Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Interplay between hydrogen bonding and n→π* interaction in an analgesic drug salicin

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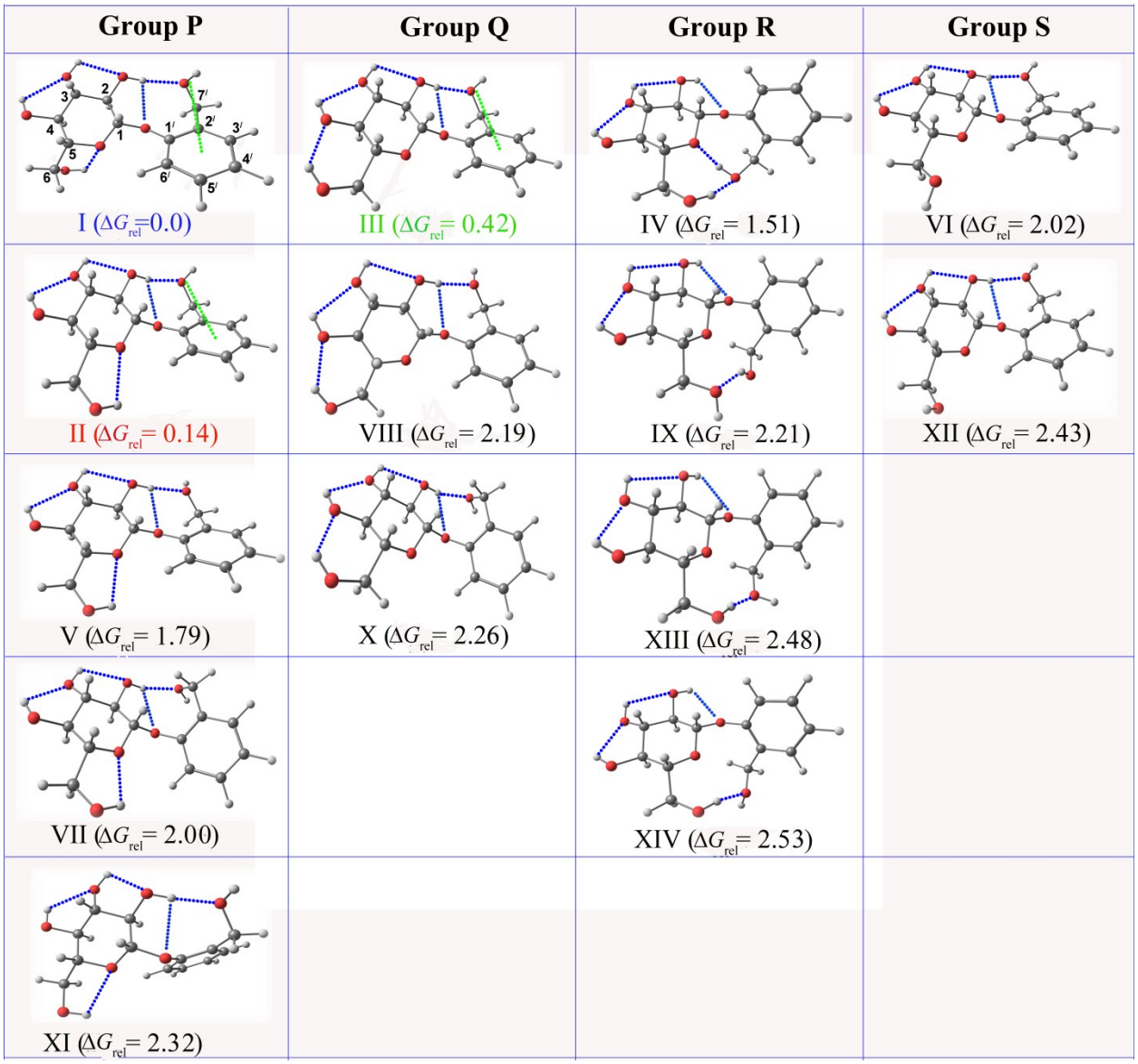


Figure S1. Structures of all the 14 low energy conformers of salicin optimized at the M06-2X/6-311++G(d,p) level of theory. ΔG_{rel} represents the relative Gibbs free energies of the conformers in kcal/mol, with respect to the most stable stable conformer I. The 14 conformers are classified into 4 groups (P, Q, R, S) depending upon their structural similarities.

2. Structural details of the conformers of salicin classified into P, Q, R, and S groups

Conformer I of group P is the global minimum. In this conformer, the -CH_2OH group of the aromatic ring (benzyl alcohol part) is strongly hydrogen bonded to the –O2H2 group of the sugar moiety. Furthermore, –O4H4, –O3H3, and –O2H2 groups of the sugar unit are weakly hydrogen bonded in a chain fashion, while the –CH_2OH group of the sugar moiety is hydrogen bonded to the oxygen atom of the sugar ring. The other conformers in group P are related by rotation of the –OH group of the benzyl alcohol moiety of salicin when retaining all the same hydrogen bonding structural motifs. The lowest energy conformer (III) in group Q is generated by rotating the -CH_2OH group of the sugar moiety along the C-C bond of conformer I by 180°. This -CH_2OH group forms a hydrogen bond with the neighboring –O4H4 group of the sugar moiety instead of the oxygen atom in the pyranose ring, while the other hydrogen bonding interactions remain intact. The remaining two conformers of group Q are again obtained from the rotation of the –OH group of the benzyl alcohol moiety of conformer III.

Conformer IV in group R is obtained by rotation of the whole benzyl alcohol moiety along the inter-ring O-C bond by 180° relative to conformer I of group P. In the R group conformers, -CH_2OH groups of the sugar moiety and aromatic ring are hydrogen bonded to each other, while all three –OH groups of the sugar ring and the inter-ring oxygen atom are weakly hydrogen bonded in a chain fashion. Different conformers in the R group originate due to rotation of either the –OH group of the benzyl alcohol group or the OH group of the -CH_2OH of the sugar moiety. Conformer VI in group S is generated by rotating the –CH_2OH group of the sugar moiety in conformer I along the C-C bond by 90° and losing the hydrogen bond to the oxygen atom of the sugar ring while keeping all other hydrogen bonding motifs the same. Another conformer in group S, namely conformer XII, arises due to rotation of the –CH_2OH group of the sugar moiety at a different angle.

