.66	0.89	0.043
25. BD (1) C 22 - H 24	/290. BD*(1) C 3 - H 8	2.69	0.89	0.044
26. CR (1) C 1	/ 94. RY*(4) C 4	0.59	11.10	0.072
26. CR (1) C 1	/227. RY*(2) C 19	0.55	10.82	0.069
27. CR (1) C 2	/149. RY*(7) C 12	0.70	11.05	0.079
27. CR (1) C 2	/255. RY*(3) C 22	0.59	11.00	0.072
27. CR (1) C 2	/294. BD*(1) C 12 - O 13	0.77	10.64	0.081
29. CR (1) C 4	/ 76. RY*(3) C 3	0.56	11.20	0.071
30. CR (1) C 12	/ 58. RY*(2) C 2	0.70	11.11	0.079
30. CR (1) C 12	/297. BD*(1) O 14 - C 15	1.19	10.44	0.100
31. CR (1) O 13	/143. RY*(1) C 12	7.09	19.81	0.336
31. CR (1) O 13	/285. BD*(1) C 2 - C 12	0.70	19.24	0.105
32. CR (1) O 14	/143. RY*(1) C 12	1.29	19.93	0.144
32. CR (1) O 14	/144. RY*(2) C 12	0.83	20.71	0.118
32. CR (1) O 14	/146. RY*(4) C 12	0.98	20.74	0.128
32. CR (1) O 14	/194. RY*(1) C 15	0.59	19.99	0.097
32. CR (1) O 14	/196. RY*(3) C 15	0.59	19.80	0.097
33. CR (1) C 15	/217. RY*(2) H 17	0.50	12.14	0.070
33. CR (1) C 15	/296. BD*(1) C 12 - O 14	0.82	10.46	0.085
33. CR (1) C 15	/297. BD*(1) O 14 - C 15	1.79	10.35	0.122
34. CR (1) C 19	/ 42. RY*(3) C 1	0.54	11.15	0.069
34. CR (1) C 19	/ 58. RY*(2) C 2	0.65	10.95	0.075
35. CR (1) C 22	/ 59. RY*(3) C 2	0.70	11.00	0.078
35. CR (1) C 22	/ 76. RY*(3) C 3	0.76	11.21	0.083
36. LP (1) O 13	/143. RY*(1) C 12	17.23	1.66	0.151
36. LP (1) O 13	/157. RY*(15) C 12	0.78	3.39	0.046
36. LP (1) O 13	/158. RY*(16) C 12	0.62	3.39	0.041
36. LP (1) O 13	/285. BD*(1) C 2 - C 12	2.32	1.10	0.045
36. LP (1) O 13	/296. BD*(1) C 12 - O 14	1.16	1.07	0.032
37. LP (2) O 13	/144. RY*(2) C 12	2.80	2.01	0.069
37. LP (2) O 13	/146. RY*(4) C 12	1.30	2.05	0.048
37. LP (2) O 13	/285. BD*(1) C 2 - C 12	16.41	0.66	0.095
37. LP (2) O 13	/296. BD*(1) C 12 - O 14	32.04	0.64	0.129
37. LP (2) O 13	/299. BD*(1) C 15 - H 17	0.78	0.67	0.021
38. LP (1) O 14	/143. RY*(1) C 12	2.61	1.53	0.057
38. LP (1) O 14	/146. RY*(4) C 12	2.29	2.34	0.066
38. LP (1) O 14	/194. RY*(1) C 15	2.15	1.59	0.053
38. LP (1) O 14	/294. BD*(1) C 12 - O 13	7.78	1.17	0.085
38. LP (1) O 14	/299. BD*(1) C 15 - H 17	2.27	0.96	0.042
38. LP (1) O 14	/300. BD*(1) C 15 - H 18	0.59	0.96	0.021
39. LP (2) O 14	/145. RY*(3) C 12	2.60	1.91	0.066
39. LP (2) O 14	/195. RY*(2) C 15	1.71	1.56	0.049
39. LP (2) O 14	/295. BD*(2) C 12 - O 13	46.36	0.34	0.113
39. LP (2) O 14	/298. BD*(1) C 15 - H 16	4.64	0.72	0.054
39. LP (2) O 14	/300. BD*(1) C 15 - H 18	4.39	0.72	0.053
295. BD*(2) C 12 - O 13	/145. RY*(3) C 12	1.53	1.56	0.130
295. BD*(2) C 12 - O 13	/153. RY*(11) C 12	0.55	2.52	0.100
295. BD*(2) C 12 - O 13	/161. RY*(2) O 13	1.46	0.65	0.082
295. BD*(2) C 12 - O 13	/287. BD*(1) C 2 - C 22	1.23	0.36	0.054
295. BD*(2) C 12 - O 13	/294. BD*(1) C 12 - O 13	1.02	0.58	0.062

2-ax



Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

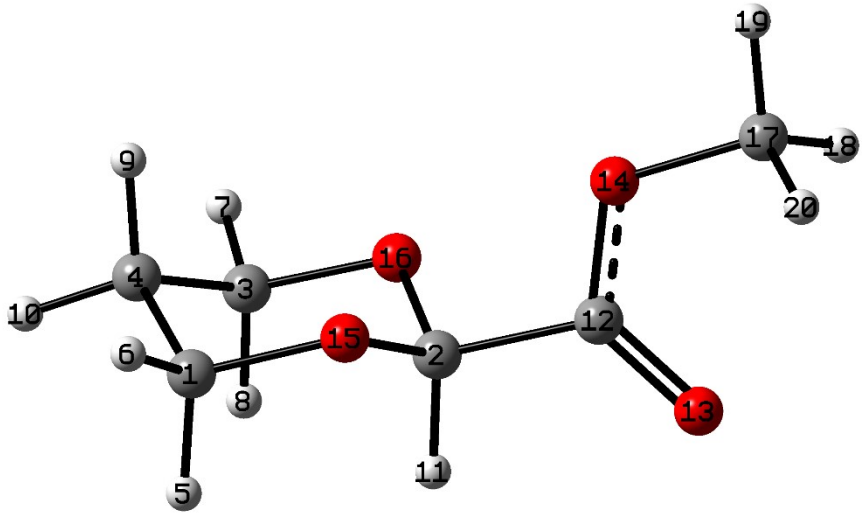
Threshold for printing: 0.50 kcal/mol

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) C 1 - C 4	/ 75. RY*(2) C 3	0.72	1.67	0.031
1. BD (1) C 1 - C 4	/194. RY*(1) O 15	0.87	1.29	0.030
1. BD (1) C 1 - C 4	/268. BD*(1) C 3 - C 4	0.52	1.01	0.020
1. BD (1) C 1 - C 4	/269. BD*(1) C 3 - H 8	1.68	1.03	0.037
1. BD (1) C 1 - C 4	/271. BD*(1) C 3 - O 16	0.54	0.90	0.020
2. BD (1) C 1 - H 6	/263. BD*(1) C 1 - O 15	0.55	0.79	0.019
2. BD (1) C 1 - H 6	/272. BD*(1) C 4 - H 10	2.53	0.91	0.043
3. BD (1) C 1 - H 7	/195. RY*(2) O 15	0.79	1.31	0.029
3. BD (1) C 1 - H 7	/266. BD*(1) C 2 - O 15	3.01	0.81	0.044
3. BD (1) C 1 - H 7	/268. BD*(1) C 3 - C 4	2.40	0.90	0.041
4. BD (1) C 1 - O 15	/ 57. RY*(1) C 2	1.88	1.82	0.052
4. BD (1) C 1 - O 15	/ 58. RY*(2) C 2	0.75	2.18	0.036
4. BD (1) C 1 - O 15	/264. BD*(1) C 2 - H 5	0.97	1.18	0.030
4. BD (1) C 1 - O 15	/273. BD*(1) C 4 - H 11	1.10	1.20	0.032
5. BD (1) C 2 - H 5	/148. RY*(6) C 12	0.57	1.96	0.030
5. BD (1) C 2 - H 5	/263. BD*(1) C 1 - O 15	3.74	0.80	0.049
5. BD (1) C 2 - H 5	/271. BD*(1) C 3 - O 16	3.96	0.80	0.050
5. BD (1) C 2 - H 5	/274. BD*(1) C 12 - O 13	1.49	1.13	0.037
5. BD (1) C 2 - H 5	/275. BD*(2) C 12 - O 13	5.24	0.53	0.049
6. BD (1) C 2 - C 12	/160. RY*(1) O 13	1.33	1.43	0.039
6. BD (1) C 2 - C 12	/177. RY*(1) O 14	0.77	1.28	0.028
6. BD (1) C 2 - C 12	/274. BD*(1) C 12 - O 13	0.75	1.25	0.027
6. BD (1) C 2 - C 12	/277. BD*(1) O 14 - C 17	4.32	0.90	0.056
7. BD (1) C 2 - O 15	/ 40. RY*(1) C 1	2.02	1.71	0.052
7. BD (1) C 2 - O 15	/262. BD*(1) C 1 - H 7	0.72	1.25	0.027
7. BD (1) C 2 - O 15	/274. BD*(1) C 12 - O 13	1.16	1.44	0.037
7. BD (1) C 2 - O 15	/275. BD*(2) C 12 - O 13	0.54	0.85	0.020
8. BD (1) C 2 - O 16	/ 74. RY*(1) C 3	1.94	1.72	0.052
8. BD (1) C 2 - O 16	/269. BD*(1) C 3 - H 8	0.62	1.26	0.025
8. BD (1) C 2 - O 16	/276. BD*(1) C 12 - O 14	1.20	1.23	0.035
9. BD (1) C 3 - C 4	/ 41. RY*(2) C 1	0.81	1.69	0.033
9. BD (1) C 3 - C 4	/211. RY*(1) O 16	0.78	1.33	0.029
9. BD (1) C 3 - C 4	/260. BD*(1) C 1 - C 4	0.53	1.00	0.021
9. BD (1) C 3 - C 4	/262. BD*(1) C 1 - H 7	1.72	1.02	0.037
9. BD (1) C 3 - C 4	/263. BD*(1) C 1 - O 15	0.53	0.90	0.020
10. BD (1) C 3 - H 8	/212. RY*(2) O 16	0.68	1.32	0.027
10. BD (1) C 3 - H 8	/260. BD*(1) C 1 - C 4	2.42	0.89	0.042

10. BD (1) C 3 - H 8	/267. BD*(1) C 2 - O 16	3.05	0.82	0.045
11. BD (1) C 3 - H 9	/271. BD*(1) C 3 - O 16	0.52	0.78	0.018
11. BD (1) C 3 - H 9	/272. BD*(1) C 4 - H 10	2.58	0.91	0.043
12. BD (1) C 3 - O 16	/ 57. RY*(1) C 2	1.47	1.82	0.046
12. BD (1) C 3 - O 16	/ 58. RY*(2) C 2	0.66	2.17	0.034
12. BD (1) C 3 - O 16	/ 59. RY*(3) C 2	0.58	2.10	0.031
12. BD (1) C 3 - O 16	/264. BD*(1) C 2 - H 5	1.00	1.18	0.031
12. BD (1) C 3 - O 16	/273. BD*(1) C 4 - H 11	1.08	1.19	0.032
13. BD (1) C 4 - H 10	/ 40. RY*(1) C 1	0.60	1.36	0.026
13. BD (1) C 4 - H 10	/ 74. RY*(1) C 3	0.65	1.36	0.027
13. BD (1) C 4 - H 10	/261. BD*(1) C 1 - H 6	2.65	0.87	0.043
13. BD (1) C 4 - H 10	/270. BD*(1) C 3 - H 9	2.53	0.88	0.042
14. BD (1) C 4 - H 11	/263. BD*(1) C 1 - O 15	3.98	0.77	0.050
14. BD (1) C 4 - H 11	/271. BD*(1) C 3 - O 16	4.03	0.77	0.050
15. BD (1) C 12 - O 13	/ 57. RY*(1) C 2	0.54	2.13	0.030
15. BD (1) C 12 - O 13	/143. RY*(1) C 12	1.64	2.12	0.053
15. BD (1) C 12 - O 13	/265. BD*(1) C 2 - C 12	0.72	1.41	0.029
16. BD (2) C 12 - O 13	/178. RY*(2) O 14	0.54	1.20	0.023
16. BD (2) C 12 - O 13	/264. BD*(1) C 2 - H 5	1.06	0.79	0.026
16. BD (2) C 12 - O 13	/266. BD*(1) C 2 - O 15	1.27	0.71	0.027
16. BD (2) C 12 - O 13	/275. BD*(2) C 12 - O 13	0.67	0.41	0.016
17. BD (1) C 12 - O 14	/ 57. RY*(1) C 2	0.60	1.97	0.031
17. BD (1) C 12 - O 14	/229. RY*(2) C 17	0.51	2.04	0.029
17. BD (1) C 12 - O 14	/230. RY*(3) C 17	0.84	1.99	0.036
17. BD (1) C 12 - O 14	/267. BD*(1) C 2 - O 16	0.73	1.26	0.027
17. BD (1) C 12 - O 14	/274. BD*(1) C 12 - O 13	0.52	1.55	0.025
18. BD (1) O 14 - C 17	/143. RY*(1) C 12	1.60	1.84	0.048
18. BD (1) O 14 - C 17	/147. RY*(5) C 12	0.69	1.87	0.032
18. BD (1) O 14 - C 17	/265. BD*(1) C 2 - C 12	2.48	1.13	0.048
19. BD (1) C 17 - H 18	/276. BD*(1) C 12 - O 14	2.85	0.90	0.046
20. BD (1) C 17 - H 19	/178. RY*(2) O 14	0.60	1.33	0.025
20. BD (1) C 17 - H 19	/277. BD*(1) O 14 - C 17	0.71	0.78	0.021
21. BD (1) C 17 - H 20	/178. RY*(2) O 14	0.61	1.33	0.025
21. BD (1) C 17 - H 20	/277. BD*(1) O 14 - C 17	0.71	0.78	0.021
22. CR (1) C 1	/ 93. RY*(3) C 4	0.87	11.21	0.088
22. CR (1) C 1	/263. BD*(1) C 1 - O 15	1.27	10.37	0.103
22. CR (1) C 1	/266. BD*(1) C 2 - O 15	0.83	10.39	0.084
23. CR (1) C 2	/263. BD*(1) C 1 - O 15	1.00	10.45	0.092
23. CR (1) C 2	/264. BD*(1) C 2 - H 5	0.78	10.56	0.081
23. CR (1) C 2	/271. BD*(1) C 3 - O 16	1.04	10.45	0.093
23. CR (1) C 2	/274. BD*(1) C 12 - O 13	0.57	10.78	0.070
24. CR (1) C 3	/ 93. RY*(3) C 4	0.77	11.21	0.083
24. CR (1) C 3	/267. BD*(1) C 2 - O 16	0.83	10.40	0.084
24. CR (1) C 3	/271. BD*(1) C 3 - O 16	1.32	10.37	0.105
25. CR (1) C 4	/ 46. RY*(7) C 1	0.68	10.96	0.077
25. CR (1) C 4	/ 80. RY*(7) C 3	0.63	11.02	0.074
25. CR (1) C 4	/133. RY*(1) H 10	0.51	11.20	0.068
26. CR (1) C 12	/ 58. RY*(2) C 2	0.64	11.58	0.077
26. CR (1) C 12	/277. BD*(1) O 14 - C 17	1.26	10.44	0.103
27. CR (1) O 13	/143. RY*(1) C 12	6.99	19.88	0.334
27. CR (1) O 13	/265. BD*(1) C 2 - C 12	0.56	19.17	0.095
28. CR (1) O 14	/143. RY*(1) C 12	1.47	20.00	0.154
28. CR (1) O 14	/144. RY*(2) C 12	0.73	20.84	0.111
28. CR (1) O 14	/146. RY*(4) C 12	0.92	20.87	0.123
28. CR (1) O 14	/228. RY*(1) C 17	0.57	19.95	0.095
28. CR (1) O 14	/274. BD*(1) C 12 - O 13	0.52	19.58	0.091
29. CR (1) O 15	/ 40. RY*(1) C 1	1.05	19.80	0.129
29. CR (1) O 15	/ 57. RY*(1) C 2	1.56	19.96	0.158
30. CR (1) O 16	/ 57. RY*(1) C 2	1.87	19.96	0.173
30. CR (1) O 16	/ 74. RY*(1) C 3	0.60	19.81	0.097
30. CR (1) O 16	/ 75. RY*(2) C 3	0.72	19.98	0.107
31. CR (1) C 17	/246. RY*(2) H 18	0.59	12.22	0.076
31. CR (1) C 17	/276. BD*(1) C 12 - O 14	0.84	10.48	0.086
31. CR (1) C 17	/277. BD*(1) O 14 - C 17	1.85	10.35	0.124
32. LP (1) O 13	/143. RY*(1) C 12	17.03	1.73	0.153
32. LP (1) O 13	/156. RY*(14) C 12	0.94	7.83	0.077
32. LP (1) O 13	/265. BD*(1) C 2 - C 12	1.74	1.03	0.038
32. LP (1) O 13	/276. BD*(1) C 12 - O 14	1.33	1.09	0.035
33. LP (2) O 13	/144. RY*(2) C 12	3.21	2.14	0.077
33. LP (2) O 13	/146. RY*(4) C 12	0.90	2.17	0.041
33. LP (2) O 13	/265. BD*(1) C 2 - C 12	20.47	0.59	0.099
33. LP (2) O 13	/276. BD*(1) C 12 - O 14	30.65	0.66	0.128
33. LP (2) O 13	/278. BD*(1) C 17 - H 18	0.69	0.68	0.020
34. LP (1) O 14	/143. RY*(1) C 12	2.63	1.59	0.058

34. LP (1) O 14	/146. RY*(4) C 12	2.19	2.46	0.066
34. LP (1) O 14	/228. RY*(1) C 17	2.07	1.55	0.051
34. LP (1) O 14	/265. BD*(1) C 2 - C 12	0.94	0.89	0.026
34. LP (1) O 14	/274. BD*(1) C 12 - O 13	8.05	1.17	0.087
34. LP (1) O 14	/278. BD*(1) C 17 - H 18	2.25	0.97	0.042
34. LP (1) O 14	/279. BD*(1) C 17 - H 19	0.53	0.96	0.020
35. LP (2) O 14	/145. RY*(3) C 12	2.78	1.93	0.069
35. LP (2) O 14	/150. RY*(8) C 12	0.56	1.20	0.025
35. LP (2) O 14	/229. RY*(2) C 17	1.17	1.43	0.039
35. LP (2) O 14	/230. RY*(3) C 17	0.81	1.38	0.032
35. LP (2) O 14	/275. BD*(2) C 12 - O 13	49.43	0.34	0.116
35. LP (2) O 14	/279. BD*(1) C 17 - H 19	4.32	0.72	0.053
35. LP (2) O 14	/280. BD*(1) C 17 - H 20	4.32	0.72	0.053
36. LP (1) O 15	/ 40. RY*(1) C 1	1.33	1.44	0.039
36. LP (1) O 15	/ 41. RY*(2) C 1	1.02	1.64	0.037
36. LP (1) O 15	/ 57. RY*(1) C 2	2.24	1.60	0.054
36. LP (1) O 15	/ 59. RY*(3) C 2	0.78	1.88	0.034
36. LP (1) O 15	/260. BD*(1) C 1 - C 4	0.74	0.96	0.024
36. LP (1) O 15	/261. BD*(1) C 1 - H 6	0.80	0.95	0.025
36. LP (1) O 15	/262. BD*(1) C 1 - H 7	2.43	0.98	0.044
36. LP (1) O 15	/264. BD*(1) C 2 - H 5	2.90	0.96	0.047
36. LP (1) O 15	/265. BD*(1) C 2 - C 12	1.31	0.88	0.031
36. LP (1) O 15	/267. BD*(1) C 2 - O 16	1.28	0.88	0.030
37. LP (2) O 15	/ 42. RY*(3) C 1	1.12	1.82	0.041
37. LP (2) O 15	/ 58. RY*(2) C 2	0.79	1.69	0.033
37. LP (2) O 15	/ 60. RY*(4) C 2	0.59	1.84	0.030
37. LP (2) O 15	/ 61. RY*(5) C 2	0.50	2.19	0.030
37. LP (2) O 15	/260. BD*(1) C 1 - C 4	4.49	0.69	0.051
37. LP (2) O 15	/261. BD*(1) C 1 - H 6	5.69	0.69	0.057
37. LP (2) O 15	/265. BD*(1) C 2 - C 12	7.55	0.62	0.061
37. LP (2) O 15	/267. BD*(1) C 2 - O 16	10.34	0.62	0.072
37. LP (2) O 15	/273. BD*(1) C 4 - H 11	0.59	0.71	0.019
37. LP (2) O 15	/275. BD*(2) C 12 - O 13	0.59	0.31	0.013
38. LP (1) O 16	/ 57. RY*(1) C 2	3.05	1.59	0.063
38. LP (1) O 16	/ 59. RY*(3) C 2	0.61	1.87	0.030
38. LP (1) O 16	/ 74. RY*(1) C 3	0.58	1.44	0.026
38. LP (1) O 16	/ 75. RY*(2) C 3	1.57	1.61	0.045
38. LP (1) O 16	/ 76. RY*(3) C 3	0.56	2.09	0.031
38. LP (1) O 16	/264. BD*(1) C 2 - H 5	3.02	0.95	0.048
38. LP (1) O 16	/265. BD*(1) C 2 - C 12	1.20	0.88	0.029
38. LP (1) O 16	/266. BD*(1) C 2 - O 15	1.47	0.86	0.032
38. LP (1) O 16	/268. BD*(1) C 3 - C 4	0.85	0.95	0.026
38. LP (1) O 16	/269. BD*(1) C 3 - H 8	2.47	0.97	0.044
38. LP (1) O 16	/270. BD*(1) C 3 - H 9	0.68	0.96	0.023
39. LP (2) O 16	/ 58. RY*(2) C 2	0.87	1.69	0.035
39. LP (2) O 16	/ 60. RY*(4) C 2	0.72	1.84	0.033
39. LP (2) O 16	/ 76. RY*(3) C 3	1.08	1.83	0.041
39. LP (2) O 16	/265. BD*(1) C 2 - C 12	7.69	0.62	0.062
39. LP (2) O 16	/266. BD*(1) C 2 - O 15	10.50	0.60	0.072
39. LP (2) O 16	/268. BD*(1) C 3 - C 4	4.27	0.69	0.049
39. LP (2) O 16	/270. BD*(1) C 3 - H 9	5.70	0.70	0.057
39. LP (2) O 16	/273. BD*(1) C 4 - H 11	0.54	0.70	0.018
39. LP (2) O 16	/276. BD*(1) C 12 - O 14	0.70	0.68	0.019
265. BD*(1) C 2 - C 12	/ 58. RY*(2) C 2	0.70	1.07	0.103
265. BD*(1) C 2 - C 12	/ 62. RY*(6) C 2	0.60	0.92	0.091
265. BD*(1) C 2 - C 12	/147. RY*(5) C 12	1.04	0.73	0.107
265. BD*(1) C 2 - C 12	/264. BD*(1) C 2 - H 5	0.67	0.07	0.024
275. BD*(2) C 12 - O 13	/145. RY*(3) C 12	1.72	1.58	0.138
275. BD*(2) C 12 - O 13	/161. RY*(2) O 13	1.42	0.55	0.075
275. BD*(2) C 12 - O 13	/264. BD*(1) C 2 - H 5	0.90	0.38	0.047
275. BD*(2) C 12 - O 13	/266. BD*(1) C 2 - O 15	1.32	0.29	0.048
275. BD*(2) C 12 - O 13	/274. BD*(1) C 12 - O 13	0.93	0.60	0.060

2-eq



Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) C 1 - C 4	/194. RY*(1) O 15	0.64	1.51	0.028
1. BD (1) C 1 - C 4	/268. BD*(1) C 3 - C 4	0.50	1.00	0.020
1. BD (1) C 1 - C 4	/269. BD*(1) C 3 - H 7	1.66	1.03	0.037
1. BD (1) C 1 - C 4	/271. BD*(1) C 3 - O 16	0.52	0.90	0.019
2. BD (1) C 1 - H 5	/263. BD*(1) C 1 - O 15	0.58	0.79	0.019
2. BD (1) C 1 - H 5	/272. BD*(1) C 4 - H 9	2.52	0.91	0.043
3. BD (1) C 1 - H 6	/195. RY*(2) O 15	0.54	1.23	0.023
3. BD (1) C 1 - H 6	/266. BD*(1) C 2 - O 15	2.75	0.81	0.043
3. BD (1) C 1 - H 6	/268. BD*(1) C 3 - C 4	2.44	0.89	0.042
4. BD (1) C 1 - O 15	/ 57. RY*(1) C 2	0.65	1.72	0.030
4. BD (1) C 1 - O 15	/265. BD*(1) C 2 - C 12	1.53	1.13	0.038
4. BD (1) C 1 - O 15	/273. BD*(1) C 4 - H 10	1.07	1.19	0.032
5. BD (1) C 2 - H 11	/276. BD*(1) C 12 - O 14	3.50	0.92	0.052
6. BD (1) C 2 - C 12	/160. RY*(1) O 13	1.34	1.36	0.038
6. BD (1) C 2 - C 12	/177. RY*(1) O 14	0.61	1.41	0.026
6. BD (1) C 2 - C 12	/182. RY*(6) O 14	0.64	2.11	0.033
6. BD (1) C 2 - C 12	/263. BD*(1) C 1 - O 15	2.53	0.93	0.043
6. BD (1) C 2 - C 12	/271. BD*(1) C 3 - O 16	2.54	0.93	0.044
6. BD (1) C 2 - C 12	/274. BD*(1) C 12 - O 13	0.78	1.26	0.028
6. BD (1) C 2 - C 12	/277. BD*(1) O 14 - C 17	4.28	0.91	0.056
7. BD (1) C 2 - O 15	/ 41. RY*(2) C 1	1.95	1.75	0.052
7. BD (1) C 2 - O 15	/262. BD*(1) C 1 - H 6	0.73	1.24	0.027
7. BD (1) C 2 - O 15	/274. BD*(1) C 12 - O 13	1.02	1.44	0.034
7. BD (1) C 2 - O 15	/275. BD*(2) C 12 - O 13	1.14	0.84	0.029
8. BD (1) C 2 - O 16	/ 75. RY*(2) C 3	1.96	1.75	0.052
8. BD (1) C 2 - O 16	/269. BD*(1) C 3 - H 7	0.74	1.24	0.027
8. BD (1) C 2 - O 16	/274. BD*(1) C 12 - O 13	1.01	1.44	0.034
8. BD (1) C 2 - O 16	/275. BD*(2) C 12 - O 13	1.16	0.84	0.029
9. BD (1) C 3 - C 4	/211. RY*(1) O 16	0.64	1.51	0.028
9. BD (1) C 3 - C 4	/262. BD*(1) C 1 - H 6	1.65	1.03	0.037
9. BD (1) C 3 - C 4	/263. BD*(1) C 1 - O 15	0.52	0.90	0.019
10. BD (1) C 3 - H 7	/212. RY*(2) O 16	0.54	1.23	0.023
10. BD (1) C 3 - H 7	/260. BD*(1) C 1 - C 4	2.45	0.89	0.042
10. BD (1) C 3 - H 7	/267. BD*(1) C 2 - O 16	2.75	0.81	0.043
11. BD (1) C 3 - H 8	/271. BD*(1) C 3 - O 16	0.58	0.79	0.019
11. BD (1) C 3 - H 8	/272. BD*(1) C 4 - H 9	2.52	0.91	0.043
12. BD (1) C 3 - O 16	/ 57. RY*(1) C 2	0.63	1.72	0.029
12. BD (1) C 3 - O 16	/265. BD*(1) C 2 - C 12	1.52	1.13	0.038
12. BD (1) C 3 - O 16	/273. BD*(1) C 4 - H 10	1.07	1.19	0.032
13. BD (1) C 4 - H 9	/ 41. RY*(2) C 1	0.60	1.40	0.026
13. BD (1) C 4 - H 9	/ 75. RY*(2) C 3	0.61	1.40	0.026
13. BD (1) C 4 - H 9	/261. BD*(1) C 1 - H 5	2.59	0.87	0.043
13. BD (1) C 4 - H 9	/270. BD*(1) C 3 - H 8	2.60	0.87	0.043
14. BD (1) C 4 - H 10	/263. BD*(1) C 1 - O 15	3.98	0.77	0.050