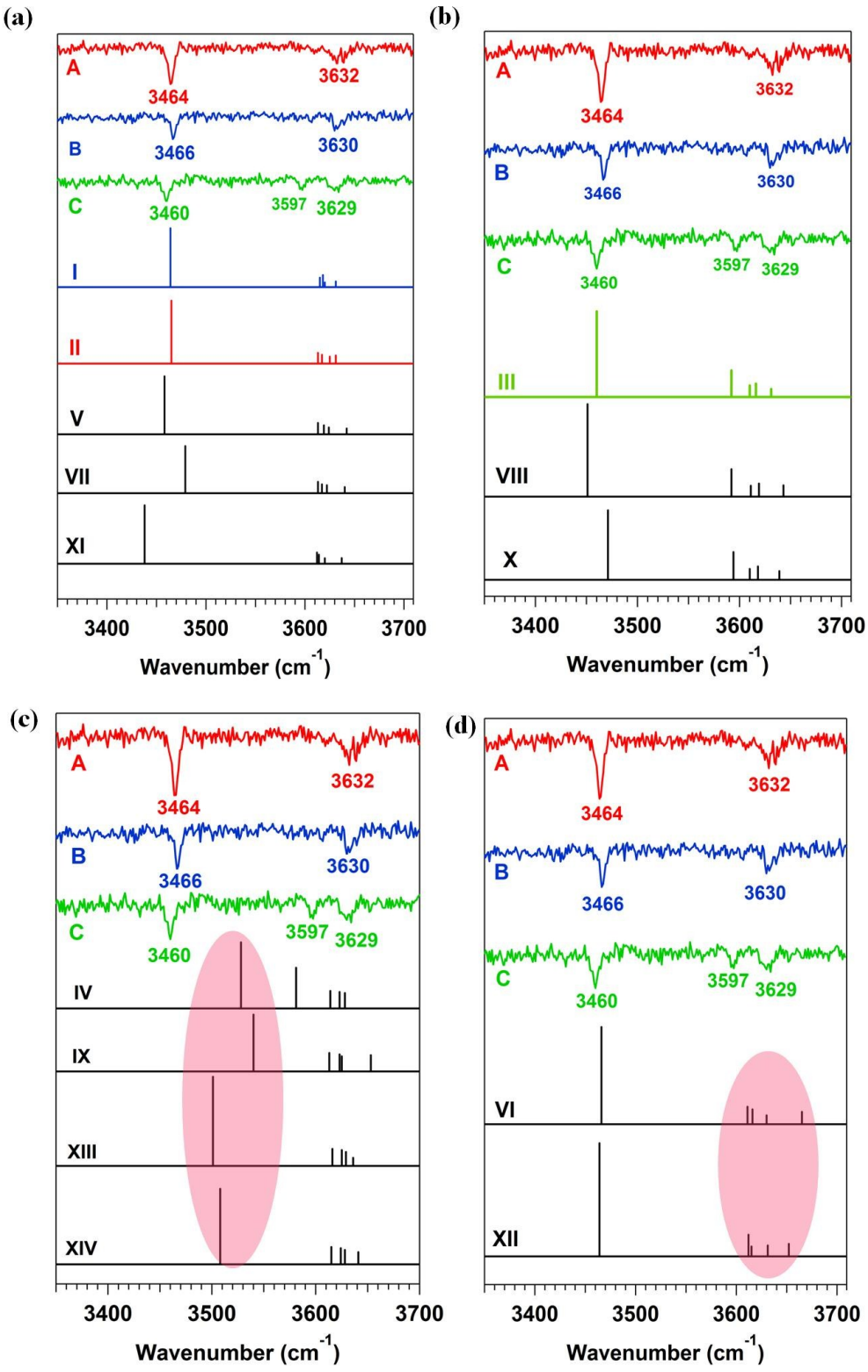


Figure S2. Experimental O-H stretching frequencies of species A, B and C in comparison with the computed O-H stretching frequencies of (a) Group P, (b) Group Q, (c) Group R, and (d) Group S conformers. The calculated [M06-2X/6-311++G(d,p) level of theory] O-H stretching frequencies shown as stick spectra are scaled by a factor of 0.9348.

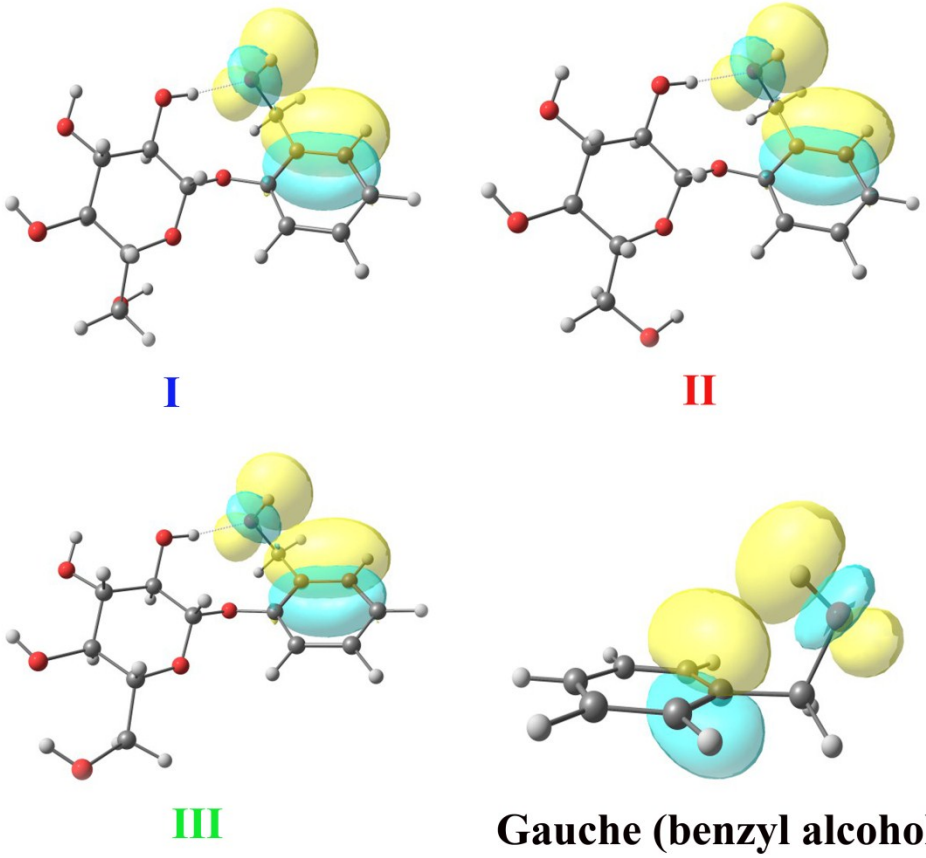


Figure S3. NBOs of the three lowest energy conformers (I, II, and III) of salicin and the gauche conformer of benzyl alcohol, showing no overlap between the π orbitals of the aromatic ring and σ^* orbital of the benzylic OH group. The electron density was calculated at the M06-2X/6-311++G(d,p) level of theory.

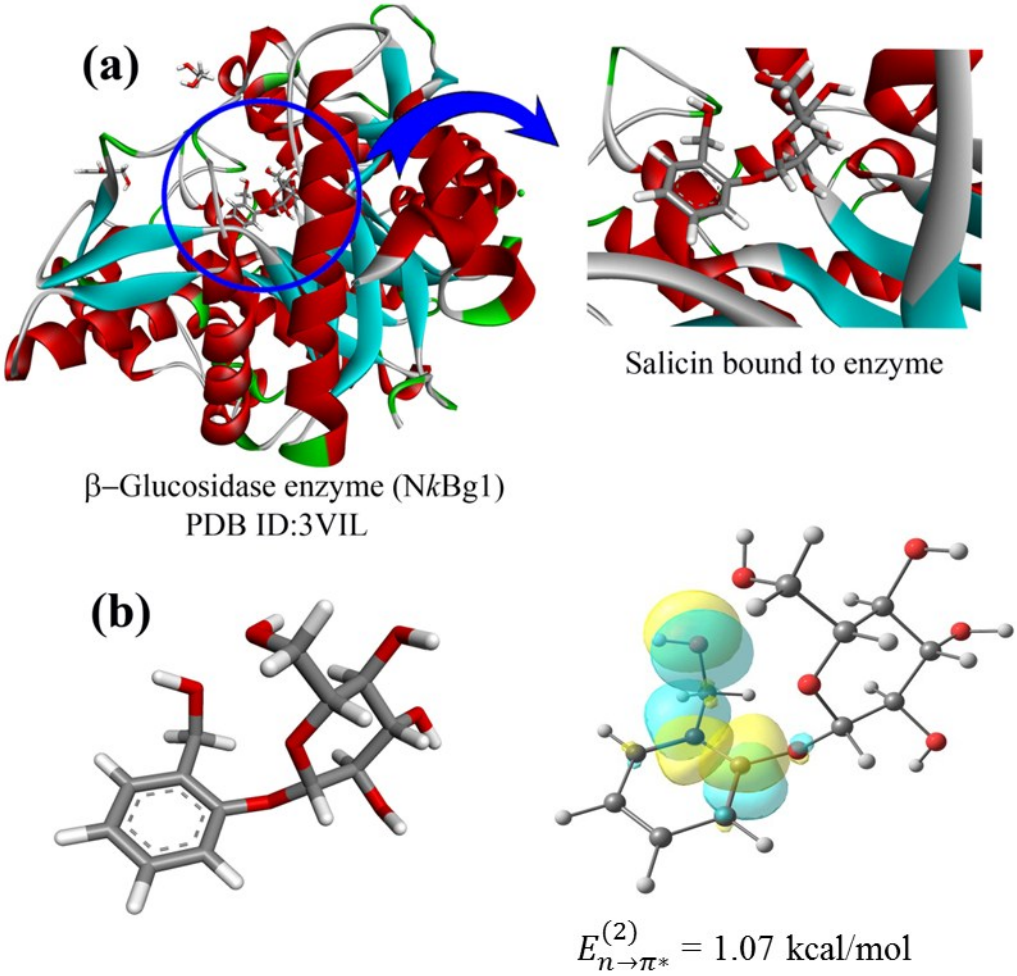


Figure S4. (a) X-ray crystal structure of the β-Glucosidase enzyme...salicin complex (PDB ID: 3VIL). (b) Structure of salicin in the enzyme bound state and one of its NBOs showing an n→π* interaction between the oxygen atom of the benzylic OH and the aromatic ring. The electron density has been calculated at the M06-2X/6-311++G(d,p) level of theory.

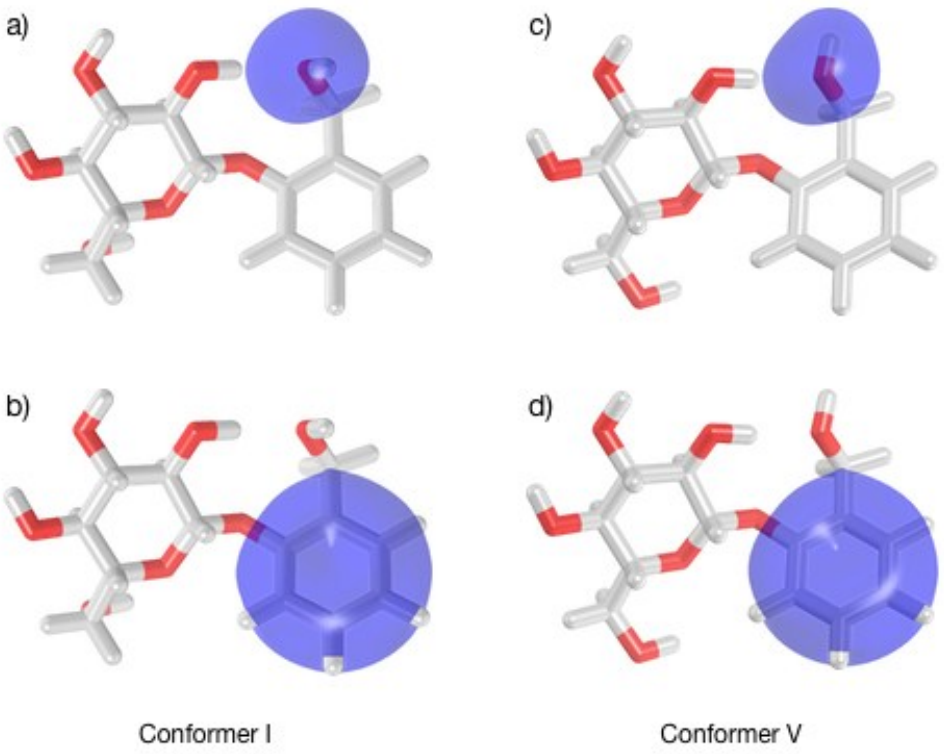


Figure S5. Zeroth-order densities from F/I-SAPT calculations on conformers I and V of salicin, isosurfaces at 0.02 electrons bohr $^{-3}$. a) and c) show the densities on the benzylic OH functional groups, and b) and d) the densities on the six carbon atoms of the phenyl functional groups.

Table S1. Comparison between the relative energies of the conformers of salicin obtained from the force field calculation (CONFLEX) and those obtained from quantum chemical optimization at the M06-2X/6-311++G(d,p) level of theory

	CONFLEX		**M06-2X**		
Conformers	**Energy (kcal/mol)**	**Relative Energy (kcal/mol)**	**E_{ZPE}[a] (E_h)**	**E_{rel}[b] (kcal/mol)**	**Conformers nomenclature**
1	115.507	0.00	-1032.3591	1.79	**V**
2	115.714	0.21	-1032.3618	0.14	**II**
3	117.730	0.22	-1032.3620	0.00	**I**
4	116.774	1.27	-1032.3587	2.08	**VI**
5	117.004	1.50	-1032.3585	2.20	**IX**
6	117.175	1.67	-1032.3613	0.41	**III**
7	117.420	1.91	-1032.3596	1.51	**IV**
8	117.913	2.41	-1032.3583	2.31	**XI**
9	118.036	2.53	-1032.3584	2.25	**X**
10	118.155	2.65	-1032.3581	2.47	**XIII**
11	118.283	2.78	-1032.3579	2.52	**XIV**
12	118.294	2.79	-1032.3588	2.02	**VII**
13	118.326	2.82	-1032.3557	3.91	
14	118.676	3.17	-1032.3565	3.47	
15	118.857	3.35	-1032.3585	2.18	**VIII**
16	119.03	3.52	-1032.3573	2.94	
17	119.112	3.60	-1032.3552	4.22	
18	119.237	3.73	-1032.3551	4.32	
19	119.384	3.88	-1032.3551	4.29	

20	119.492	3.98	-1032.3553	4.19	
21	119.495	3.99	-1032.3581	2.42	**XII**
22	119.512	4.00	-1032.35461	4.64	
23	119.518	4.01	-1032.35884	4.60	
24	119.711	4.2	-1032.35467	3.76	
25	119.773	4.27	-1032.35601	4.36	
26	120.067	4.56	-1032.35505	2.29	
27	120.320	4.81	-1032.35835	2.29	
28	120.508	5.00	-1032.35835	3.90	
29	121.030	5.52	-1032.35579	3.15	
30	121.049	5.54	-1032.35698	4.30	
31	121.824	6.32	-1032.35515	6.41	
32	123.066	7.56	-1032.35179	6.53	
33	123.087	7.58	-1032.35160	4.64	
34	123.359	7.85	-1032.35460	6.53	
35	124.012	8.50	-1032.35160	6.35	

[a]Absolute ZPE (zero point energy) corrected energies. [b]ZPE corrected relative energies of the conformers.

Table S2. Zero-point energy (ZPE) corrected relative energies (kcal/mol) of various conformers of salicin, calculated at different levels of theory

Method	I	II	III	IV	V	VI
M06-2X/6-311++G(d,p)	0.00	0.14	0.41	1.51	1.78	2.02
M05-2X/6-311++G(d,p)	0.00	0.16	0.52	1.51	1.80	2.19
M05-2X/6-31+G(d)	0.00	0.12	0.33	1.86	1.93	2.33
M05-2X/cc-pVTZ	0.00	0.10	0.49	1.74	1.83	1.91
M05-2X/aug-cc-pVDZ	0.00	0.04	0.59	1.68	1.64	1.87

Table S3. Relative electronic energies (E_{rel}) and relative Gibbs Free energies (ΔG_{rel}) of 14 low energy conformers of salicin calculated at 10 K

Conformer	E_{rel} (kcal/mol)	ΔG_{rel} (kcal/mol)
I	0.00	0.00
II	0.14	0.14
III	0.41	0.42
IV	1.51	1.51
V	1.80	1.80
VI	2.03	2.02
VII	2.09	2.00
VIII	2.19	2.19
IX	2.21	2.21
X	2.26	2.26
XI	2.32	2.32
XII	2.42	2.43
XIII	2.48	2.48
XIV	2.53	2.53

Table S4. Scaling factors obtained from different molecules having OH group. The theoretical OH stretching frequencies are calculated at the M06-2X/6-311++G(d,p) level of theory

Molecule	ν_{OH} (exp)	ν_{OH} (theory)	Scaling factor
Methanol	3666 cm^{-1} [a]	3918	0.9356
Ethanol (Anti conformer)	3660 cm^{-1} [b]	3915	0.9348
Benzyl Alcohol (Gauche conformer)	3649 cm^{-1} [c]	3888	0.9385

[a]Han *et al., J. Phys. Chem.*, 1996, **100**, 17124-17132.
[b]Coussan *et al., J. Phys. Chem. A*, 1998, **102**, 5789-5793.
[c]Mons *et al*., *J. Phys. Chem. A*, 2000, **104**, 1430-1437.

Table S5. Experimental and theoretical red-shift ($\Delta\nu$) in the OH stretching frequencies of the observed salicin conformers with respect to the experimental and theoretical OH stretching frequency of ethanol. Theoretical harmonic OH stretching frequencies are calculated at the M06-

	I		II		III	
OH groups	$\Delta\nu_{exp}$[a] (cm^{-1})	$\Delta\nu_{theor}$ (cm^{-1})	$\Delta\nu_{exp}$[a] (cm^{-1})	$\Delta\nu_{theor}$ (cm^{-1})	$\Delta\nu_{exp}$[a] (cm^{-1})	$\Delta\nu_{theor}$ (cm^{-1})
O2-H2	-194	-209	-196	-208	-200	-213
O3-H3	-30	-47	-28	-45	-27	-46
O4-H4	-30	-42	-28	-49	-27	-53
O6-H6	-30	-44	-21	-37	-63	-72
O7′-H7′	-30	-30	-21	-30	-27	-30

2X/6-311++G(d,p) level of theory and used without scaling to determine the red-shift

[a]Values of experimental frequencies of several O-H groups are reported to be the same because they could not be resolved properly from the experiment. The peak position of the broad IR band has been assigned for all the O-H groups appearing in a similar region.

Table S6: Experimental 0_0^0 band transitions of species A, B and C in comparison with the TDDFT calculated [TD-M06-2X/6-311++G(d)] vertical excitation energies of conformers I, II and III

Observed Species	Experimental 0_0^0 band transitions (cm^{-1})[a]	Assigned conformer	Calculated vertical excitation energies (cm^{-1})[b]
A	36422 (0)	II	42877 (0)
B	36435 (13)	I	42912 (35)
C	36452 (30)	III	42930 (53)

[a]Values in parentheses represent the relative frequencies with respect to the 0_0^0 band transition of species A. [b]Values in parentheses represent the relative frequencies with respect to the calculated vertical excitation energy of conformer II.

Table S7: Experimental and Franck-Condon simulated low frequency intramolecular vibrational modes of the three observed conformers of salicin.