14. BD (1) C 4 - H 10	/271. BD*(1) C 3 - O 16	3.97	0.77	0.050
15. BD (1) C 12 - O 13	/ 58. RY*(2) C 2	0.64	2.29	0.034
15. BD (1) C 12 - O 13	/143. RY*(1) C 12	1.58	2.13	0.052
15. BD (1) C 12 - O 13	/265. BD*(1) C 2 - C 12	1.02	1.44	0.035
16. BD (2) C 12 - O 13	/178. RY*(2) O 14	0.52	1.23	0.023
16. BD (2) C 12 - O 13	/266. BD*(1) C 2 - O 15	1.83	0.70	0.032
16. BD (2) C 12 - O 13	/267. BD*(1) C 2 - O 16	1.85	0.70	0.032
16. BD (2) C 12 - O 13	/275. BD*(2) C 12 - O 13	0.51	0.40	0.014
17. BD (1) C 12 - O 14	/ 58. RY*(2) C 2	0.72	2.15	0.035
17. BD (1) C 12 - O 14	/229. RY*(2) C 17	1.48	1.85	0.047
17. BD (1) C 12 - O 14	/274. BD*(1) C 12 - O 13	0.59	1.56	0.027
18. BD (1) O 14 - C 17	/143. RY*(1) C 12	1.72	1.85	0.051
18. BD (1) O 14 - C 17	/148. RY*(6) C 12	0.80	1.85	0.034
18. BD (1) O 14 - C 17	/265. BD*(1) C 2 - C 12	2.72	1.16	0.051
19. BD (1) C 17 - H 18	/178. RY*(2) O 14	0.64	1.35	0.026
19. BD (1) C 17 - H 18	/277. BD*(1) O 14 - C 17	0.73	0.78	0.021
20. BD (1) C 17 - H 19	/180. RY*(4) O 14	0.67	2.04	0.033
20. BD (1) C 17 - H 19	/276. BD*(1) C 12 - O 14	2.73	0.91	0.045
21. BD (1) C 17 - H 20	/178. RY*(2) O 14	0.64	1.35	0.026
21. BD (1) C 17 - H 20	/277. BD*(1) O 14 - C 17	0.73	0.78	0.021
22. CR (1) C 1	/ 93. RY*(3) C 4	0.82	11.18	0.086
22. CR (1) C 1	/263. BD*(1) C 1 - O 15	1.29	10.37	0.104
22. CR (1) C 1	/266. BD*(1) C 2 - O 15	0.80	10.39	0.082
23. CR (1) C 2	/148. RY*(6) C 12	0.51	11.20	0.068
23. CR (1) C 2	/263. BD*(1) C 1 - O 15	0.96	10.45	0.090
23. CR (1) C 2	/271. BD*(1) C 3 - O 16	0.96	10.45	0.090
24. CR (1) C 3	/ 93. RY*(3) C 4	0.82	11.18	0.086
24. CR (1) C 3	/267. BD*(1) C 2 - O 16	0.80	10.39	0.082
24. CR (1) C 3	/271. BD*(1) C 3 - O 16	1.29	10.37	0.104
25. CR (1) C 4	/ 46. RY*(7) C 1	0.51	11.19	0.068
25. CR (1) C 4	/ 80. RY*(7) C 3	0.52	11.18	0.068
25. CR (1) C 4	/128. RY*(1) H 9	0.53	11.22	0.069
26. CR (1) C 12	/ 62. RY*(6) C 2	1.39	11.38	0.112
26. CR (1) C 12	/277. BD*(1) O 14 - C 17	1.27	10.45	0.103
27. CR (1) O 13	/143. RY*(1) C 12	6.68	19.89	0.327
27. CR (1) O 13	/265. BD*(1) C 2 - C 12	0.62	19.20	0.100
28. CR (1) O 14	/143. RY*(1) C 12	1.57	20.01	0.159
28. CR (1) O 14	/144. RY*(2) C 12	0.67	20.84	0.106
28. CR (1) O 14	/146. RY*(4) C 12	0.91	20.96	0.123
28. CR (1) O 14	/228. RY*(1) C 17	0.51	20.00	0.091
28. CR (1) O 14	/229. RY*(2) C 17	0.68	19.88	0.104
28. CR (1) O 14	/274. BD*(1) C 12 - O 13	0.55	19.58	0.093
29. CR (1) O 15	/ 40. RY*(1) C 1	0.95	19.98	0.123
29. CR (1) O 15	/ 57. RY*(1) C 2	1.59	19.86	0.159
29. CR (1) O 15	/ 58. RY*(2) C 2	0.65	20.13	0.102
30. CR (1) O 16	/ 57. RY*(1) C 2	1.55	19.86	0.157
30. CR (1) O 16	/ 58. RY*(2) C 2	0.69	20.13	0.105
30. CR (1) O 16	/ 74. RY*(1) C 3	0.93	19.98	0.122
31. CR (1) C 17	/251. RY*(2) H 19	0.73	12.25	0.084
31. CR (1) C 17	/276. BD*(1) C 12 - O 14	0.78	10.49	0.083
31. CR (1) C 17	/277. BD*(1) O 14 - C 17	1.89	10.35	0.125
32. LP (1) O 13	/143. RY*(1) C 12	16.20	1.75	0.150
32. LP (1) O 13	/159. RY*(17) C 12	1.23	4.44	0.066
32. LP (1) O 13	/265. BD*(1) C 2 - C 12	1.86	1.06	0.040
32. LP (1) O 13	/276. BD*(1) C 12 - O 14	1.38	1.10	0.035
33. LP (2) O 13	/144. RY*(2) C 12	3.10	2.15	0.075
33. LP (2) O 13	/146. RY*(4) C 12	0.69	2.27	0.037
33. LP (2) O 13	/265. BD*(1) C 2 - C 12	18.26	0.62	0.097
33. LP (2) O 13	/276. BD*(1) C 12 - O 14	29.91	0.67	0.128
33. LP (2) O 13	/279. BD*(1) C 17 - H 19	0.68	0.68	0.020
34. LP (1) O 14	/143. RY*(1) C 12	2.48	1.61	0.057
34. LP (1) O 14	/146. RY*(4) C 12	2.27	2.56	0.069
34. LP (1) O 14	/228. RY*(1) C 17	2.04	1.59	0.051
34. LP (1) O 14	/229. RY*(2) C 17	0.54	1.47	0.025
34. LP (1) O 14	/265. BD*(1) C 2 - C 12	0.93	0.91	0.026
34. LP (1) O 14	/274. BD*(1) C 12 - O 13	8.38	1.18	0.089
34. LP (1) O 14	/278. BD*(1) C 17 - H 18	0.52	0.96	0.020
34. LP (1) O 14	/279. BD*(1) C 17 - H 19	2.25	0.97	0.042
35. LP (2) O 14	/145. RY*(3) C 12	2.96	1.94	0.072
35. LP (2) O 14	/150. RY*(8) C 12	0.54	1.89	0.030
35. LP (2) O 14	/230. RY*(3) C 17	1.68	1.69	0.051
35. LP (2) O 14	/275. BD*(2) C 12 - O 13	52.22	0.33	0.118
35. LP (2) O 14	/278. BD*(1) C 17 - H 18	4.25	0.72	0.052
35. LP (2) O 14	/280. BD*(1) C 17 - H 20	4.29	0.72	0.053

36. LP (1) O 15	/ 40. RY*(1) C 1	2.14	1.62	0.053
36. LP (1) O 15	/ 42. RY*(3) C 1	0.52	2.11	0.030
36. LP (1) O 15	/ 57. RY*(1) C 2	1.80	1.50	0.047
36. LP (1) O 15	/ 58. RY*(2) C 2	0.66	1.77	0.031
36. LP (1) O 15	/ 61. RY*(5) C 2	0.76	2.45	0.039
36. LP (1) O 15	/260. BD*(1) C 1 - C 4	0.61	0.96	0.022
36. LP (1) O 15	/261. BD*(1) C 1 - H 5	0.80	0.96	0.025
36. LP (1) O 15	/262. BD*(1) C 1 - H 6	2.34	0.98	0.043
36. LP (1) O 15	/264. BD*(1) C 2 - H 11	1.21	0.95	0.030
36. LP (1) O 15	/265. BD*(1) C 2 - C 12	1.85	0.92	0.037
36. LP (1) O 15	/267. BD*(1) C 2 - O 16	0.52	0.88	0.019
37. LP (2) O 15	/ 40. RY*(1) C 1	0.53	1.35	0.024
37. LP (2) O 15	/ 42. RY*(3) C 1	1.09	1.84	0.041
37. LP (2) O 15	/ 60. RY*(4) C 2	0.80	2.16	0.038
37. LP (2) O 15	/260. BD*(1) C 1 - C 4	4.68	0.69	0.052
37. LP (2) O 15	/261. BD*(1) C 1 - H 5	5.18	0.69	0.054
37. LP (2) O 15	/264. BD*(1) C 2 - H 11	5.26	0.68	0.054
37. LP (2) O 15	/267. BD*(1) C 2 - O 16	12.41	0.61	0.078
37. LP (2) O 15	/273. BD*(1) C 4 - H 10	0.57	0.71	0.018
38. LP (1) O 16	/ 57. RY*(1) C 2	1.75	1.50	0.046
38. LP (1) O 16	/ 58. RY*(2) C 2	0.70	1.77	0.032
38. LP (1) O 16	/ 61. RY*(5) C 2	0.76	2.45	0.039
38. LP (1) O 16	/ 74. RY*(1) C 3	2.12	1.62	0.053
38. LP (1) O 16	/ 76. RY*(3) C 3	0.53	2.11	0.030
38. LP (1) O 16	/264. BD*(1) C 2 - H 11	1.22	0.95	0.030
38. LP (1) O 16	/265. BD*(1) C 2 - C 12	1.84	0.92	0.037
38. LP (1) O 16	/266. BD*(1) C 2 - O 15	0.51	0.88	0.019
38. LP (1) O 16	/268. BD*(1) C 3 - C 4	0.60	0.96	0.022
38. LP (1) O 16	/269. BD*(1) C 3 - H 7	2.34	0.98	0.043
38. LP (1) O 16	/270. BD*(1) C 3 - H 8	0.80	0.96	0.025
39. LP (2) O 16	/ 60. RY*(4) C 2	0.80	2.16	0.038
39. LP (2) O 16	/ 74. RY*(1) C 3	0.52	1.35	0.024
39. LP (2) O 16	/ 76. RY*(3) C 3	1.09	1.84	0.041
39. LP (2) O 16	/264. BD*(1) C 2 - H 11	5.25	0.68	0.054
39. LP (2) O 16	/266. BD*(1) C 2 - O 15	12.43	0.61	0.078
39. LP (2) O 16	/268. BD*(1) C 3 - C 4	4.69	0.69	0.052
39. LP (2) O 16	/270. BD*(1) C 3 - H 8	5.17	0.69	0.054
39. LP (2) O 16	/273. BD*(1) C 4 - H 10	0.58	0.71	0.018
275. BD*(2) C 12 - O 13	/145. RY*(3) C 12	1.64	1.61	0.136
275. BD*(2) C 12 - O 13	/161. RY*(2) O 13	1.63	0.54	0.079
275. BD*(2) C 12 - O 13	/266. BD*(1) C 2 - O 15	1.62	0.30	0.053
275. BD*(2) C 12 - O 13	/267. BD*(1) C 2 - O 16	1.64	0.30	0.053

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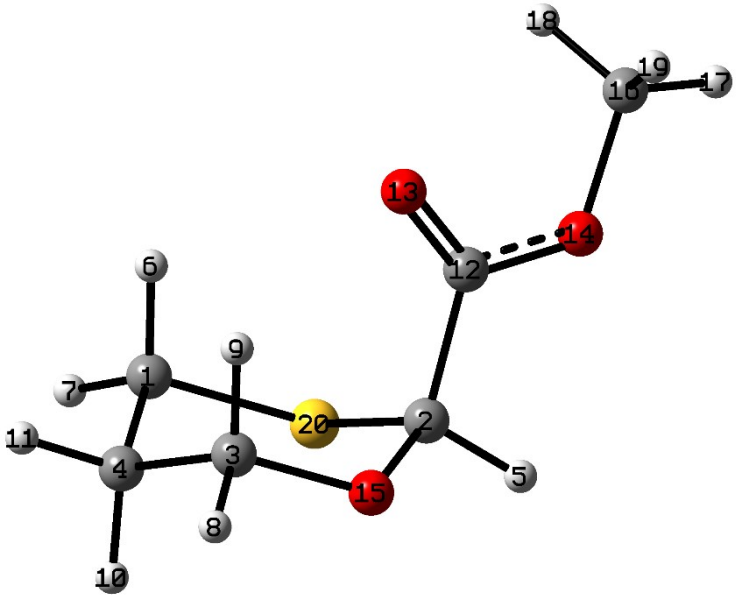

Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) C 1 - C 4	/ 78. RY*(1) C 3	1.22	1.53	0.039
1. BD (1) C 1 - C 4	/270. BD*(1) C 1 - H 7	0.55	1.03	0.021
1. BD (1) C 1 - C 4	/276. BD*(1) C 3 - C 4	0.55	1.02	0.021
1. BD (1) C 1 - C 4	/277. BD*(1) C 3 - H 8	1.35	1.03	0.033
2. BD (1) C 1 - H 6	/247. RY*(1) S 20	0.58	1.12	0.023
2. BD (1) C 1 - H 6	/280. BD*(1) C 4 - H 10	2.60	0.92	0.044
3. BD (1) C 1 - H 7	/ 96. RY*(2) C 4	0.59	1.16	0.023
3. BD (1) C 1 - H 7	/248. RY*(2) S 20	0.55	1.32	0.024
3. BD (1) C 1 - H 7	/275. BD*(1) C 2 - S 20	1.33	0.64	0.026
3. BD (1) C 1 - H 7	/276. BD*(1) C 3 - C 4	2.82	0.90	0.045
4. BD (1) C 1 - S 20	/ 95. RY*(1) C 4	0.97	1.36	0.033
4. BD (1) C 1 - S 20	/272. BD*(1) C 2 - H 5	1.07	0.98	0.029
4. BD (1) C 1 - S 20	/281. BD*(1) C 4 - H 11	2.32	0.98	0.043
5. BD (1) C 2 - H 5	/199. RY*(2) O 15	0.91	1.40	0.032
5. BD (1) C 2 - H 5	/271. BD*(1) C 1 - S 20	1.04	0.68	0.024
5. BD (1) C 2 - H 5	/279. BD*(1) C 3 - O 15	4.43	0.80	0.053
5. BD (1) C 2 - H 5	/282. BD*(1) C 12 - O 13	4.88	1.12	0.066
5. BD (1) C 2 - H 5	/283. BD*(2) C 12 - O 13	0.72	0.54	0.019
5. BD (1) C 2 - H 5	/284. BD*(1) C 12 - O 14	0.76	0.90	0.024
6. BD (1) C 2 - C 12	/164. RY*(1) O 13	1.11	1.47	0.036
6. BD (1) C 2 - C 12	/181. RY*(1) O 14	0.74	1.19	0.027
6. BD (1) C 2 - C 12	/186. RY*(6) O 14	0.54	2.12	0.030
6. BD (1) C 2 - C 12	/282. BD*(1) C 12 - O 13	1.30	1.26	0.036
6. BD (1) C 2 - C 12	/285. BD*(1) O 14 - C 16	4.12	0.92	0.055
7. BD (1) C 2 - O 15	/ 78. RY*(1) C 3	0.84	1.77	0.035
7. BD (1) C 2 - O 15	/ 79. RY*(2) C 3	0.99	1.81	0.038
7. BD (1) C 2 - O 15	/284. BD*(1) C 12 - O 14	1.04	1.24	0.033
8. BD (1) C 2 - S 20	/ 44. RY*(1) C 1	0.60	1.39	0.026
8. BD (1) C 2 - S 20	/151. RY*(5) C 12	0.78	1.39	0.030
8. BD (1) C 2 - S 20	/198. RY*(1) O 15	1.24	1.26	0.035
8. BD (1) C 2 - S 20	/270. BD*(1) C 1 - H 7	1.22	0.98	0.031
8. BD (1) C 2 - S 20	/283. BD*(2) C 12 - O 13	5.52	0.58	0.053
9. BD (1) C 3 - C 4	/ 44. RY*(1) C 1	0.99	1.43	0.034
9. BD (1) C 3 - C 4	/198. RY*(1) O 15	0.92	1.30	0.031
9. BD (1) C 3 - C 4	/268. BD*(1) C 1 - C 4	0.67	1.00	0.023
9. BD (1) C 3 - C 4	/270. BD*(1) C 1 - H 7	1.74	1.02	0.038
10. BD (1) C 3 - H 8	/199. RY*(2) O 15	0.52	1.37	0.024
10. BD (1) C 3 - H 8	/268. BD*(1) C 1 - C 4	2.99	0.89	0.046
10. BD (1) C 3 - H 8	/274. BD*(1) C 2 - O 15	3.58	0.81	0.048
11. BD (1) C 3 - H 9	/279. BD*(1) C 3 - O 15	0.56	0.78	0.019
11. BD (1) C 3 - H 9	/280. BD*(1) C 4 - H 10	2.74	0.91	0.045
12. BD (1) C 3 - O 15	/ 61. RY*(1) C 2	1.42	1.62	0.043
12. BD (1) C 3 - O 15	/ 62. RY*(2) C 2	0.90	1.81	0.036
12. BD (1) C 3 - O 15	/272. BD*(1) C 2 - H 5	0.95	1.19	0.030
12. BD (1) C 3 - O 15	/281. BD*(1) C 4 - H 11	0.90	1.19	0.029
13. BD (1) C 4 - H 10	/269. BD*(1) C 1 - H 6	2.85	0.89	0.045
13. BD (1) C 4 - H 10	/278. BD*(1) C 3 - H 9	2.49	0.89	0.042
14. BD (1) C 4 - H 11	/271. BD*(1) C 1 - S 20	4.91	0.64	0.050
14. BD (1) C 4 - H 11	/279. BD*(1) C 3 - O 15	4.97	0.76	0.055
15. BD (1) C 12 - O 13	/147. RY*(1) C 12	1.64	2.02	0.052
15. BD (1) C 12 - O 13	/273. BD*(1) C 2 - C 12	1.31	1.44	0.040
16. BD (2) C 12 - O 13	/274. BD*(1) C 2 - O 15	0.56	0.71	0.018
16. BD (2) C 12 - O 13	/275. BD*(1) C 2 - S 20	1.73	0.53	0.027
16. BD (2) C 12 - O 13	/283. BD*(2) C 12 - O 13	0.81	0.41	0.017
17. BD (1) C 12 - O 14	/ 62. RY*(2) C 2	0.50	1.96	0.028
17. BD (1) C 12 - O 14	/217. RY*(3) C 16	1.36	1.82	0.044
17. BD (1) C 12 - O 14	/274. BD*(1) C 2 - O 15	0.99	1.25	0.032
17. BD (1) C 12 - O 14	/282. BD*(1) C 12 - O 13	0.51	1.54	0.025
18. BD (1) O 14 - C 16	/147. RY*(1) C 12	1.59	1.75	0.047
18. BD (1) O 14 - C 16	/273. BD*(1) C 2 - C 12	2.59	1.16	0.050
19. BD (1) C 16 - H 17	/284. BD*(1) C 12 - O 14	2.82	0.89	0.046
20. BD (1) C 16 - H 18	/182. RY*(2) O 14	0.68	1.28	0.026
20. BD (1) C 16 - H 18	/285. BD*(1) O 14 - C 16	0.72	0.78	0.021
21. BD (1) C 16 - H 19	/182. RY*(2) O 14	0.56	1.28	0.024
21. BD (1) C 16 - H 19	/285. BD*(1) O 14 - C 16	0.69	0.78	0.021
22. CR (1) C 1	/ 97. RY*(3) C 4	0.81	11.22	0.085
22. CR (1) C 1	/271. BD*(1) C 1 - S 20	1.21	10.22	0.100