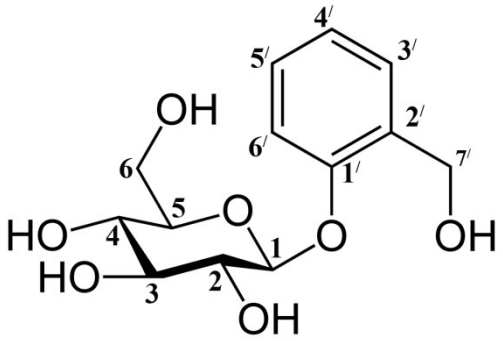
A	**II**		**B**	**I**		**C**	**III**	
Obs. (cm^{-1})	Cal. (cm^{-1})	Assign.	Obs. (cm^{-1})	Cal. (cm^{-1})	Assign.	Obs. (cm^{-1})	Cal. (cm^{-1})	Assign.
28	27	α	28	28	α	28	29	α
47	47	β	47	48	β	-	48	β
57	55	2α	56	56	2α	56	58	2α
	59	γ						
75	74	α+β	75	76	α+ β	-	78	α + β
	79	δ						
85	86	α+ γ	83	84	3α	82	88	3α
89	92	ε	-	88	α+γ	-		
	94	2β		97	2β			
103	102	2α+β	102	103	α+δ	-		
	106	β+γ		104	2α+β		107	2α + β
111	113	2α+γ	111	112	4α	-		
				116	2α+γ		118	2α + γ
118	119	α+ε	123	124	α+2β	-	126	α + 2β
121	121	α+2β	130	131	2α+δ	-		

131	134	2α+δ	136	132	3α + β	-	136	3α + β
146	148	2α+2β	139	144	3α + γ	-		

Table S8. Important geometrical parameters[a] of low energy conformers of salicin calculated at the M06-2X/6-311++G(d,p) level of theory

	I	II	III	V	VIII
O3-H3…O2	2.43	2.45	2.46	2.47	2.48
∠O3-H3…O2	101.1	104.6	104.3	104.0	103.7
O5-H5…O3	2.41	2.38	2.36	2.38	2.36
∠O5-H5…O3	105.1	107.4	107.3	107.5	107.4
O6-H6…O5	2.30	2.34	-	2.33	-
∠O6-H6…O5	106.2	104.5	-	104.9	-
O6-H6…O4	-	-	2.05	-	2.04
∠O6-H6…O4	-	-	134.4	-	134.5
O2-H2… O7/	1.94	1.95	1.93	1.94	1.92
∠O2-H2… O7/	164	164.2	164.4	172.6	172.4
O7/…Ar[b]	3.68	3.67	3.68	3.64	3.64
O7/-H7/…Ar[b]	3.65	3.65	3.65	4.52	4.53
∠O6-C6-C5-O5	–56.5	57.5	164.9	57.7	164.9
∠H6-O6-C6-C5	55.2	–58.9	53.1	–58.2	53.0
∠H7/-O7/-C7/-C2/	57.3	57.6	57.0	167.2	166.4
∠O7/-C7/-C2/-C1/	64.6	64.2	64.7	65.8	66.2

[a]Hydrogen bond distances have been measured between hydrogen and oxygen atoms. All the distances are in Å and angles (∠) are in degrees. [b]Ar stands for aromatic ring.



Skeletal structure of salicin showing atom numbering scheme

Table S9. Electron density (ρ) and Laplacian of electron density ($\nabla^2\rho$) of O2-H2…O7/ hydrogen bonding interaction, calculated using AIM for all the conformers of group P and Q, in comparison with the amount of red shift ($\Delta\nu$) in the unscaled theoretical stretching frequency of the O2-H2 group of salicin with respect to unscaled theoretical free -OH stretching frequency of ethanol. NBO second order perturbative energy value ($E^{(2)}_{i\rightarrow j*}$) for O2-H2…O7/ hydrogen bonding interaction and n→π* interaction of all the conformers of group P and Q are included for comparison

Conformers	O2-H2…O7/		$\Delta\nu$ (O2-H2) (cm^{-1})	$E^{(2)}_{n\rightarrow\sigma*}$ (kcal/mol)	$E^{(2)}_{n\rightarrow\pi*}$ (kcal/mol)
	ρ (a.u.)	$\nabla^2\rho$ (a.u.)			
I[a]	0.02381210	0.09465644	-209	8.93	1.13
II[a]	0.02319848	0.09206186	-208	8.59	1.15
III[a]	0.02410016	0.0956791	-200	9.17	1.13
V	0.02350143	0.09359325	-215	9.46	0.31
VIII	0.02432022	0.09676899	-223	10.01	0.31
XI	0.02961733	0.11595896	-237	13.74	0.38
VII	0.02326949	0.09438093	-193	7.28	0.77
X	0.02371155	0.09584836	-201	7.72	0.73

[a]Experimental red-shift values in the O2-H2 stretching frequencies of conformers I, II, and III with respect to experimental O-H stretching frequency of ethanol are 194, 196, and 200 cm^{-1}.

Table S10. Effect of dispersion on the equilibrium geometry of selected conformers of salicin. $RMSD_{disp}$ is the RMSD between B3LYP and B3LYP-D optimized structures, ΔO-centroid is the change in the O7′ to phenyl ring centroid distance when the dispersion correction is added to B3LYP, and $RMSD_{M06}$ is the RMSD between B3LYP-D and M06-2X optimized structures. The 6-311++G(d,p) basis is used throughout, and all distances are in Å.

Conformer	$RMSD_{disp}$	ΔO-centroid	$RMSD_{M06}$
I	0.030	–0.018	0.036
II	0.047	–0.018	0.046
III	0.033	–0.019	0.049
IV	0.073	–0.008	0.054
V	0.047	–0.014	0.053
VI	0.043	–0.019	0.055
VII	0.051	–0.013	0.118
VIII	0.028	–0.014	0.072
IX	0.051	–0.015	0.053
X	0.047	–0.015	0.150

Table S11. NBO second order perturbative energy values of all the hydrogen bonding interactions and n→π* interaction in the conformers I, II, III, V and VIII of salicin, calculated at the M06-2X and HF levels of theory using 6-311++G(d,p) basis set

	$E_{i\to j*}^{(2)}$ **(kcal/mol)**									
	M06-2X/6-311++G(d,p)					**HF/6-311++G(d,p)**				
	I	**II**	**III**	**V**	**VIII**	**I**	**II**	**III**	**V**	**VIII**
n_p (O7′)→σ*(O2-H2)	5.65	5.35	5.90	7.07	7.61	6.07	5.72	6.34	6.91	7.51
n_s (O7′)→σ*(O2-H2)	3.28	3.24	3.27	2.39	2.40	3.13	3.10	2.92	2.75	2.77
n_p (O2)→σ*(O3-H3)	0.18	0.16	0.16	-	0.14	0.14	0.13	0.13	-	-
n_s (O2)→σ*(O3-H3)	0.17	0.15	0.14	0.15	0.10	0.15	0.14	0.13	0.13	0.12
n_p (O3)→σ*(O4-H4)	0.15	0.20	0.20	0.23	0.22	0.12	0.16	0.16	0.18	0.17
n_s (O3)→σ*(O4-H4)	0.18	0.20	0.24	0.20	0.24	0.16	0.18	0.23	0.18	0.22
n_p (O5)→σ*(O6-H6)	0.14	0.21	-	0.23	-	0.14	0.17	-	0.19	-
n_s (O5)→σ*(O6-H6)	0.44	0.33	-	0.34	-	0.42	0.33	-	0.34	-
n_p (O4)→σ*(O6-H6)	-	-	0.69	-	0.68	-	-	0.49	-	0.56
n_s (O4)→σ*(O6-H6)	-	-	2.60	-	2.61	-	-	2.80	-	2.68
n_p (O7′)→π*(C2′-C3′)	0.80	0.83	0.78	-	-	0.75	0.77	0.73	-	-
n_s(O7′)→ π*(C2′-C3′)	0.33	0.32	0.35	0.31	0.31	0.39	0.37	0.42	0.34	0.35

Table S12. Theoretical red-shift in the O-H stretching frequencies of the observed conformers of salicin in comparison with geometrical parameters of the hydrogen bonding interactions present in the observed conformers of salicin. The geometrical parameters of hydrogen bonding interactions include hydrogen bond distance (O**H...O)** , hydrogen bond angle (**∠O-H...O**) and O-H distance (**r_{O-H}).**