23. CR (1) C 2	/148. RY*(2) C 12	0.55	11.96	0.073
23. CR (1) C 2	/154. RY*(8) C 12	0.53	11.40	0.069
23. CR (1) C 2	/272. BD*(1) C 2 - H 5	0.83	10.55	0.084
23. CR (1) C 2	/275. BD*(1) C 2 - S 20	0.54	10.28	0.067
23. CR (1) C 2	/279. BD*(1) C 3 - O 15	1.12	10.43	0.097
23. CR (1) C 2	/282. BD*(1) C 12 - O 13	0.74	10.75	0.080
24. CR (1) C 3	/ 96. RY*(2) C 4	0.52	10.74	0.067
24. CR (1) C 3	/ 97. RY*(3) C 4	0.60	11.24	0.073
24. CR (1) C 3	/274. BD*(1) C 2 - O 15	0.92	10.39	0.088
24. CR (1) C 3	/279. BD*(1) C 3 - O 15	1.47	10.36	0.111
25. CR (1) C 4	/ 45. RY*(2) C 1	1.06	10.82	0.096
26. CR (1) C 12	/ 61. RY*(1) C 2	0.68	11.02	0.077
26. CR (1) C 12	/285. BD*(1) O 14 - C 16	1.22	10.45	0.101
27. CR (1) O 13	/147. RY*(1) C 12	7.01	19.78	0.334
27. CR (1) O 13	/273. BD*(1) C 2 - C 12	0.66	19.20	0.103
28. CR (1) O 14	/147. RY*(1) C 12	1.51	19.91	0.155
28. CR (1) O 14	/148. RY*(2) C 12	0.70	20.78	0.108
28. CR (1) O 14	/150. RY*(4) C 12	0.96	20.69	0.126
28. CR (1) O 14	/215. RY*(1) C 16	0.55	19.98	0.094
28. CR (1) O 14	/217. RY*(3) C 16	0.57	19.85	0.095
28. CR (1) O 14	/282. BD*(1) C 12 - O 13	0.54	19.57	0.092
29. CR (1) O 15	/ 61. RY*(1) C 2	2.23	19.77	0.188
29. CR (1) O 15	/ 79. RY*(2) C 3	1.30	19.89	0.143
30. CR (1) C 16	/284. BD*(1) C 12 - O 14	0.83	10.47	0.085
30. CR (1) C 16	/285. BD*(1) O 14 - C 16	1.84	10.35	0.124
36. LP (1) O 13	/147. RY*(1) C 12	16.86	1.64	0.149
36. LP (1) O 13	/148. RY*(2) C 12	0.56	2.51	0.033
36. LP (1) O 13	/163. RY*(17) C 12	0.92	5.42	0.063
36. LP (1) O 13	/273. BD*(1) C 2 - C 12	2.16	1.05	0.043
36. LP (1) O 13	/284. BD*(1) C 12 - O 14	1.31	1.08	0.034
37. LP (2) O 13	/148. RY*(2) C 12	2.84	2.08	0.071
37. LP (2) O 13	/150. RY*(4) C 12	1.14	2.00	0.044
37. LP (2) O 13	/273. BD*(1) C 2 - C 12	18.85	0.62	0.098
37. LP (2) O 13	/284. BD*(1) C 12 - O 14	30.98	0.65	0.128
37. LP (2) O 13	/286. BD*(1) C 16 - H 17	0.68	0.68	0.020
38. LP (1) O 14	/147. RY*(1) C 12	2.89	1.50	0.059
38. LP (1) O 14	/150. RY*(4) C 12	2.18	2.29	0.064
38. LP (1) O 14	/215. RY*(1) C 16	2.12	1.58	0.052
38. LP (1) O 14	/273. BD*(1) C 2 - C 12	0.68	0.92	0.023
38. LP (1) O 14	/274. BD*(1) C 2 - O 15	0.50	0.88	0.019
38. LP (1) O 14	/282. BD*(1) C 12 - O 13	8.24	1.17	0.088
38. LP (1) O 14	/286. BD*(1) C 16 - H 17	2.24	0.97	0.042
38. LP (1) O 14	/287. BD*(1) C 16 - H 18	0.53	0.96	0.020
39. LP (2) O 14	/149. RY*(3) C 12	2.68	1.94	0.068
39. LP (2) O 14	/153. RY*(7) C 12	0.51	1.85	0.029
39. LP (2) O 14	/216. RY*(2) C 16	1.63	1.52	0.047
39. LP (2) O 14	/283. BD*(2) C 12 - O 13	48.46	0.34	0.115
39. LP (2) O 14	/287. BD*(1) C 16 - H 18	4.22	0.72	0.052
39. LP (2) O 14	/288. BD*(1) C 16 - H 19	4.45	0.72	0.053
40. LP (1) O 15	/ 61. RY*(1) C 2	2.77	1.37	0.055
40. LP (1) O 15	/ 62. RY*(2) C 2	0.59	1.56	0.027
40. LP (1) O 15	/ 65. RY*(5) C 2	0.60	2.09	0.032
40. LP (1) O 15	/ 79. RY*(2) C 3	1.91	1.49	0.048
40. LP (1) O 15	/ 80. RY*(3) C 3	0.66	2.06	0.033
40. LP (1) O 15	/272. BD*(1) C 2 - H 5	3.32	0.94	0.050
40. LP (1) O 15	/273. BD*(1) C 2 - C 12	2.04	0.89	0.038
40. LP (1) O 15	/275. BD*(1) C 2 - S 20	2.17	0.67	0.034
40. LP (1) O 15	/276. BD*(1) C 3 - C 4	0.52	0.94	0.020
40. LP (1) O 15	/277. BD*(1) C 3 - H 8	2.59	0.95	0.045
40. LP (1) O 15	/278. BD*(1) C 3 - H 9	1.19	0.95	0.030
41. LP (2) O 15	/ 63. RY*(3) C 2	1.57	1.68	0.047
41. LP (2) O 15	/ 64. RY*(4) C 2	0.80	1.55	0.032
41. LP (2) O 15	/ 79. RY*(2) C 3	0.64	1.26	0.026
41. LP (2) O 15	/ 80. RY*(3) C 3	0.81	1.83	0.035
41. LP (2) O 15	/273. BD*(1) C 2 - C 12	6.62	0.66	0.059
41. LP (2) O 15	/275. BD*(1) C 2 - S 20	11.99	0.44	0.065
41. LP (2) O 15	/276. BD*(1) C 3 - C 4	5.09	0.71	0.055
41. LP (2) O 15	/278. BD*(1) C 3 - H 9	4.46	0.72	0.052
41. LP (2) O 15	/281. BD*(1) C 4 - H 11	0.52	0.71	0.017
42. LP (1) S 20	/ 64. RY*(4) C 2	0.68	1.88	0.032
42. LP (1) S 20	/268. BD*(1) C 1 - C 4	0.69	1.03	0.024
42. LP (1) S 20	/274. BD*(1) C 2 - O 15	1.17	0.95	0.030
43. LP (2) S 20	/ 61. RY*(1) C 2	0.54	1.06	0.022
43. LP (2) S 20	/268. BD*(1) C 1 - C 4	2.37	0.62	0.035

43. LP (2) S 20	/269. BD*(1) C 1 - H 6	4.44	0.64	0.048
43. LP (2) S 20	/273. BD*(1) C 2 - C 12	3.88	0.58	0.042
43. LP (2) S 20	/274. BD*(1) C 2 - O 15	4.37	0.55	0.044
43. LP (2) S 20	/281. BD*(1) C 4 - H 11	0.71	0.64	0.019
43. LP (2) S 20	/283. BD*(2) C 12 - O 13	2.80	0.24	0.024
283. BD*(2) C 12 - O 13	/149. RY*(3) C 12	1.85	1.60	0.137
283. BD*(2) C 12 - O 13	/165. RY*(2) O 13	1.44	0.55	0.072
283. BD*(2) C 12 - O 13	/274. BD*(1) C 2 - O 15	1.12	0.30	0.043
283. BD*(2) C 12 - O 13	/275. BD*(1) C 2 - S 20	4.15	0.12	0.050
283. BD*(2) C 12 - O 13	/282. BD*(1) C 12 - O 13	1.24	0.59	0.065

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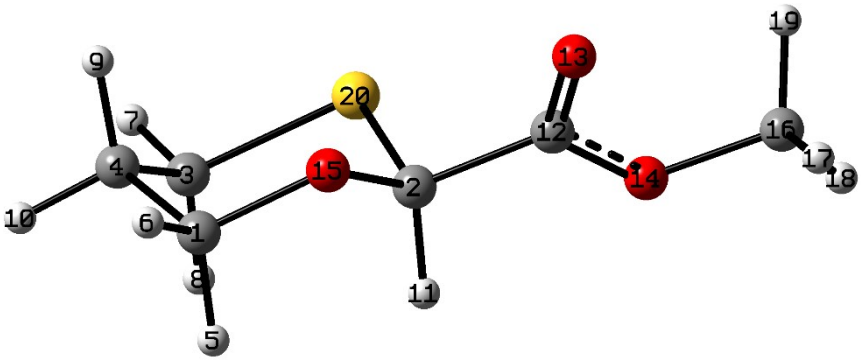


Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

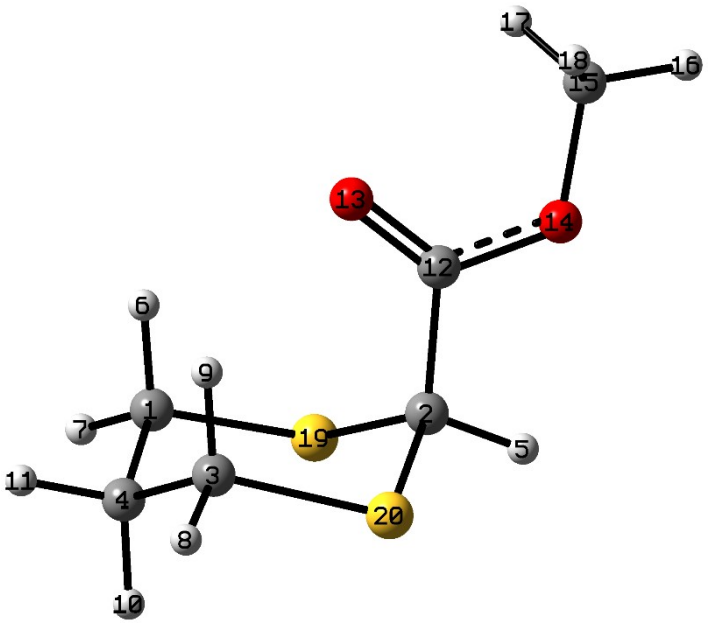
Threshold for printing: 0.50 kcal/mol

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) C 1 - C 4	/ 78. RY*(1) C 3	0.75	1.41	0.029
1. BD (1) C 1 - C 4	/198. RY*(1) O 15	0.84	1.33	0.030
1. BD (1) C 1 - C 4	/276. BD*(1) C 3 - C 4	0.66	1.00	0.023
1. BD (1) C 1 - C 4	/277. BD*(1) C 3 - H 7	1.72	1.02	0.037
2. BD (1) C 1 - H 5	/271. BD*(1) C 1 - O 15	0.64	0.79	0.020
2. BD (1) C 1 - H 5	/280. BD*(1) C 4 - H 9	2.62	0.92	0.044
3. BD (1) C 1 - H 6	/199. RY*(2) O 15	0.58	1.35	0.025
3. BD (1) C 1 - H 6	/274. BD*(1) C 2 - O 15	3.07	0.82	0.045
3. BD (1) C 1 - H 6	/276. BD*(1) C 3 - C 4	2.91	0.89	0.046
4. BD (1) C 1 - O 15	/ 61. RY*(1) C 2	1.29	1.57	0.040
4. BD (1) C 1 - O 15	/273. BD*(1) C 2 - C 12	1.53	1.15	0.038
4. BD (1) C 1 - O 15	/281. BD*(1) C 4 - H 10	0.91	1.19	0.029
5. BD (1) C 2 - H 11	/198. RY*(1) O 15	0.55	1.24	0.023
5. BD (1) C 2 - H 11	/282. BD*(1) C 12 - O 13	3.59	1.14	0.057
5. BD (1) C 2 - H 11	/283. BD*(2) C 12 - O 13	1.93	0.54	0.030
6. BD (1) C 2 - C 12	/164. RY*(1) O 13	1.26	1.41	0.038
6. BD (1) C 2 - C 12	/181. RY*(1) O 14	0.76	1.29	0.028
6. BD (1) C 2 - C 12	/185. RY*(5) O 14	0.69	2.20	0.035
6. BD (1) C 2 - C 12	/199. RY*(2) O 15	0.78	1.51	0.031
6. BD (1) C 2 - C 12	/271. BD*(1) C 1 - O 15	2.75	0.95	0.046
6. BD (1) C 2 - C 12	/282. BD*(1) C 12 - O 13	1.50	1.28	0.039
6. BD (1) C 2 - C 12	/285. BD*(1) O 14 - C 16	4.14	0.92	0.055
7. BD (1) C 2 - O 15	/ 44. RY*(1) C 1	1.11	1.80	0.040
7. BD (1) C 2 - O 15	/ 45. RY*(2) C 1	0.78	1.83	0.034
7. BD (1) C 2 - O 15	/ 49. RY*(6) C 1	0.51	2.39	0.031
7. BD (1) C 2 - O 15	/147. RY*(1) C 12	0.83	1.84	0.035
7. BD (1) C 2 - O 15	/270. BD*(1) C 1 - H 6	0.53	1.27	0.023
7. BD (1) C 2 - O 15	/284. BD*(1) C 12 - O 14	1.49	1.23	0.039
8. BD (1) C 2 - S 20	/ 78. RY*(1) C 3	0.94	1.37	0.032
8. BD (1) C 2 - S 20	/151. RY*(5) C 12	0.95	1.45	0.033
8. BD (1) C 2 - S 20	/198. RY*(1) O 15	1.50	1.28	0.039
8. BD (1) C 2 - S 20	/277. BD*(1) C 3 - H 7	1.30	0.98	0.032
8. BD (1) C 2 - S 20	/282. BD*(1) C 12 - O 13	0.81	1.18	0.028