Hydrogen bonding interactions	**I**					**II**					**III**				
	$\Delta\nu_{theo}$ r (cm^{-1})	**r_{O-H} (Å)**	**OH... O (Å)**	**∠O-H...O (°)**	**$E^{(2)}_{n\to\sigma*}$ (kcal/mol)**	**$\Delta\nu_{theo}$ r (cm^{-1})**	**r_{O-H} (Å)**	**OH... O (Å)**	**∠O-H... O (°)**	**$E^{(2)}_{n\to\sigma*}$ (kcal/mol)**	**$\Delta\nu_{theo}$ r (cm^{-1})**	**r_{O-H} (Å)**	**OH... O (Å)**	**∠O-H...O (°)**	**$E^{(2)}_{n\to\sigma*}$ (kcal/mol)**
O2-H2…O7/	-209	0.97	1.94	164	8.93	-208	0.97	1.95	164	8.59	-213	0.97	1.93	164	9.17
O3-H3…O2	-47	0.96	2.43	105	0.35	-45	0.96	2.45	104	0.31	-46	0.96	2.46	104	0.3
O4-H4…O3	-42	0.96	2.41	106	0.33	-49	0.96	2.38	107	0.40	-53	0.96	2.36	107	0.44
O6-H6…O5	-44	0.96	2.31	106	0.58	-37	0.96	2.34	104	0.54	-	-	-	-	-
O6-H6…O4	-	-	-	-	-	-	-	-	-	-	-72	0.96	2.04	134	3.29

NBO output

Salicin (Conformer I)

Summary of Natural Population Analysis:

Atom No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
O 1	-0.64267	2.00000	6.61961	0.02306	8.64267
O 2	-0.58652	2.00000	6.56250	0.02403	8.58652
O 3	-0.76064	2.00000	6.74681	0.01383	8.76064
O 4	-0.75213	2.00000	6.73862	0.01351	8.75213
O 5	-0.78545	2.00000	6.77057	0.01488	8.78545
O 6	-0.74076	2.00000	6.72716	0.01360	8.74076
O 7	-0.75836	2.00000	6.74425	0.01412	8.75836
C 8	0.09707	1.99999	3.87680	0.02614	5.90293
C 9	0.08872	1.99999	3.88443	0.02685	5.91128
C 10	0.07578	1.99999	3.89770	0.02653	5.92422
C 11	0.09468	1.99999	3.88172	0.02361	5.90532
C 12	0.44950	1.99999	3.51756	0.03295	5.55050
C 13	-0.03356	1.99999	4.00969	0.02387	6.03356
C 14	0.33608	1.99999	3.63989	0.02403	5.66392
C 15	-0.11560	1.99999	4.09985	0.01575	6.11560
C 16	-0.26290	1.99999	4.24630	0.01660	6.26290
C 17	-0.19048	1.99999	4.17368	0.01680	6.19048
C 18	-0.03537	1.99999	4.01236	0.02302	6.03537
C 19	-0.19009	1.99999	4.17315	0.01694	6.19009
C 20	-0.22714	1.99999	4.21041	0.01674	6.22714
H 21	0.17309	0.00000	0.82385	0.00307	0.82691
H 22	0.19155	0.00000	0.80530	0.00315	0.80845
H 23	0.18443	0.00000	0.81281	0.00276	0.81557
H 24	0.18480	0.00000	0.81275	0.00244	0.81520
H 25	0.15832	0.00000	0.83880	0.00288	0.84168
H 26	0.20455	0.00000	0.79367	0.00177	0.79545
H 27	0.16309	0.00000	0.83453	0.00238	0.83691
H 28	0.48537	0.00000	0.51060	0.00403	0.51463
H 29	0.48269	0.00000	0.51328	0.00402	0.51731
H 30	0.51396	0.00000	0.48178	0.00426	0.48604
H 31	0.46987	0.00000	0.52566	0.00447	0.53013
H 32	0.23491	0.00000	0.76225	0.00284	0.76509
H 33	0.21379	0.00000	0.78444	0.00176	0.78621
H 34	0.17243	0.00000	0.82543	0.00214	0.82757
H 35	0.20229	0.00000	0.79558	0.00213	0.79771
H 36	0.21559	0.00000	0.78272	0.00169	0.78441
H 37	0.21721	0.00000	0.78110	0.00169	0.78279
H 38	0.47188	0.00000	0.52427	0.00385	0.52812
* Total *	0.00000	39.99990	111.54187	0.45822	152.00000