8. BD (1) C 2 - S 20	/283. BD*(2) C 12 - O 13	5.63	0.58	0.054
9. BD (1) C 3 - C 4	/ 44. RY*(1) C 1	1.05	1.57	0.036
9. BD (1) C 3 - C 4	/268. BD*(1) C 1 - C 4	0.55	1.01	0.021
9. BD (1) C 3 - C 4	/270. BD*(1) C 1 - H 6	1.37	1.03	0.034
9. BD (1) C 3 - C 4	/277. BD*(1) C 3 - H 7	0.56	1.03	0.021
10. BD (1) C 3 - H 7	/ 96. RY*(2) C 4	0.56	1.17	0.023
10. BD (1) C 3 - H 7	/268. BD*(1) C 1 - C 4	2.86	0.90	0.045
10. BD (1) C 3 - H 7	/275. BD*(1) C 2 - S 20	1.15	0.63	0.024
11. BD (1) C 3 - H 8	/ 95. RY*(1) C 4	0.56	1.29	0.024
11. BD (1) C 3 - H 8	/247. RY*(1) S 20	0.58	1.16	0.023
11. BD (1) C 3 - H 8	/280. BD*(1) C 4 - H 9	2.61	0.92	0.044
12. BD (1) C 3 - S 20	/ 62. RY*(2) C 2	0.62	1.88	0.031
12. BD (1) C 3 - S 20	/ 95. RY*(1) C 4	0.96	1.36	0.032
12. BD (1) C 3 - S 20	/273. BD*(1) C 2 - C 12	1.13	0.93	0.029
12. BD (1) C 3 - S 20	/281. BD*(1) C 4 - H 10	2.22	0.97	0.042
13. BD (1) C 4 - H 9	/269. BD*(1) C 1 - H 5	2.65	0.87	0.043
13. BD (1) C 4 - H 9	/278. BD*(1) C 3 - H 8	2.84	0.88	0.045
14. BD (1) C 4 - H 10	/271. BD*(1) C 1 - O 15	4.69	0.77	0.054
14. BD (1) C 4 - H 10	/279. BD*(1) C 3 - S 20	5.01	0.64	0.051
15. BD (1) C 12 - O 13	/147. RY*(1) C 12	1.56	2.08	0.051
15. BD (1) C 12 - O 13	/273. BD*(1) C 2 - C 12	1.57	1.45	0.043
16. BD (2) C 12 - O 13	/272. BD*(1) C 2 - H 11	0.73	0.78	0.021
16. BD (2) C 12 - O 13	/275. BD*(1) C 2 - S 20	1.79	0.52	0.028
16. BD (2) C 12 - O 13	/283. BD*(2) C 12 - O 13	0.74	0.41	0.016
17. BD (1) C 12 - O 14	/217. RY*(3) C 16	1.01	1.93	0.040
17. BD (1) C 12 - O 14	/274. BD*(1) C 2 - O 15	0.92	1.25	0.031
17. BD (1) C 12 - O 14	/282. BD*(1) C 12 - O 13	0.58	1.55	0.027
18. BD (1) O 14 - C 16	/147. RY*(1) C 12	1.59	1.80	0.048
18. BD (1) O 14 - C 16	/152. RY*(6) C 12	0.56	2.42	0.033
18. BD (1) O 14 - C 16	/273. BD*(1) C 2 - C 12	2.57	1.17	0.050
19. BD (1) C 16 - H 17	/182. RY*(2) O 14	0.58	1.29	0.024
19. BD (1) C 16 - H 17	/285. BD*(1) O 14 - C 16	0.72	0.78	0.021
20. BD (1) C 16 - H 18	/184. RY*(4) O 14	0.61	1.91	0.030
20. BD (1) C 16 - H 18	/284. BD*(1) C 12 - O 14	2.76	0.90	0.045
21. BD (1) C 16 - H 19	/182. RY*(2) O 14	0.58	1.29	0.024
21. BD (1) C 16 - H 19	/285. BD*(1) O 14 - C 16	0.72	0.78	0.021
22. CR (1) C 1	/ 96. RY*(2) C 4	0.59	10.75	0.071
22. CR (1) C 1	/ 97. RY*(3) C 4	0.60	11.22	0.073
22. CR (1) C 1	/271. BD*(1) C 1 - O 15	1.34	10.37	0.106
22. CR (1) C 1	/274. BD*(1) C 2 - O 15	0.95	10.41	0.089
23. CR (1) C 2	/148. RY*(2) C 12	0.57	11.92	0.073
23. CR (1) C 2	/153. RY*(7) C 12	0.73	11.28	0.081
23. CR (1) C 2	/271. BD*(1) C 1 - O 15	1.09	10.44	0.096
23. CR (1) C 2	/272. BD*(1) C 2 - H 11	0.53	10.53	0.067
23. CR (1) C 2	/275. BD*(1) C 2 - S 20	0.59	10.28	0.071
23. CR (1) C 2	/282. BD*(1) C 12 - O 13	0.65	10.76	0.075
24. CR (1) C 3	/ 97. RY*(3) C 4	0.70	11.20	0.079
24. CR (1) C 3	/279. BD*(1) C 3 - S 20	1.23	10.22	0.100
25. CR (1) C 4	/ 79. RY*(2) C 3	1.04	10.80	0.095
25. CR (1) C 4	/132. RY*(1) H 9	0.52	11.21	0.068
26. CR (1) C 12	/ 64. RY*(4) C 2	1.43	11.12	0.113
26. CR (1) C 12	/285. BD*(1) O 14 - C 16	1.21	10.44	0.101
27. CR (1) O 13	/147. RY*(1) C 12	6.90	19.83	0.332
27. CR (1) O 13	/273. BD*(1) C 2 - C 12	0.72	19.20	0.107
28. CR (1) O 14	/147. RY*(1) C 12	1.58	19.96	0.159
28. CR (1) O 14	/148. RY*(2) C 12	0.68	20.74	0.106
28. CR (1) O 14	/150. RY*(4) C 12	0.96	20.73	0.126
28. CR (1) O 14	/215. RY*(1) C 16	0.57	19.99	0.096
28. CR (1) O 14	/282. BD*(1) C 12 - O 13	0.56	19.59	0.094
29. CR (1) O 15	/ 45. RY*(2) C 1	1.19	19.90	0.138
29. CR (1) O 15	/ 61. RY*(1) C 2	2.41	19.71	0.195
30. CR (1) C 16	/238. RY*(2) H 18	0.51	12.11	0.070
30. CR (1) C 16	/284. BD*(1) C 12 - O 14	0.79	10.47	0.083
30. CR (1) C 16	/285. BD*(1) O 14 - C 16	1.86	10.35	0.124
32. CR (2) S 20	/ 65. RY*(5) C 2	0.65	9.99	0.072
36. LP (1) O 13	/147. RY*(1) C 12	16.43	1.69	0.149
36. LP (1) O 13	/150. RY*(4) C 12	0.52	2.46	0.032
36. LP (1) O 13	/161. RY*(15) C 12	0.64	2.91	0.039
36. LP (1) O 13	/273. BD*(1) C 2 - C 12	2.07	1.06	0.042
36. LP (1) O 13	/284. BD*(1) C 12 - O 14	1.53	1.08	0.037
37. LP (2) O 13	/148. RY*(2) C 12	3.07	2.04	0.073
37. LP (2) O 13	/150. RY*(4) C 12	1.28	2.03	0.047
37. LP (2) O 13	/273. BD*(1) C 2 - C 12	19.67	0.63	0.101
37. LP (2) O 13	/284. BD*(1) C 12 - O 14	31.33	0.65	0.129

37. LP (2) O 13	/287. BD*(1) C 16 - H 18	0.67	0.67	0.020
38. LP (1) O 14	/147. RY*(1) C 12	2.86	1.56	0.060
38. LP (1) O 14	/150. RY*(4) C 12	2.12	2.33	0.063
38. LP (1) O 14	/215. RY*(1) C 16	2.16	1.59	0.053
38. LP (1) O 14	/273. BD*(1) C 2 - C 12	0.71	0.93	0.023
38. LP (1) O 14	/274. BD*(1) C 2 - O 15	0.67	0.89	0.022
38. LP (1) O 14	/282. BD*(1) C 12 - O 13	8.21	1.18	0.088
38. LP (1) O 14	/286. BD*(1) C 16 - H 17	0.51	0.96	0.020
38. LP (1) O 14	/287. BD*(1) C 16 - H 18	2.22	0.97	0.042
39. LP (2) O 14	/149. RY*(3) C 12	2.81	1.91	0.069
39. LP (2) O 14	/216. RY*(2) C 16	1.29	1.44	0.041
39. LP (2) O 14	/217. RY*(3) C 16	0.71	1.32	0.029
39. LP (2) O 14	/283. BD*(2) C 12 - O 13	48.65	0.34	0.115
39. LP (2) O 14	/286. BD*(1) C 16 - H 17	4.32	0.72	0.053
39. LP (2) O 14	/288. BD*(1) C 16 - H 19	4.30	0.72	0.053
40. LP (1) O 15	/ 45. RY*(2) C 1	1.96	1.52	0.049
40. LP (1) O 15	/ 46. RY*(3) C 1	0.75	2.08	0.036
40. LP (1) O 15	/ 61. RY*(1) C 2	2.50	1.33	0.052
40. LP (1) O 15	/ 62. RY*(2) C 2	1.14	1.86	0.041
40. LP (1) O 15	/269. BD*(1) C 1 - H 5	1.51	0.94	0.034
40. LP (1) O 15	/270. BD*(1) C 1 - H 6	2.37	0.96	0.043
40. LP (1) O 15	/272. BD*(1) C 2 - H 11	2.14	0.94	0.040
40. LP (1) O 15	/273. BD*(1) C 2 - C 12	1.97	0.91	0.038
40. LP (1) O 15	/275. BD*(1) C 2 - S 20	0.86	0.68	0.022
41. LP (2) O 15	/ 45. RY*(2) C 1	0.72	1.28	0.028
41. LP (2) O 15	/ 46. RY*(3) C 1	0.87	1.84	0.037
41. LP (2) O 15	/ 62. RY*(2) C 2	0.52	1.62	0.027
41. LP (2) O 15	/ 63. RY*(3) C 2	1.81	1.89	0.053
41. LP (2) O 15	/268. BD*(1) C 1 - C 4	5.69	0.70	0.058
41. LP (2) O 15	/269. BD*(1) C 1 - H 5	4.01	0.70	0.048
41. LP (2) O 15	/272. BD*(1) C 2 - H 11	4.73	0.69	0.052
41. LP (2) O 15	/275. BD*(1) C 2 - S 20	14.09	0.44	0.071
41. LP (2) O 15	/281. BD*(1) C 4 - H 10	0.60	0.71	0.019
42. LP (1) S 20	/ 65. RY*(5) C 2	0.60	1.84	0.030
42. LP (1) S 20	/276. BD*(1) C 3 - C 4	0.58	1.03	0.022
43. LP (2) S 20	/ 61. RY*(1) C 2	0.81	1.01	0.026
43. LP (2) S 20	/ 79. RY*(2) C 3	0.55	1.01	0.021
43. LP (2) S 20	/272. BD*(1) C 2 - H 11	3.12	0.62	0.039
43. LP (2) S 20	/274. BD*(1) C 2 - O 15	6.48	0.55	0.054
43. LP (2) S 20	/276. BD*(1) C 3 - C 4	2.79	0.62	0.038
43. LP (2) S 20	/278. BD*(1) C 3 - H 8	4.11	0.63	0.046
43. LP (2) S 20	/281. BD*(1) C 4 - H 10	0.64	0.63	0.018
283. BD*(2) C 12 - O 13	/149. RY*(3) C 12	1.65	1.56	0.133
283. BD*(2) C 12 - O 13	/165. RY*(2) O 13	1.07	0.66	0.070
283. BD*(2) C 12 - O 13	/272. BD*(1) C 2 - H 11	0.59	0.37	0.036
283. BD*(2) C 12 - O 13	/275. BD*(1) C 2 - S 20	3.92	0.11	0.049
283. BD*(2) C 12 - O 13	/282. BD*(1) C 12 - O 13	0.88	0.60	0.058

4-ax



Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

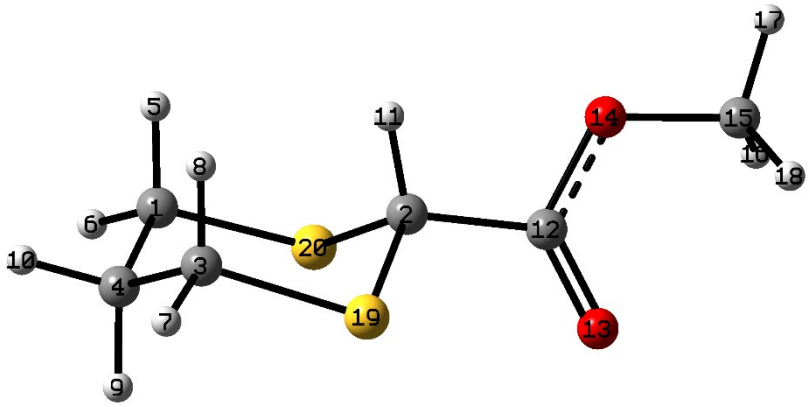
Threshold for printing: 0.50 kcal/mol

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) C 1 - C 4	/ 82. RY*(1) C 3	1.25	1.41	0.038
1. BD (1) C 1 - C 4	/278. BD*(1) C 1 - H 7	0.53	1.02	0.021
1. BD (1) C 1 - C 4	/284. BD*(1) C 3 - C 4	0.72	1.01	0.024
1. BD (1) C 1 - C 4	/285. BD*(1) C 3 - H 8	1.46	1.02	0.035
2. BD (1) C 1 - H 6	/234. RY*(1) S 19	0.61	1.02	0.022
2. BD (1) C 1 - H 6	/288. BD*(1) C 4 - H 10	2.70	0.91	0.044
3. BD (1) C 1 - H 7	/100. RY*(2) C 4	0.59	1.18	0.024
3. BD (1) C 1 - H 7	/235. RY*(2) S 19	0.79	1.35	0.029
3. BD (1) C 1 - H 7	/282. BD*(1) C 2 - S 19	1.69	0.65	0.030
3. BD (1) C 1 - H 7	/284. BD*(1) C 3 - C 4	3.13	0.89	0.047
4. BD (1) C 1 - S 19	/ 66. RY*(2) C 2	0.64	1.45	0.027
4. BD (1) C 1 - S 19	/ 99. RY*(1) C 4	1.02	1.29	0.033
4. BD (1) C 1 - S 19	/280. BD*(1) C 2 - H 5	1.31	0.98	0.032
4. BD (1) C 1 - S 19	/289. BD*(1) C 4 - H 11	1.96	0.98	0.039
5. BD (1) C 2 - H 5	/154. RY*(4) C 12	0.51	2.14	0.030
5. BD (1) C 2 - H 5	/235. RY*(2) S 19	0.54	1.38	0.025
5. BD (1) C 2 - H 5	/256. RY*(2) S 20	0.56	1.37	0.025
5. BD (1) C 2 - H 5	/279. BD*(1) C 1 - S 19	1.34	0.69	0.027
5. BD (1) C 2 - H 5	/287. BD*(1) C 3 - S 20	1.36	0.69	0.027
5. BD (1) C 2 - H 5	/290. BD*(1) C 12 - O 13	5.60	1.13	0.071
5. BD (1) C 2 - H 5	/292. BD*(1) C 12 - O 14	1.10	0.90	0.029
6. BD (1) C 2 - C 12	/168. RY*(1) O 13	1.24	1.44	0.038
6. BD (1) C 2 - C 12	/185. RY*(1) O 14	0.54	1.19	0.023
6. BD (1) C 2 - C 12	/290. BD*(1) C 12 - O 13	1.74	1.28	0.042
6. BD (1) C 2 - C 12	/293. BD*(1) O 14 - C 15	4.07	0.93	0.055
7. BD (1) C 2 - S 19	/ 48. RY*(1) C 1	0.89	1.39	0.032
7. BD (1) C 2 - S 19	/155. RY*(5) C 12	0.83	1.28	0.029
7. BD (1) C 2 - S 19	/278. BD*(1) C 1 - H 7	0.96	1.00	0.028
7. BD (1) C 2 - S 19	/291. BD*(2) C 12 - O 13	3.72	0.60	0.045
7. BD (1) C 2 - S 19	/292. BD*(1) C 12 - O 14	1.06	0.97	0.029
8. BD (1) C 2 - S 20	/ 82. RY*(1) C 3	0.89	1.40	0.032
8. BD (1) C 2 - S 20	/155. RY*(5) C 12	0.81	1.29	0.029
8. BD (1) C 2 - S 20	/285. BD*(1) C 3 - H 8	0.95	1.01	0.028
8. BD (1) C 2 - S 20	/291. BD*(2) C 12 - O 13	2.77	0.61	0.039
8. BD (1) C 2 - S 20	/292. BD*(1) C 12 - O 14	1.49	0.97	0.035
9. BD (1) C 3 - C 4	/ 48. RY*(1) C 1	1.25	1.41	0.038
9. BD (1) C 3 - C 4	/276. BD*(1) C 1 - C 4	0.72	1.01	0.024
9. BD (1) C 3 - C 4	/278. BD*(1) C 1 - H 7	1.46	1.02	0.035
9. BD (1) C 3 - C 4	/285. BD*(1) C 3 - H 8	0.53	1.02	0.021
10. BD (1) C 3 - H 8	/100. RY*(2) C 4	0.59	1.18	0.024

10. BD (1) C 3 - H 8	/256. RY*(2) S 20	0.79	1.35	0.029
10. BD (1) C 3 - H 8	/276. BD*(1) C 1 - C 4	3.14	0.89	0.047
10. BD (1) C 3 - H 8	/283. BD*(1) C 2 - S 20	1.70	0.65	0.030
11. BD (1) C 3 - H 9	/ 99. RY*(1) C 4	0.51	1.22	0.022
11. BD (1) C 3 - H 9	/255. RY*(1) S 20	0.61	1.02	0.022
11. BD (1) C 3 - H 9	/288. BD*(1) C 4 - H 10	2.70	0.91	0.044
12. BD (1) C 3 - S 20	/ 66. RY*(2) C 2	0.58	1.45	0.026
12. BD (1) C 3 - S 20	/ 99. RY*(1) C 4	1.01	1.29	0.032
12. BD (1) C 3 - S 20	/280. BD*(1) C 2 - H 5	1.32	0.98	0.032
12. BD (1) C 3 - S 20	/283. BD*(1) C 2 - S 20	0.50	0.72	0.017
12. BD (1) C 3 - S 20	/289. BD*(1) C 4 - H 11	1.96	0.98	0.039
13. BD (1) C 4 - H 10	/277. BD*(1) C 1 - H 6	2.76	0.89	0.044
13. BD (1) C 4 - H 10	/286. BD*(1) C 3 - H 9	2.76	0.90	0.044
14. BD (1) C 4 - H 11	/279. BD*(1) C 1 - S 19	5.50	0.64	0.053
14. BD (1) C 4 - H 11	/287. BD*(1) C 3 - S 20	5.50	0.64	0.053
15. BD (1) C 12 - O 13	/ 66. RY*(2) C 2	0.50	1.97	0.028
15. BD (1) C 12 - O 13	/151. RY*(1) C 12	1.71	1.96	0.052
15. BD (1) C 12 - O 13	/281. BD*(1) C 2 - C 12	1.77	1.45	0.046
16. BD (2) C 12 - O 13	/186. RY*(2) O 14	0.57	1.06	0.022
16. BD (2) C 12 - O 13	/282. BD*(1) C 2 - S 19	1.28	0.53	0.024
16. BD (2) C 12 - O 13	/283. BD*(1) C 2 - S 20	1.03	0.54	0.021
16. BD (2) C 12 - O 13	/291. BD*(2) C 12 - O 13	0.90	0.40	0.018
17. BD (1) C 12 - O 14	/ 66. RY*(2) C 2	0.61	1.81	0.030
17. BD (1) C 12 - O 14	/204. RY*(3) C 15	1.61	1.73	0.047
17. BD (1) C 12 - O 14	/282. BD*(1) C 2 - S 19	0.59	1.08	0.023
17. BD (1) C 12 - O 14	/283. BD*(1) C 2 - S 20	0.82	1.08	0.027
18. BD (1) O 14 - C 15	/151. RY*(1) C 12	1.66	1.68	0.047
18. BD (1) O 14 - C 15	/157. RY*(7) C 12	0.53	1.75	0.027
18. BD (1) O 14 - C 15	/281. BD*(1) C 2 - C 12	2.87	1.17	0.053
19. BD (1) C 15 - H 16	/292. BD*(1) C 12 - O 14	2.84	0.89	0.046
20. BD (1) C 15 - H 17	/186. RY*(2) O 14	0.64	1.19	0.025
20. BD (1) C 15 - H 17	/293. BD*(1) O 14 - C 15	0.72	0.78	0.021
21. BD (1) C 15 - H 18	/186. RY*(2) O 14	0.59	1.19	0.024
21. BD (1) C 15 - H 18	/293. BD*(1) O 14 - C 15	0.71	0.78	0.021
22. CR (1) C 1	/101. RY*(3) C 4	0.91	10.86	0.089
22. CR (1) C 1	/279. BD*(1) C 1 - S 19	1.28	10.22	0.103
23. CR (1) C 2	/116. RY*(1) H 5	0.60	11.39	0.074
23. CR (1) C 2	/152. RY*(2) C 12	0.77	11.91	0.086
23. CR (1) C 2	/157. RY*(7) C 12	0.72	11.07	0.079
23. CR (1) C 2	/280. BD*(1) C 2 - H 5	0.87	10.53	0.086
23. CR (1) C 2	/282. BD*(1) C 2 - S 19	0.50	10.27	0.065
23. CR (1) C 2	/283. BD*(1) C 2 - S 20	0.52	10.27	0.066
23. CR (1) C 2	/290. BD*(1) C 12 - O 13	0.82	10.73	0.084
24. CR (1) C 3	/101. RY*(3) C 4	0.88	10.86	0.087
24. CR (1) C 3	/287. BD*(1) C 3 - S 20	1.28	10.22	0.103
25. CR (1) C 4	/ 49. RY*(2) C 1	1.02	10.81	0.094
25. CR (1) C 4	/ 83. RY*(2) C 3	1.01	10.82	0.093
26. CR (1) C 12	/ 65. RY*(1) C 2	1.45	10.89	0.112
26. CR (1) C 12	/293. BD*(1) O 14 - C 15	1.19	10.44	0.100
27. CR (1) O 13	/151. RY*(1) C 12	7.17	19.71	0.337
27. CR (1) O 13	/281. BD*(1) C 2 - C 12	0.71	19.20	0.106
28. CR (1) O 14	/151. RY*(1) C 12	1.58	19.84	0.159
28. CR (1) O 14	/152. RY*(2) C 12	0.66	20.76	0.105
28. CR (1) O 14	/154. RY*(4) C 12	1.04	20.58	0.131
28. CR (1) O 14	/202. RY*(1) C 15	0.55	19.99	0.094
28. CR (1) O 14	/204. RY*(3) C 15	0.64	19.76	0.100
28. CR (1) O 14	/290. BD*(1) C 12 - O 13	0.54	19.57	0.092
29. CR (1) C 15	/292. BD*(1) C 12 - O 14	0.84	10.46	0.086
29. CR (1) C 15	/293. BD*(1) O 14 - C 15	1.85	10.35	0.124
31. CR (2) S 19	/ 67. RY*(3) C 2	1.20	9.44	0.095
31. CR (2) S 19	/283. BD*(1) C 2 - S 20	0.52	8.93	0.062
36. CR (2) S 20	/ 67. RY*(3) C 2	1.06	9.44	0.089
36. CR (2) S 20	/282. BD*(1) C 2 - S 19	0.53	8.93	0.062
40. LP (1) O 13	/151. RY*(1) C 12	17.27	1.57	0.147
40. LP (1) O 13	/152. RY*(2) C 12	0.54	2.49	0.033
40. LP (1) O 13	/154. RY*(4) C 12	0.61	2.31	0.034
40. LP (1) O 13	/167. RY*(17) C 12	0.88	5.84	0.064
40. LP (1) O 13	/281. BD*(1) C 2 - C 12	2.33	1.06	0.045
40. LP (1) O 13	/292. BD*(1) C 12 - O 14	1.31	1.07	0.034
41. LP (2) O 13	/152. RY*(2) C 12	2.85	2.06	0.071
41. LP (2) O 13	/154. RY*(4) C 12	1.23	1.88	0.045
41. LP (2) O 13	/281. BD*(1) C 2 - C 12	18.25	0.63	0.097
41. LP (2) O 13	/292. BD*(1) C 12 - O 14	31.55	0.64	0.129
41. LP (2) O 13	/294. BD*(1) C 15 - H 16	0.69	0.67	0.020

42. LP (1) O 14	/151. RY*(1) C 12	3.19	1.44	0.061
42. LP (1) O 14	/154. RY*(4) C 12	2.21	2.18	0.062
42. LP (1) O 14	/202. RY*(1) C 15	2.10	1.59	0.052
42. LP (1) O 14	/290. BD*(1) C 12 - O 13	8.23	1.17	0.088
42. LP (1) O 14	/294. BD*(1) C 15 - H 16	2.22	0.97	0.042
42. LP (1) O 14	/295. BD*(1) C 15 - H 17	0.52	0.96	0.020
43. LP (2) O 14	/153. RY*(3) C 12	2.82	1.94	0.070
43. LP (2) O 14	/203. RY*(2) C 15	1.80	1.54	0.050
43. LP (2) O 14	/291. BD*(2) C 12 - O 13	49.72	0.33	0.116
43. LP (2) O 14	/295. BD*(1) C 15 - H 17	4.26	0.72	0.052
43. LP (2) O 14	/296. BD*(1) C 15 - H 18	4.37	0.72	0.053
44. LP (1) S 19	/ 67. RY*(3) C 2	0.78	1.29	0.029
44. LP (1) S 19	/276. BD*(1) C 1 - C 4	0.75	1.03	0.025
44. LP (1) S 19	/283. BD*(1) C 2 - S 20	2.13	0.78	0.037
45. LP (2) S 19	/ 65. RY*(1) C 2	0.58	0.93	0.021
45. LP (2) S 19	/276. BD*(1) C 1 - C 4	3.16	0.63	0.040
45. LP (2) S 19	/277. BD*(1) C 1 - H 6	3.97	0.65	0.046
45. LP (2) S 19	/281. BD*(1) C 2 - C 12	4.54	0.59	0.046
45. LP (2) S 19	/283. BD*(1) C 2 - S 20	4.77	0.38	0.038
45. LP (2) S 19	/289. BD*(1) C 4 - H 11	0.62	0.64	0.018
45. LP (2) S 19	/291. BD*(2) C 12 - O 13	1.81	0.24	0.019
46. LP (1) S 20	/ 67. RY*(3) C 2	0.64	1.29	0.026
46. LP (1) S 20	/281. BD*(1) C 2 - C 12	0.62	0.99	0.023
46. LP (1) S 20	/282. BD*(1) C 2 - S 19	2.10	0.78	0.036
46. LP (1) S 20	/284. BD*(1) C 3 - C 4	0.73	1.03	0.024
47. LP (2) S 20	/ 65. RY*(1) C 2	0.58	0.93	0.021
47. LP (2) S 20	/281. BD*(1) C 2 - C 12	4.74	0.59	0.047
47. LP (2) S 20	/282. BD*(1) C 2 - S 19	5.07	0.38	0.039
47. LP (2) S 20	/284. BD*(1) C 3 - C 4	3.18	0.63	0.041
47. LP (2) S 20	/286. BD*(1) C 3 - H 9	3.96	0.65	0.046
47. LP (2) S 20	/289. BD*(1) C 4 - H 11	0.62	0.64	0.018
47. LP (2) S 20	/291. BD*(2) C 12 - O 13	1.19	0.24	0.016
291. BD*(2) C 12 - O 13	/153. RY*(3) C 12	1.86	1.61	0.135
291. BD*(2) C 12 - O 13	/169. RY*(2) O 13	1.98	0.52	0.080
291. BD*(2) C 12 - O 13	/282. BD*(1) C 2 - S 19	3.42	0.14	0.050
291. BD*(2) C 12 - O 13	/283. BD*(1) C 2 - S 20	2.99	0.14	0.047