(Occupancy) Bond orbital / Coefficients / Hybrids

---------- Lewis ----------

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 21. (1.95864) LP ( 1) O  1           s( 41.98%)p 1.38( 57.99%)d 0.00(  0.03%)
                                       0.0000  0.6477  0.0152  0.0011  0.0000
                                      -0.2420  0.0011  0.0003 -0.0015 -0.4952
                                      -0.0062 -0.0018 -0.0007  0.5254  0.0019
                                      -0.0012 -0.0005 -0.0081  0.0057  0.0125
                                       0.0059 -0.0047
 22. (1.92830) LP ( 2) O  1           s(  0.02%)p99.99( 99.95%)d 2.27(  0.04%)
                                       0.0000  0.0098  0.0072 -0.0035 -0.0001
                                       0.4275  0.0072  0.0002  0.0000  0.5580
                                       0.0130  0.0060 -0.0016  0.7107  0.0035
                                      -0.0013 -0.0034  0.0084 -0.0017  0.0019
                                      -0.0047 -0.0163
 23. (1.95768) LP ( 1) O  2           s( 34.12%)p 1.93( 65.84%)d 0.00(  0.03%)
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```
                                    0.0000  0.5840  0.0126  0.0014  0.0001
                                   -0.0608  0.0042  0.0026 -0.0004  0.5782
                                    0.0068  0.0020 -0.0010  0.5659  0.0065
                                   -0.0028 -0.0003  0.0014  0.0001 -0.0149
                                    0.0069 -0.0086
24. (1.86714) LP ( 2) O  2          s(  2.31%)p42.23( 97.64%)d 0.02(  0.05%)
                                    0.0000  0.1519  0.0034 -0.0049  0.0004
                                    0.2666 -0.0012 -0.0020  0.0016 -0.7266
                                   -0.0061 -0.0017  0.0035  0.6142  0.0049
                                   -0.0070 -0.0029 -0.0018 -0.0064  0.0082
                                   -0.0057 -0.0177
25. (1.98034) LP ( 1) O  3          s( 47.80%)p 1.09( 52.17%)d 0.00(  0.03%)
                                    0.0000  0.6913  0.0087  0.0023  0.0001
                                    0.6687  0.0053  0.0011  0.0015  0.0321
                                   -0.0067  0.0014 -0.0010  0.2709  0.0009
                                    0.0006  0.0000 -0.0014 -0.0095 -0.0003
                                   -0.0149  0.0026
26. (1.96008) LP ( 2) O  3          s(  0.02%)p99.99( 99.94%)d 3.06(  0.05%)
                                    0.0000  0.0117 -0.0025  0.0032  0.0001
                                    0.3644  0.0076 -0.0024 -0.0006  0.0112
                                    0.0019  0.0006  0.0007 -0.9306 -0.0172
                                   -0.0019  0.0038 -0.0006  0.0162 -0.0006
                                   -0.0074  0.0122
27. (1.98043) LP ( 1) O  4          s( 48.24%)p 1.07( 51.73%)d 0.00(  0.03%)
                                    0.0000  0.6945  0.0083  0.0023  0.0001
                                    0.2387 -0.0036  0.0009  0.0002 -0.5663
                                   -0.0054  0.0003 -0.0022 -0.3736 -0.0010
                                   -0.0013  0.0000  0.0100  0.0032 -0.0124
                                    0.0088  0.0002
28. (1.96067) LP ( 2) O  4          s(  0.00%)p 1.00( 99.95%)d 0.00(  0.05%)
                                    0.0000  0.0055  0.0042 -0.0016  0.0000
                                   -0.4872 -0.0106 -0.0003  0.0003  0.3336
                                    0.0050 -0.0024 -0.0012 -0.8065 -0.0148
                                   -0.0022  0.0031 -0.0111 -0.0003 -0.0112
                                   -0.0029 -0.0152
29. (1.97884) LP ( 1) O  5          s( 44.87%)p 1.23( 55.09%)d 0.00(  0.03%)
                                    0.0000  0.6698  0.0095  0.0025  0.0002
                                    0.2299  0.0057 -0.0035  0.0012  0.4537
                                    0.0020  0.0028  0.0010 -0.5405 -0.0043
                                   -0.0011  0.0000 -0.0078  0.0062  0.0126
                                    0.0056 -0.0054
30. (1.95380) LP ( 2) O  5          s(  0.18%)p99.99( 99.78%)d 0.24(  0.04%)
                                    0.0000  0.0423 -0.0026  0.0036  0.0002
                                    0.3538  0.0058 -0.0028 -0.0005  0.6054
                                    0.0139  0.0012 -0.0011  0.7111  0.0143
                                    0.0049 -0.0022 -0.0093  0.0000 -0.0019
                                    0.0064  0.0175
31. (1.98164) LP ( 1) O  6          s( 48.78%)p 1.05( 51.19%)d 0.00(  0.04%)
                                    0.0000  0.6983  0.0110  0.0004  0.0000
                                    0.5804  0.0049  0.0023  0.0019 -0.0292
                                   -0.0026 -0.0029 -0.0002  0.4172  0.0021
                                    0.0030  0.0010  0.0013 -0.0162  0.0021
                                   -0.0090  0.0023
32. (1.95607) LP ( 2) O  6          s(  0.05%)p99.99( 99.89%)d 1.03(  0.05%)
                                    0.0000  0.0222 -0.0010  0.0057  0.0001
                                   -0.1420 -0.0045 -0.0041  0.0003 -0.9848
                                   -0.0215 -0.0001  0.0034  0.0914  0.0028
                                   -0.0005  0.0001  0.0189 -0.0007  0.0121
                                    0.0062 -0.0013
33. (1.97544) LP ( 1) O  7          s( 44.37%)p 1.25( 55.59%)d 0.00(  0.03%)
                                    0.0000  0.6661  0.0072 -0.0003  0.0000
                                    0.3730 -0.0004 -0.0056  0.0013  0.5858
                                    0.0088 -0.0063 -0.0008  0.2710  0.0046
                                    0.0035  0.0008 -0.0120 -0.0060 -0.0094
                                    0.0019  0.0061
34. (1.95801) LP ( 2) O  7          s(  4.26%)p22.45( 95.70%)d 0.01(  0.04%)
                                    0.0000  0.2062  0.0103 -0.0005 -0.0001
                                    0.7393  0.0190 -0.0010  0.0002 -0.5720
                                   -0.0117  0.0003  0.0024 -0.2877 -0.0030
                                    0.0054  0.0006  0.0013 -0.0009  0.0076
                                   -0.0171  0.0060
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82. (0.00735) BD*( 1) O  3- H 28
            ( 25.43%)   0.5043* O  3 s( 20.92%)p 3.77( 78.94%)d 0.01(  0.14%)
                                      0.0000 -0.4573  0.0083 -0.0007  0.0002
                                      0.4444  0.0055 -0.0022  0.0001 -0.7520
                                      0.0317 -0.0055 -0.0022  0.1592  0.0021
                                      0.0003 -0.0003  0.0290 -0.0118  0.0107
                                     -0.0006  0.0159
            ( 74.57%)  -0.8635* H 28 s( 99.87%)p 0.00(  0.13%)
                                     -0.9994  0.0034  0.0005 -0.0001 -0.0140
                                      0.0324 -0.0029
83. (0.01774) BD*( 1) O  4- C  9
            ( 33.77%)   0.5812* O  4 s( 31.02%)p 2.22( 68.90%)d 0.00(  0.08%)
                                      0.0000 -0.5568  0.0090  0.0058  0.0000
                                      0.6870 -0.0084 -0.0056  0.0023 -0.0915
                                     -0.0020  0.0068  0.0002 -0.4566  0.0057
                                      0.0044  0.0004  0.0102  0.0221 -0.0108
                                     -0.0098  0.0022
            ( 66.23%)  -0.8138* C  9 s( 21.25%)p 3.70( 78.53%)d 0.01(  0.21%)
                                      0.0000 -0.4589  0.0434  0.0022  0.0008
                                     -0.7564  0.0419  0.0024 -0.0040  0.0682
                                     -0.0161 -0.0009  0.0016  0.4542 -0.0078
                                     -0.0091  0.0058  0.0034  0.0382 -0.0017
                                     -0.0256  0.0039
84. (0.00708) BD*( 1) O  4- H 29
            ( 25.59%)   0.5059* O  4 s( 20.72%)p 3.82( 79.15%)d 0.01(  0.14%)
                                      0.0000 -0.4551  0.0077 -0.0018  0.0001
                                     -0.4816  0.0268 -0.0062 -0.0011 -0.7470
                                      0.0105 -0.0009 -0.0008 -0.0211 -0.0122
                                      0.0014 -0.0001 -0.0197 -0.0025 -0.0111
                                      0.0236  0.0173
            ( 74.41%)  -0.8626* H 29 s( 99.87%)p 0.00(  0.13%)
                                     -0.9993  0.0030 -0.0010  0.0000  0.0231
                                      0.0274 -0.0030
85. (0.01896) BD*( 1) O  5- C 10
            ( 34.15%)   0.5843* O  5 s( 30.98%)p 2.23( 68.94%)d 0.00(  0.08%)
                                      0.0000 -0.5565  0.0086  0.0043 -0.0003
                                     -0.4078  0.0121  0.0010 -0.0023  0.6498
                                     -0.0089 -0.0055 -0.0001 -0.3172  0.0035
                                      0.0019  0.0007  0.0122 -0.0054  0.0202
                                      0.0131  0.0053
            ( 65.85%)  -0.8115* C 10 s( 21.81%)p 3.58( 77.99%)d 0.01(  0.21%)
                                      0.0000 -0.4651  0.0413 -0.0023  0.0002
                                      0.4636  0.0085  0.0019  0.0025 -0.6910
                                     -0.0409 -0.0016  0.0055  0.2926 -0.0034
                                     -0.0062  0.0072  0.0307 -0.0163  0.0228
                                      0.0105  0.0153
86. (0.02211) BD*( 1) O  5- H 30
            ( 23.41%)   0.4838* O  5 s( 23.94%)p 3.17( 75.93%)d 0.01(  0.13%)
                                      0.0000 -0.4892  0.0085  0.0002  0.0007
                                      0.8082 -0.0262 -0.0014  0.0026 -0.0655
                                      0.0214 -0.0053  0.0001 -0.3173 -0.0040
                                      0.0023  0.0009 -0.0072  0.0261  0.0057
                                     -0.0216  0.0052
            ( 76.59%)  -0.8752* H 30 s( 99.84%)p 0.00(  0.16%)
                                     -0.9992  0.0061  0.0001  0.0004 -0.0383
                                      0.0073  0.0087
87. (0.01035) BD*( 1) O  6- C 13
            ( 33.67%)   0.5803* O  6 s( 30.36%)p 2.29( 69.55%)d 0.00(  0.09%)
                                      0.0000 -0.5508  0.0144  0.0033 -0.0001
                                      0.0687  0.0097 -0.0078  0.0001  0.0547
                                     -0.0076  0.0009 -0.0007  0.8291 -0.0098
                                     -0.0054  0.0027  0.0010 -0.0146 -0.0008
                                     -0.0057 -0.0259
            ( 66.33%)  -0.8144* C 13 s( 21.89%)p 3.56( 77.87%)d 0.01(  0.24%)
                                      0.0000 -0.4655  0.0476 -0.0014  0.0003
                                     -0.0452 -0.0271  0.0021  0.0011 -0.0420
                                      0.0215 -0.0027  0.0008 -0.8779 -0.0534
                                      0.0004  0.0081  0.0022 -0.0003 -0.0073
                                      0.0025 -0.0479
88. (0.00936) BD*( 1) O  6- H 31
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              ( 26.11%)   0.5110* O  6 s( 20.81%)p 3.80( 79.05%)d 0.01(  0.14%)
                                        0.0000 -0.4561  0.0074 -0.0026  0.0001
                                        0.7975 -0.0195 -0.0019  0.0004 -0.1585
                                        0.0053  0.0003  0.0005 -0.3577  0.0300
                                       -0.0047 -0.0007  0.0116  0.0091 -0.0019
                                       -0.0311  0.0162
              ( 73.89%)  -0.8596* H 31 s( 99.87%)p 0.00(  0.13%)
                                       -0.9993  0.0042  0.0003 -0.0002 -0.0295
                                        0.0087  0.0198

107. (0.35181) BD*( 2) C 15- C 17
              ( 47.86%)   0.6918* C 15 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.03%)
                                        0.0000 -0.0019  0.0031 -0.0002 -0.1084
                                        0.0014 -0.0017  0.0008 -0.4526 -0.0038
                                       -0.0161 -0.0026  0.8846 -0.0136  0.0062
                                       -0.0089  0.0056 -0.0065 -0.0083 -0.0034
                                       -0.0139
              ( 52.14%)  -0.7221* C 17 s(  0.00%)p 1.00( 99.95%)d 0.00(  0.05%)
                                        0.0000  0.0000 -0.0045  0.0004 -0.0016
                                       -0.1113 -0.0031 -0.0026  0.0000 -0.4653
                                       -0.0078 -0.0091  0.0004  0.8776  0.0126
                                        0.0110 -0.0044 -0.0111  0.0189 -0.0006
                                       -0.0043  0.0046
108. (0.02853) BD*( 1) C 15- C 18
              ( 48.33%)   0.6952* C 15 s( 30.58%)p 2.27( 69.38%)d 0.00(  0.04%)
                                        0.0000 -0.5530 -0.0075  0.0000 -0.0068
                                        0.0117 -0.0038  0.0005 -0.7405 -0.0042
                                        0.0050  0.0043 -0.3809  0.0008  0.0081
                                        0.0025 -0.0008 -0.0025 -0.0149  0.0110
                                        0.0075
              ( 51.67%)  -0.7188* C 18 s( 30.96%)p 2.23( 68.99%)d 0.00(  0.05%)
                                        0.0000 -0.5563  0.0101 -0.0007  0.0020
                                        0.0069 -0.0122 -0.0021 -0.0005  0.7372
                                       -0.0070 -0.0028  0.0037  0.3822  0.0097
                                        0.0009  0.0003  0.0005 -0.0008 -0.0172
                                        0.0145  0.0027



SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

     Threshold for printing:   0.10 kcal/mol
                                                                 E(2) E(NL)-E(L) F(L,NL)
      Donor (L) NBO              Acceptor (NL) NBO              kcal/mol   a.u.    a.u.
 ===========================================================================================

 within unit  1
   21. LP ( 1) O  1            79. BD*( 1) O  2- C 12      5.56    0.97   0.066
   21. LP ( 1) O  1            83. BD*( 1) O  4- C  9      0.13    0.98   0.010
   21. LP ( 1) O  1            85. BD*( 1) O  5- C 10      0.14    0.98   0.010
   21. LP ( 1) O  1            88. BD*( 1) O  6- H 31      0.44    1.12   0.020
   21. LP ( 1) O  1            94. BD*( 1) C  9- C 11      0.91    1.03   0.027
   21. LP ( 1) O  1            95. BD*( 1) C  9- H 22      0.12    1.06   0.010
   21. LP ( 1) O  1            96. BD*( 1) C 10- C 12      0.91    1.02   0.027
   21. LP ( 1) O  1            97. BD*( 1) C 10- H 23      0.14    1.04   0.011
   21. LP ( 1) O  1            98. BD*( 1) C 11- C 13      1.77    1.04   0.038
   21. LP ( 1) O  1            99. BD*( 1) C 11- H 24      1.00    1.05   0.029
   21. LP ( 1) O  1           100. BD*( 1) C 12- H 25      0.93    1.02   0.027
   21. LP ( 1) O  1           101. BD*( 1) C 13- H 26      0.51    1.08   0.021
   21. LP ( 1) O  1           110. BD*( 1) C 16- H 32      0.12    1.10   0.010
   21. LP ( 1) O  1           126. RY ( 8) O  1            0.14    1.91   0.015
   21. LP ( 1) O  1           289. RY ( 1) C 11            1.24    1.55   0.039
   21. LP ( 1) O  1           290. RY ( 2) C 11            1.23    1.99   0.044
   21. LP ( 1) O  1           299. RY (11) C 11            0.12    2.21   0.014
   21. LP ( 1) O  1           306. RY ( 1) C 12            2.28    1.80   0.057
   21. LP ( 1) O  1           307. RY ( 2) C 12            0.13    3.15   0.018
   21. LP ( 1) O  1           308. RY ( 3) C 12            0.17    2.36   0.018
   21. LP ( 1) O  1           309. RY ( 4) C 12            0.20    2.16   0.018
   21. LP ( 1) O  1           310. RY ( 5) C 12            0.34    2.26   0.025
   21. LP ( 1) O  1           313. RY ( 8) C 12            0.12    2.33   0.015
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21. LP (1) O 1	316. RY (11) C 12	0.13	3.35	0.019
21. LP (1) O 1	322. RY (17) C 12	0.12	3.35	0.018
22. LP (2) O 1	83. BD*(1) O 4- C 9	0.97	0.78	0.025
22. LP (2) O 1	85. BD*(1) O 5- C 10	0.97	0.78	0.025
22. LP (2) O 1	88. BD*(1) O 6- H 31	0.14	0.92	0.010
22. LP (2) O 1	94. BD*(1) C 9- C 11	5.96	0.83	0.063
22. LP (2) O 1	96. BD*(1) C 10- C 12	6.43	0.82	0.065
22. LP (2) O 1	99. BD*(1) C 11- H 24	7.28	0.85	0.070
22. LP (2) O 1	100. BD*(1) C 12- H 25	8.04	0.82	0.073
22. LP (2) O 1	110. BD*(1) C 16- H 32	0.36	0.90	0.016
22. LP (2) O 1	122. RY (4) O 1	0.12	1.75	0.013
22. LP (2) O 1	272. RY (1) C 10	0.16	1.49	0.014
22. LP (2) O 1	289. RY (1) C 11	0.14	1.35	0.012
22. LP (2) O 1	291. RY (3) C 11	0.64	2.53	0.036
22. LP (2) O 1	294. RY (6) C 11	0.31	2.03	0.022
22. LP (2) O 1	307. RY (2) C 12	0.12	2.95	0.017
22. LP (2) O 1	308. RY (3) C 12	0.12	2.16	0.014
22. LP (2) O 1	309. RY (4) C 12	0.48	1.96	0.027
22. LP (2) O 1	310. RY (5) C 12	0.61	2.06	0.032
22. LP (2) O 1	311. RY (6) C 12	0.40	2.52	0.028
22. LP (2) O 1	475. RY (1) H 24	0.25	1.20	0.015
22. LP (2) O 1	481. RY (1) H 25	0.20	1.32	0.014
23. LP (1) O 2	78. BD*(1) O 1- C 12	0.54	0.94	0.020
23. LP (1) O 2	85. BD*(1) O 5- C 10	0.10	0.96	0.009
23. LP (1) O 2	86. BD*(1) O 5- H 30	0.15	1.09	0.012
23. LP (1) O 2	92. BD*(1) C 8- C 10	0.57	1.02	0.021
23. LP (1) O 2	96. BD*(1) C 10- C 12	2.20	1.00	0.042
23. LP (1) O 2	100. BD*(1) C 12- H 25	2.52	1.00	0.045
23. LP (1) O 2	103. BD*(1) C 14- C 15	1.11	1.18	0.032
23. LP (1) O 2	104. BD*(1) C 14- C 16	6.35	1.19	0.078
23. LP (1) O 2	105. BD*(2) C 14- C 16	1.24	0.62	0.025
23. LP (1) O 2	106. BD*(1) C 15- C 17	0.22	1.20	0.014
23. LP (1) O 2	108. BD*(1) C 15- C 18	0.14	1.04	0.011
23. LP (1) O 2	109. BD*(1) C 16- C 19	0.22	1.19	0.014
23. LP (1) O 2	110. BD*(1) C 16- H 32	0.23	1.08	0.014
23. LP (1) O 2	113. BD*(1) C 18- H 34	0.40	1.02	0.018
23. LP (1) O 2	273. RY (2) C 10	0.14	1.96	0.015
23. LP (1) O 2	307. RY (2) C 12	1.59	3.12	0.063
23. LP (1) O 2	308. RY (3) C 12	0.26	2.34	0.022
23. LP (1) O 2	309. RY (4) C 12	0.11	2.14	0.014
23. LP (1) O 2	310. RY (5) C 12	0.11	2.23	0.014
23. LP (1) O 2	312. RY (7) C 12	0.22	2.36	0.020
23. LP (1) O 2	313. RY (8) C 12	0.16	2.30	0.017
23. LP (1) O 2	318. RY (13) C 12	0.16	4.20	0.023
23. LP (1) O 2	340. RY (1) C 14	1.93	1.75	0.052
23. LP (1) O 2	342. RY (3) C 14	0.11	2.94	0.016
23. LP (1) O 2	343. RY (4) C 14	0.38	2.38	0.027
23. LP (1) O 2	344. RY (5) C 14	0.21	1.51	0.016
23. LP (1) O 2	345. RY (6) C 14	0.13	2.22	0.015
23. LP (1) O 2	351. RY (12) C 14	0.14	2.71	0.017
24. LP (2) O 2	77. BD*(1) O 1- C 11	0.54	0.77	0.018
24. LP (2) O 2	78. BD*(1) O 1- C 12	15.40	0.78	0.098
24. LP (2) O 2	79. BD*(1) O 2- C 12	0.16	0.79	0.010
24. LP (2) O 2	86. BD*(1) O 5- H 30	0.21	0.94	0.013
24. LP (2) O 2	92. BD*(1) C 8- C 10	0.18	0.86	0.011
24. LP (2) O 2	96. BD*(1) C 10- C 12	0.75	0.84	0.022
24. LP (2) O 2	97. BD*(1) C 10- H 23	0.19	0.86	0.011
24. LP (2) O 2	100. BD*(1) C 12- H 25	3.67	0.84	0.050
24. LP (2) O 2	103. BD*(1) C 14- C 15	2.14	1.02	0.042
24. LP (2) O 2	104. BD*(1) C 14- C 16	1.33	1.03	0.033
24. LP (2) O 2	105. BD*(2) C 14- C 16	24.64	0.47	0.096
24. LP (2) O 2	106. BD*(1) C 15- C 17	0.13	1.04	0.011
24. LP (2) O 2	107. BD*(2) C 15- C 17	0.13	0.47	0.007
24. LP (2) O 2	121. RY (3) O 1	0.12	1.29	0.011
24. LP (2) O 2	306. RY (1) C 12	0.60	1.61	0.028
24. LP (2) O 2	308. RY (3) C 12	0.22	2.18	0.019
24. LP (2) O 2	310. RY (5) C 12	0.12	2.08	0.014
24. LP (2) O 2	311. RY (6) C 12	0.58	2.53	0.034
24. LP (2) O 2	316. RY (11) C 12	0.12	3.17	0.018
24. LP (2) O 2	341. RY (2) C 14	0.18	1.65	0.015
24. LP (2) O 2	342. RY (3) C 14	0.97	2.78	0.046