4-eq



Second Order Perturbation Theory Analysis of Fock Matrix in NBO Basis

Threshold for printing: 0.50 kcal/mol

Donor NBO (i)	Acceptor NBO (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
within unit 1				
1. BD (1) C 1 - C 4	/ 82. RY*(1) C 3	1.01	1.41	0.034
1. BD (1) C 1 - C 4	/278. BD*(1) C 1 - H 6	0.55	1.03	0.021
1. BD (1) C 1 - C 4	/284. BD*(1) C 3 - C 4	0.72	1.01	0.024
1. BD (1) C 1 - C 4	/285. BD*(1) C 3 - H 7	1.45	1.03	0.034
2. BD (1) C 1 - H 5	/ 99. RY*(1) C 4	0.52	1.20	0.022
2. BD (1) C 1 - H 5	/255. RY*(1) S 20	0.57	1.03	0.022
2. BD (1) C 1 - H 5	/288. BD*(1) C 4 - H 9	2.66	0.92	0.044
3. BD (1) C 1 - H 6	/100. RY*(2) C 4	0.58	1.17	0.023

3. BD (1) C 1 - H 6	/256. RY*(2) S 20	0.76	1.33	0.028
3. BD (1) C 1 - H 6	/283. BD*(1) C 2 - S 20	1.34	0.64	0.026
3. BD (1) C 1 - H 6	/284. BD*(1) C 3 - C 4	3.17	0.89	0.048
4. BD (1) C 1 - S 20	/ 67. RY*(3) C 2	0.99	1.68	0.037
4. BD (1) C 1 - S 20	/ 99. RY*(1) C 4	1.06	1.27	0.033
4. BD (1) C 1 - S 20	/281. BD*(1) C 2 - C 12	1.46	0.93	0.033
4. BD (1) C 1 - S 20	/289. BD*(1) C 4 - H 10	1.93	0.98	0.039
5. BD (1) C 2 - H 11	/154. RY*(4) C 12	0.57	2.15	0.031
5. BD (1) C 2 - H 11	/290. BD*(1) C 12 - O 13	5.23	1.14	0.069
5. BD (1) C 2 - H 11	/292. BD*(1) C 12 - O 14	1.05	0.91	0.028
6. BD (1) C 2 - C 12	/168. RY*(1) O 13	1.17	1.40	0.036
6. BD (1) C 2 - C 12	/186. RY*(2) O 14	0.81	1.33	0.030
6. BD (1) C 2 - C 12	/290. BD*(1) C 12 - O 13	1.86	1.29	0.044
6. BD (1) C 2 - C 12	/293. BD*(1) O 14 - C 15	4.08	0.93	0.055
7. BD (1) C 2 - S 19	/ 82. RY*(1) C 3	1.33	1.38	0.038
7. BD (1) C 2 - S 19	/155. RY*(5) C 12	0.82	1.40	0.030
7. BD (1) C 2 - S 19	/285. BD*(1) C 3 - H 7	1.10	1.00	0.030
7. BD (1) C 2 - S 19	/291. BD*(2) C 12 - O 13	3.05	0.60	0.040
7. BD (1) C 2 - S 19	/292. BD*(1) C 12 - O 14	1.73	0.97	0.037
8. BD (1) C 2 - S 20	/ 48. RY*(1) C 1	1.32	1.38	0.038
8. BD (1) C 2 - S 20	/155. RY*(5) C 12	1.06	1.39	0.034
8. BD (1) C 2 - S 20	/278. BD*(1) C 1 - H 6	1.10	1.00	0.030
8. BD (1) C 2 - S 20	/291. BD*(2) C 12 - O 13	4.08	0.59	0.046
8. BD (1) C 2 - S 20	/292. BD*(1) C 12 - O 14	1.05	0.96	0.029
9. BD (1) C 3 - C 4	/ 48. RY*(1) C 1	1.00	1.41	0.034
9. BD (1) C 3 - C 4	/276. BD*(1) C 1 - C 4	0.72	1.01	0.024
9. BD (1) C 3 - C 4	/278. BD*(1) C 1 - H 6	1.45	1.03	0.034
9. BD (1) C 3 - C 4	/285. BD*(1) C 3 - H 7	0.56	1.03	0.021
10. BD (1) C 3 - H 7	/100. RY*(2) C 4	0.58	1.17	0.023
10. BD (1) C 3 - H 7	/235. RY*(2) S 19	0.75	1.32	0.028
10. BD (1) C 3 - H 7	/276. BD*(1) C 1 - C 4	3.18	0.89	0.048
10. BD (1) C 3 - H 7	/282. BD*(1) C 2 - S 19	1.34	0.65	0.026
11. BD (1) C 3 - H 8	/ 99. RY*(1) C 4	0.52	1.20	0.022
11. BD (1) C 3 - H 8	/234. RY*(1) S 19	0.58	1.03	0.022
11. BD (1) C 3 - H 8	/288. BD*(1) C 4 - H 9	2.67	0.92	0.044
12. BD (1) C 3 - S 19	/ 67. RY*(3) C 2	0.96	1.68	0.036
12. BD (1) C 3 - S 19	/ 99. RY*(1) C 4	1.06	1.27	0.033
12. BD (1) C 3 - S 19	/281. BD*(1) C 2 - C 12	1.51	0.93	0.034
12. BD (1) C 3 - S 19	/289. BD*(1) C 4 - H 10	1.94	0.98	0.039
13. BD (1) C 4 - H 9	/277. BD*(1) C 1 - H 5	2.84	0.88	0.045
13. BD (1) C 4 - H 9	/286. BD*(1) C 3 - H 8	2.85	0.88	0.045
14. BD (1) C 4 - H 10	/279. BD*(1) C 1 - S 20	5.48	0.64	0.053
14. BD (1) C 4 - H 10	/287. BD*(1) C 3 - S 19	5.46	0.64	0.053
15. BD (1) C 12 - O 13	/151. RY*(1) C 12	1.64	2.00	0.051
15. BD (1) C 12 - O 13	/281. BD*(1) C 2 - C 12	1.81	1.46	0.047
16. BD (2) C 12 - O 13	/282. BD*(1) C 2 - S 19	0.83	0.54	0.019
16. BD (2) C 12 - O 13	/283. BD*(1) C 2 - S 20	1.20	0.53	0.023
16. BD (2) C 12 - O 13	/291. BD*(2) C 12 - O 13	0.79	0.40	0.017
17. BD (1) C 12 - O 14	/204. RY*(3) C 15	1.68	1.72	0.048
17. BD (1) C 12 - O 14	/282. BD*(1) C 2 - S 19	0.81	1.08	0.027
17. BD (1) C 12 - O 14	/283. BD*(1) C 2 - S 20	0.56	1.08	0.022
18. BD (1) O 14 - C 15	/151. RY*(1) C 12	1.63	1.71	0.047
18. BD (1) O 14 - C 15	/281. BD*(1) C 2 - C 12	2.87	1.17	0.052
19. BD (1) C 15 - H 16	/293. BD*(1) O 14 - C 15	0.73	0.77	0.021
20. BD (1) C 15 - H 17	/188. RY*(4) O 14	0.60	1.82	0.030
20. BD (1) C 15 - H 17	/292. BD*(1) C 12 - O 14	2.80	0.89	0.046
21. BD (1) C 15 - H 18	/185. RY*(1) O 14	0.60	1.03	0.022
21. BD (1) C 15 - H 18	/293. BD*(1) O 14 - C 15	0.73	0.77	0.021
22. CR (1) C 1	/101. RY*(3) C 4	0.89	10.84	0.088
22. CR (1) C 1	/279. BD*(1) C 1 - S 20	1.27	10.23	0.102
23. CR (1) C 2	/146. RY*(1) H 11	0.53	11.17	0.068
23. CR (1) C 2	/152. RY*(2) C 12	0.63	11.88	0.077
23. CR (1) C 2	/157. RY*(7) C 12	0.81	10.93	0.084
23. CR (1) C 2	/280. BD*(1) C 2 - H 11	0.63	10.53	0.073
23. CR (1) C 2	/282. BD*(1) C 2 - S 19	0.55	10.27	0.068
23. CR (1) C 2	/283. BD*(1) C 2 - S 20	0.55	10.26	0.068
23. CR (1) C 2	/290. BD*(1) C 12 - O 13	0.78	10.73	0.082
24. CR (1) C 3	/101. RY*(3) C 4	0.90	10.84	0.088
24. CR (1) C 3	/287. BD*(1) C 3 - S 19	1.26	10.23	0.102
25. CR (1) C 4	/ 49. RY*(2) C 1	1.00	10.77	0.093
25. CR (1) C 4	/ 83. RY*(2) C 3	1.00	10.77	0.092
26. CR (1) C 12	/ 68. RY*(4) C 2	1.47	10.99	0.114
26. CR (1) C 12	/293. BD*(1) O 14 - C 15	1.20	10.44	0.100
27. CR (1) O 13	/151. RY*(1) C 12	7.07	19.74	0.335

27. CR (1) O 13	/281. BD*(1) C 2 - C 12	0.70	19.21	0.105
28. CR (1) O 14	/151. RY*(1) C 12	1.55	19.87	0.157
28. CR (1) O 14	/152. RY*(2) C 12	0.68	20.73	0.106
28. CR (1) O 14	/154. RY*(4) C 12	1.11	20.59	0.135
28. CR (1) O 14	/202. RY*(1) C 15	0.56	20.00	0.095
28. CR (1) O 14	/204. RY*(3) C 15	0.60	19.75	0.097
28. CR (1) O 14	/290. BD*(1) C 12 - O 13	0.55	19.58	0.093
29. CR (1) C 15	/292. BD*(1) C 12 - O 14	0.81	10.47	0.084
29. CR (1) C 15	/293. BD*(1) O 14 - C 15	1.87	10.35	0.125
31. CR (2) S 19	/ 65. RY*(1) C 2	0.81	9.55	0.079
31. CR (2) S 19	/ 66. RY*(2) C 2	0.64	9.41	0.069
36. CR (2) S 20	/ 66. RY*(2) C 2	1.38	9.41	0.102
40. LP (1) O 13	/151. RY*(1) C 12	17.14	1.60	0.148
40. LP (1) O 13	/154. RY*(4) C 12	0.62	2.32	0.034
40. LP (1) O 13	/167. RY*(17) C 12	1.31	3.32	0.059
40. LP (1) O 13	/281. BD*(1) C 2 - C 12	2.14	1.06	0.043
40. LP (1) O 13	/292. BD*(1) C 12 - O 14	1.39	1.08	0.035
41. LP (2) O 13	/152. RY*(2) C 12	3.06	2.03	0.073
41. LP (2) O 13	/154. RY*(4) C 12	1.20	1.89	0.044
41. LP (2) O 13	/281. BD*(1) C 2 - C 12	18.38	0.63	0.098
41. LP (2) O 13	/292. BD*(1) C 12 - O 14	31.59	0.65	0.129
41. LP (2) O 13	/295. BD*(1) C 15 - H 17	0.70	0.68	0.020
42. LP (1) O 14	/151. RY*(1) C 12	3.15	1.47	0.061
42. LP (1) O 14	/154. RY*(4) C 12	2.32	2.19	0.064
42. LP (1) O 14	/202. RY*(1) C 15	2.09	1.60	0.052
42. LP (1) O 14	/281. BD*(1) C 2 - C 12	0.51	0.93	0.020
42. LP (1) O 14	/290. BD*(1) C 12 - O 13	8.27	1.18	0.088
42. LP (1) O 14	/295. BD*(1) C 15 - H 17	2.20	0.97	0.042
43. LP (2) O 14	/153. RY*(3) C 12	3.01	1.93	0.072
43. LP (2) O 14	/160. RY*(10) C 12	0.51	1.84	0.029
43. LP (2) O 14	/203. RY*(2) C 15	1.77	1.54	0.049
43. LP (2) O 14	/291. BD*(2) C 12 - O 13	50.44	0.33	0.116
43. LP (2) O 14	/294. BD*(1) C 15 - H 16	4.24	0.72	0.052
43. LP (2) O 14	/296. BD*(1) C 15 - H 18	4.28	0.72	0.053
44. LP (1) S 19	/280. BD*(1) C 2 - H 11	0.76	1.03	0.025
44. LP (1) S 19	/283. BD*(1) C 2 - S 20	1.13	0.77	0.027
44. LP (1) S 19	/286. BD*(1) C 3 - H 8	0.67	1.03	0.024
45. LP (2) S 19	/ 66. RY*(2) C 2	0.52	0.85	0.019
45. LP (2) S 19	/ 83. RY*(2) C 3	0.59	0.98	0.022
45. LP (2) S 19	/280. BD*(1) C 2 - H 11	3.24	0.64	0.041
45. LP (2) S 19	/283. BD*(1) C 2 - S 20	7.09	0.38	0.046
45. LP (2) S 19	/284. BD*(1) C 3 - C 4	3.70	0.63	0.044
45. LP (2) S 19	/286. BD*(1) C 3 - H 8	3.53	0.64	0.043
45. LP (2) S 19	/289. BD*(1) C 4 - H 10	0.65	0.64	0.018
46. LP (1) S 20	/ 66. RY*(2) C 2	0.52	1.25	0.023
46. LP (1) S 20	/277. BD*(1) C 1 - H 5	0.67	1.03	0.024
46. LP (1) S 20	/280. BD*(1) C 2 - H 11	0.72	1.04	0.025
46. LP (1) S 20	/282. BD*(1) C 2 - S 19	1.10	0.78	0.026
47. LP (2) S 20	/ 49. RY*(2) C 1	0.58	0.98	0.022
47. LP (2) S 20	/276. BD*(1) C 1 - C 4	3.70	0.63	0.044
47. LP (2) S 20	/277. BD*(1) C 1 - H 5	3.50	0.64	0.043
47. LP (2) S 20	/280. BD*(1) C 2 - H 11	3.16	0.64	0.041
47. LP (2) S 20	/282. BD*(1) C 2 - S 19	6.90	0.38	0.046
47. LP (2) S 20	/289. BD*(1) C 4 - H 10	0.65	0.64	0.018
291. BD*(2) C 12 - O 13	/153. RY*(3) C 12	1.63	1.59	0.131
291. BD*(2) C 12 - O 13	/160. RY*(10) C 12	0.68	1.51	0.083
291. BD*(2) C 12 - O 13	/169. RY*(2) O 13	0.74	0.89	0.066
291. BD*(2) C 12 - O 13	/282. BD*(1) C 2 - S 19	2.46	0.14	0.044
291. BD*(2) C 12 - O 13	/283. BD*(1) C 2 - S 20	3.13	0.14	0.048

Table S4: Dipole moment of the compounds 1-4 optimized at CBS-QB3 level.

	Dipole Moment (debye)		Dipole Moment (debye)
1-ax	2.4	**1-eq**	2.4
2-ax	3.4	**2-eq**	4.7
3-ax	1.4	**3-eq**	4.5
4-ax	1.4	**4-eq**	3.7

Table S5: Cartesian Co-ordinates of optimization at CBS-QB3 method with SMD(chloroform) solvation model:

1-ax

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.398203	1.431121	-0.562750
6	0.107024	-0.126004	1.003598
6	1.960059	-1.041985	-0.509026
6	2.506942	0.379185	-0.704260
1	-0.272418	-0.177379	2.031815
1	0.679568	1.316825	-1.384990
1	1.815674	2.439146	-0.654737
1	2.777598	-1.769565	-0.547088
1	1.283231	-1.287665	-1.334020
1	3.285351	0.576226	0.044973
1	2.987888	0.465855	-1.684285
6	-1.111188	-0.419164	0.135763
8	-1.275525	-1.402847	-0.549894
8	-2.044626	0.546555	0.253745
6	-3.266337	0.347241	-0.485477
1	-3.887818	1.211838	-0.260235
1	-3.064019	0.296792	-1.556700
1	-3.763763	-0.570005	-0.165542
6	0.667808	1.298486	0.780639
1	1.372722	1.509378	1.593244
1	-0.136875	2.031968	0.859465
6	1.204578	-1.189058	0.821131
1	0.769145	-2.188288	0.897974
1	1.912393	-1.083733	1.651611

1-eq

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.381455	-1.045966	-0.524781
6	-0.055191	-0.049176	-0.332624
6	-2.107042	1.411822	0.035832
6	-2.969280	0.156668	0.225794
1	-2.439884	-0.861990	-1.605378
1	-2.978094	-1.942714	-0.328815
1	-2.509145	2.242144	0.625478
1	-2.146667	1.724962	-1.015347
1	-3.029794	-0.080188	1.295773
1	-3.993225	0.348563	-0.111176
1	-0.023021	0.207427	-1.396580
6	1.371572	-0.276381	0.122383
8	1.711218	-0.972423	1.052764
8	2.245358	0.432571	-0.620638
6	3.631982	0.345339	-0.231936
1	3.982488	-0.686574	-0.286354
1	4.173320	0.965713	-0.943624
1	3.771654	0.724147	0.782129
6	-0.920757	-1.303730	-0.130868
1	-0.866580	-1.603228	0.921036
1	-0.511329	-2.134109	-0.715249
6	-0.645869	1.161750	0.432205
1	-0.040426	2.051914	0.236481
1	-0.585667	0.960793	1.508583

2-ax

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.262442	1.424046	-0.411442
6	0.224482	-0.179691	0.987941
6	1.839421	-0.985594	-0.553974
6	2.380929	0.431764	-0.711578
1	-0.064046	-0.308718	2.034221
1	0.483533	1.382062	-1.185917
1	1.626455	2.449975	-0.353829
1	2.632814	-1.732740	-0.580422
1	1.118205	-1.220801	-1.345200
1	3.204248	0.591045	-0.008819
1	2.760864	0.581420	-1.726912
6	-1.054859	-0.446192	0.145834
8	-1.303719	-1.489367	-0.406166
8	-1.880056	0.605537	0.185447
8	0.684169	1.143344	0.875419
8	1.210118	-1.138918	0.733970
6	-3.157637	0.434213	-0.468899
1	-3.679557	1.379645	-0.338648

2-eq

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.916412	1.399809	0.110017
6	0.135237	-0.060134	-0.348894
6	2.276842	-0.988403	-0.476569
6	2.837326	0.198198	0.302756
1	1.958475	1.761466	-0.927552
1	2.171456	2.225607	0.774444
1	2.797272	-1.916978	-0.242167
1	2.350819	-0.812504	-1.559588
1	2.884803	-0.055783	1.365657
1	3.849351	0.434841	-0.040093
1	0.164563	0.213461	-1.416953
6	-1.308403	-0.354784	0.069007
8	-1.656492	-1.262450	0.777707
8	-2.126333	0.559238	-0.465340
8	0.560267	1.039309	0.428152
8	0.899466	-1.208260	-0.125769
6	-3.523413	0.444819	-0.115275
1	-3.655208	0.551131	0.962410

1	-3.017818	0.219576	-1.529248	1	-4.021286	1.257269	-0.639921
1	-3.717459	-0.377516	-0.001877	1	-3.919516	-0.518240	-0.440492

3-ax

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.752959	0.799084	1.045295
6	0.043320	0.023075	-0.934919
6	-1.695592	-1.465180	-0.090122
6	-2.572832	-0.361817	0.487060
1	0.449711	0.314854	-1.902596
1	-1.104726	0.477081	1.863780
1	-2.394118	1.599805	1.418225
1	-2.309137	-2.247818	-0.537505
1	-1.071136	-1.911416	0.686675
1	-3.259225	0.007321	-0.280980
1	-3.175012	-0.797316	1.292555
6	1.208994	-0.366935	-0.025459
8	1.151582	-1.130168	0.910659
8	2.322484	0.272497	-0.407041
8	-0.861024	-1.011519	-1.180083
6	3.492843	0.068999	0.416260
1	4.280895	0.653939	-0.052620
1	3.308145	0.423834	1.431384
1	3.763518	-0.987366	0.437967
16	-0.733494	1.577328	-0.270866

3-eq

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.070477	1.353013	0.420001
6	0.017930	0.244585	0.361780
6	-2.336626	-1.155502	0.170638
6	-2.898747	0.221115	-0.178935
1	-2.067330	1.292770	1.518110
1	-2.472516	2.324562	0.131839
1	-2.890314	-1.952420	-0.328827
1	-2.382368	-1.338167	1.247947
1	-2.942271	0.341352	-1.265087
1	-3.921609	0.299371	0.207019
1	-0.026518	0.125395	1.451547
6	1.469349	0.447031	-0.059882
8	1.855033	1.307027	-0.807121
8	2.253334	-0.467390	0.526588
8	-0.716826	1.350216	-0.056881
6	3.659219	-0.406532	0.196692
1	4.077771	0.555803	0.494529
1	4.122915	-1.213098	0.760046
1	3.805858	-0.556923	-0.873716
16	-0.592489	-1.351233	-0.381616

4-ax

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.638527	1.334427	0.751996
6	0.219148	-0.047302	-0.878068
6	-1.791216	-1.227015	0.740146
6	-2.543208	0.102789	0.768802
1	0.664260	-0.067828	-1.871883
1	-0.940816	1.325965	1.590730
1	-2.234208	2.247722	0.816948
1	-2.492604	-2.063077	0.784513
1	-1.105313	-1.312991	1.583487
1	-3.254612	0.149691	-0.060984
1	-3.124191	0.132636	1.698805
6	1.329795	-0.083182	0.159377
8	1.172445	-0.165052	1.356300
8	2.527905	0.003844	-0.434402
6	3.677725	0.010915	0.442499
1	4.538670	0.130188	-0.211298
1	3.614245	0.841854	1.146221
1	3.742064	-0.930459	0.990229
16	-0.682451	1.549615	-0.800898
16	-0.850836	-1.531355	-0.808506

4-eq

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.298249	1.285744	0.180029
6	0.118795	-0.000103	0.542759
6	-2.298343	-1.285631	0.180027
6	-2.903909	0.000080	-0.384350
1	-2.407934	1.329600	1.267402
1	-2.801547	2.160355	-0.237140
1	-2.801730	-2.160204	-0.237111
1	-2.408004	-1.329455	1.267404
1	-2.826839	0.000081	-1.475162
1	-3.971907	0.000115	-0.132559
1	-0.183362	-0.000033	1.589269
6	1.637989	-0.000080	0.537236
8	2.305554	0.000030	1.542612
8	2.133837	-0.000154	-0.703429
6	3.575562	0.000086	-0.818107
1	3.992324	-0.892991	-0.350889
1	3.778094	0.000701	-1.886525
1	3.992114	0.892670	-0.349789
16	-0.527165	-1.535481	-0.237311
16	-0.527047	1.535454	-0.237309

Table S6: Cartesian Co-ordinates of optimization at B3LYP/6-311+G(d,p)/SMD(chloroform):

1-ax

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.026984	-1.726036	0.027972
6	-0.722543	0.800855	0.281205
6	-2.986096	-0.300057	0.777024
6	-2.299308	-1.668712	0.885017
1	-0.018164	1.539450	0.684238
1	-1.298938	-1.654507	-1.033651
1	-0.525369	-2.691148	0.155306
1	-3.847323	-0.255878	1.452046
1	-3.377651	-0.169072	-0.237395
1	-2.034129	-1.862727	1.932961
1	-2.992605	-2.461988	0.586000
6	-0.939292	1.237780	-1.162222
8	-1.973192	1.663370	-1.630090
8	0.196312	1.143935	-1.882875
6	0.128744	1.567368	-3.260389
1	1.132686	1.425868	-3.656464
1	-0.585405	0.956600	-3.814976
1	-0.158594	2.617902	-3.326069
6	-2.023353	0.852884	1.103107
1	-2.521618	1.814436	0.955990
1	-1.744777	0.798156	2.162166
6	-0.057214	-0.592077	0.388103
1	0.275469	-0.720296	1.424769
1	0.836545	-0.630867	-0.237900

1-eq

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.069589	-1.709369	0.616602
6	-0.250682	-0.247275	-0.373329
6	-2.390336	0.803659	0.514014
6	-2.707441	-0.484251	1.285578
1	-2.545137	-1.879126	-0.358191
1	-2.256740	-2.607332	1.214411
1	-2.798929	1.672526	1.040629
1	-2.882658	0.771643	-0.466567
1	-2.326351	-0.393620	2.311032
1	-3.791407	-0.618254	1.364545
1	-0.683215	-0.329291	-1.376314
6	1.238031	-0.027383	-0.542635
8	2.098749	-0.368785	0.240249
8	1.511703	0.640378	-1.681819
6	2.895854	0.969438	-1.925727
1	3.494516	0.061783	-2.017211
1	2.902338	1.520466	-2.864250
1	3.290952	1.590237	-1.120216
6	-0.557905	-1.527632	0.420346
1	-0.062646	-1.469809	1.395518
1	-0.135598	-2.395806	-0.095955
6	-0.880335	0.991532	0.313113
1	-0.686450	1.886549	-0.285317
1	-0.395660	1.141060	1.285518

2-ax

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.946109	-1.480990	-0.156235
6	-0.350962	0.234300	0.218029
6	-2.503134	0.523006	1.198453
6	-2.773527	-0.966132	1.015660
1	0.703240	0.347855	0.483512
1	-2.300971	-1.056674	-1.105927
1	-1.975645	-2.567533	-0.237953
1	-2.918205	0.903666	2.131690
1	-2.924233	1.105299	0.371456
1	-2.497757	-1.509157	1.924735
1	-3.838681	-1.132594	0.827662
6	-0.560021	1.053131	-1.089962
8	-1.077561	2.143109	-1.141766
8	-0.010174	0.427589	-2.134259
8	-0.558367	-1.143813	0.033070
8	-1.082842	0.768922	1.283095
6	-0.034838	1.132468	-3.397597
1	0.458165	0.470577	-4.106197

2-eq

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-1.942415	-1.650765	0.815799
6	-0.409479	-0.409036	-0.455440
6	-2.287261	0.765700	0.318945
6	-2.565467	-0.351996	1.319470
1	-2.467945	-2.018218	-0.076406
1	-1.955898	-2.434410	1.573326
1	-2.553900	1.746413	0.712644
1	-2.840081	0.603528	-0.616697
1	-2.134879	-0.090672	2.290421
1	-3.644894	-0.479649	1.448289
1	-0.942064	-0.674418	-1.381125
6	1.077008	-0.264568	-0.794953
8	1.510530	-0.423911	-1.913363
8	1.807556	0.049923	0.269211
8	-0.553612	-1.442279	0.488163
8	-0.877364	0.827880	0.024225
6	3.229966	0.208036	0.056717
1	3.418421	1.010204	-0.657836

1	-1.063377	1.322081	-3.707128	1	3.638671	0.464125	1.031585
1	0.506969	2.075554	-3.314727	1	3.664228	-0.724495	-0.305873

3-ax

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.404509	-1.657629	-0.012590
6	-0.303087	0.174896	0.005229
6	-2.383767	0.548994	1.234729
6	-2.811788	-0.912607	1.256053
1	0.765611	0.268679	0.194367
1	-2.871012	-1.224985	-0.900852
1	-2.682277	-2.711864	0.035602
1	-2.627973	1.034792	2.179842
1	-2.880381	1.088502	0.425673
1	-2.390238	-1.413762	2.132791
1	-3.903418	-0.938160	1.351682
6	-0.619917	0.881647	-1.313263
8	-1.689291	1.357199	-1.622199
8	0.463249	0.893362	-2.101132
8	-0.950447	0.720303	1.116213
6	0.296703	1.450750	-3.424995
1	1.263413	1.336121	-3.910446
1	-0.471253	0.902773	-3.972595
1	0.026466	2.505462	-3.360684
16	-0.574115	-1.653808	-0.217813

3-eq

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.200808	-1.581085	0.169896
6	-0.170218	-0.379513	-0.039436
6	-2.407594	0.790799	1.044026
6	-2.852987	-0.661608	1.196432
1	-2.478776	-1.283920	-0.851257
1	-2.508366	-2.616050	0.321572
1	-2.823131	1.420862	1.832156
1	-2.722734	1.203297	0.081418
1	-2.623980	-1.019490	2.204270
1	-3.939485	-0.717308	1.062557
1	-0.498436	-0.023884	-1.023231
6	1.343146	-0.564242	-0.049864
8	1.930015	-1.485953	0.458226
8	1.928290	0.448667	-0.700389
8	-0.766731	-1.597007	0.278841
6	3.374552	0.442235	-0.742690
1	3.734990	-0.453328	-1.249949
1	3.649573	1.333296	-1.302694
1	3.781738	0.487818	0.268168
16	-0.577937	0.967810	1.189049

4-ax

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.472774	-1.634881	0.067975
6	-0.145867	-0.016251	-0.150298
6	-2.504561	0.605313	1.317925
6	-2.880000	-0.875312	1.329354
1	0.940391	-0.043255	-0.077518
1	-2.908711	-1.183466	-0.824843
1	-2.809903	-2.672220	0.121054
1	-2.855008	1.095417	2.228724
1	-2.947011	1.120736	0.464356
1	-2.459721	-1.362995	2.214025
1	-3.972126	-0.937120	1.412086
6	-0.532292	0.671494	-1.448374
8	-1.663659	0.915967	-1.804298
8	0.559612	0.967340	-2.168585
6	0.339151	1.599791	-3.451173
1	1.330544	1.737607	-3.877427
1	-0.264771	0.956102	-4.091951
1	-0.156379	2.562265	-3.318299
16	-0.653188	-1.782819	-0.172850
16	-0.691757	0.926953	1.325726

4-eq

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	-2.408099	-1.582935	-0.038504
6	-0.012060	-0.216262	0.203925
6	-2.433342	0.663614	1.210251
6	-2.996559	-0.752947	1.102242
1	-2.563516	-1.093792	-1.004404
1	-2.886432	-2.563400	-0.084317
1	-2.929645	1.211697	2.013552
1	-2.589346	1.223053	0.283210
1	-2.867359	-1.279319	2.052128
1	-4.075609	-0.665346	0.922767
1	-0.340962	0.281787	-0.707468
6	1.505806	-0.222937	0.243035
8	2.172544	-0.613774	1.171583
8	2.009493	0.262895	-0.897830
6	3.453322	0.307155	-0.998513
1	3.869396	-0.697284	-0.912526
1	3.658923	0.721470	-1.982930
1	3.865492	0.950052	-0.219995
16	-0.646117	0.736358	1.645510
16	-0.614809	-1.958693	0.145384

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