24. LP (2) O 2	343. RY (4) C 14	0.32	2.23	0.024
24. LP (2) O 2	345. RY (6) C 14	0.14	2.06	0.015
25. LP (1) O 3	84. BD*(1) O 4- H 29	0.18	1.14	0.013
25. LP (1) O 3	91. BD*(1) C 8- C 9	1.74	1.07	0.039
25. LP (1) O 3	92. BD*(1) C 8- C 10	1.32	1.07	0.034
25. LP (1) O 3	93. BD*(1) C 8- H 21	0.88	1.06	0.027
25. LP (1) O 3	94. BD*(1) C 9- C 11	0.36	1.05	0.017
25. LP (1) O 3	96. BD*(1) C 10- C 12	0.15	1.05	0.011
25. LP (1) O 3	97. BD*(1) C 10- H 23	0.19	1.07	0.013
25. LP (1) O 3	238. RY (1) C 8	1.81	1.57	0.048
25. LP (1) O 3	240. RY (3) C 8	0.75	1.64	0.031
25. LP (1) O 3	241. RY (4) C 8	0.17	2.17	0.017
25. LP (1) O 3	242. RY (5) C 8	0.39	2.25	0.026
25. LP (1) O 3	245. RY (8) C 8	0.15	3.22	0.020
25. LP (1) O 3	251. RY (14) C 8	0.12	2.19	0.015
25. LP (1) O 3	257. RY (3) C 9	0.11	1.56	0.012
25. LP (1) O 3	500. RY (2) H 28	1.09	2.56	0.047
26. LP (2) O 3	84. BD*(1) O 4- H 29	0.15	0.90	0.010
26. LP (2) O 3	85. BD*(1) O 5- C 10	0.19	0.77	0.011
26. LP (2) O 3	92. BD*(1) C 8- C 10	5.93	0.83	0.063
26. LP (2) O 3	93. BD*(1) C 8- H 21	8.91	0.83	0.077
26. LP (2) O 3	95. BD*(1) C 9- H 22	0.10	0.85	0.008
26. LP (2) O 3	96. BD*(1) C 10- C 12	0.73	0.81	0.022
26. LP (2) O 3	238. RY (1) C 8	0.14	1.34	0.012
26. LP (2) O 3	239. RY (2) C 8	0.45	1.53	0.023
26. LP (2) O 3	241. RY (4) C 8	1.07	1.93	0.041
26. LP (2) O 3	242. RY (5) C 8	0.15	2.02	0.015
26. LP (2) O 3	248. RY (11) C 8	0.16	1.38	0.013
26. LP (2) O 3	272. RY (1) C 10	0.14	1.48	0.013
26. LP (2) O 3	457. RY (1) H 21	0.18	1.17	0.013
26. LP (2) O 3	499. RY (1) H 28	1.68	2.04	0.052
27. LP (1) O 4	77. BD*(1) O 1- C 11	0.70	0.97	0.023
27. LP (1) O 4	91. BD*(1) C 8- C 9	1.40	1.06	0.034
27. LP (1) O 4	92. BD*(1) C 8- C 10	0.15	1.06	0.011
27. LP (1) O 4	93. BD*(1) C 8- H 21	0.20	1.06	0.013
27. LP (1) O 4	94. BD*(1) C 9- C 11	1.69	1.05	0.038
27. LP (1) O 4	95. BD*(1) C 9- H 22	0.73	1.07	0.025
27. LP (1) O 4	101. BD*(1) C 13- H 26	0.15	1.09	0.011
27. LP (1) O 4	255. RY (1) C 9	1.51	1.55	0.043
27. LP (1) O 4	256. RY (2) C 9	0.11	1.81	0.013
27. LP (1) O 4	257. RY (3) C 9	0.91	1.55	0.033
27. LP (1) O 4	258. RY (4) C 9	0.16	2.19	0.017
27. LP (1) O 4	259. RY (5) C 9	0.47	2.33	0.030
27. LP (1) O 4	289. RY (1) C 11	0.24	1.57	0.017
27. LP (1) O 4	506. RY (2) H 29	1.17	2.56	0.049
28. LP (2) O 4	81. BD*(1) O 3- C 8	0.18	0.76	0.011
28. LP (2) O 4	91. BD*(1) C 8- C 9	5.61	0.83	0.061
28. LP (2) O 4	92. BD*(1) C 8- C 10	0.76	0.83	0.022
28. LP (2) O 4	94. BD*(1) C 9- C 11	0.12	0.82	0.009
28. LP (2) O 4	95. BD*(1) C 9- H 22	9.01	0.84	0.078
28. LP (2) O 4	99. BD*(1) C 11- H 24	0.12	0.84	0.009
28. LP (2) O 4	238. RY (1) C 8	0.21	1.33	0.015
28. LP (2) O 4	256. RY (2) C 9	0.30	1.57	0.019
28. LP (2) O 4	258. RY (4) C 9	1.30	1.95	0.045
28. LP (2) O 4	259. RY (5) C 9	0.17	2.10	0.017
28. LP (2) O 4	463. RY (1) H 22	0.20	1.18	0.014
28. LP (2) O 4	505. RY (1) H 29	1.79	2.05	0.054
29. LP (1) O 5	78. BD*(1) O 1- C 12	0.14	0.96	0.010
29. LP (1) O 5	82. BD*(1) O 3- H 28	0.17	1.11	0.012
29. LP (1) O 5	91. BD*(1) C 8- C 9	0.40	1.05	0.018
29. LP (1) O 5	92. BD*(1) C 8- C 10	2.04	1.05	0.041
29. LP (1) O 5	96. BD*(1) C 10- C 12	1.13	1.03	0.030
29. LP (1) O 5	97. BD*(1) C 10- H 23	1.53	1.05	0.036
29. LP (1) O 5	100. BD*(1) C 12- H 25	0.24	1.02	0.014
29. LP (1) O 5	272. RY (1) C 10	1.97	1.69	0.052
29. LP (1) O 5	273. RY (2) C 10	0.11	1.98	0.013
29. LP (1) O 5	274. RY (3) C 10	0.69	1.86	0.032
29. LP (1) O 5	276. RY (5) C 10	0.40	2.40	0.028
29. LP (1) O 5	285. RY (14) C 10	0.21	3.53	0.024
29. LP (1) O 5	511. RY (1) H 30	1.03	2.50	0.045
29. LP (1) O 5	513. RY (3) H 30	0.16	2.18	0.017

30. LP (2) O 5	78. BD*(1) O 1- C 12	1.31	0.75	0.028
30. LP (2) O 5	79. BD*(1) O 2- C 12	0.20	0.76	0.011
30. LP (2) O 5	82. BD*(1) O 3- H 28	0.18	0.89	0.011
30. LP (2) O 5	93. BD*(1) C 8- H 21	0.12	0.83	0.009
30. LP (2) O 5	96. BD*(1) C 10- C 12	7.48	0.81	0.069
30. LP (2) O 5	97. BD*(1) C 10- H 23	8.44	0.83	0.075
30. LP (2) O 5	272. RY (1) C 10	0.26	1.47	0.018
30. LP (2) O 5	273. RY (2) C 10	0.14	1.77	0.014
30. LP (2) O 5	274. RY (3) C 10	0.35	1.65	0.021
30. LP (2) O 5	275. RY (4) C 10	0.97	1.79	0.037
30. LP (2) O 5	276. RY (5) C 10	0.10	2.18	0.013
30. LP (2) O 5	277. RY (6) C 10	0.15	2.67	0.018
30. LP (2) O 5	306. RY (1) C 12	0.25	1.58	0.018
30. LP (2) O 5	469. RY (1) H 23	0.18	1.28	0.014
30. LP (2) O 5	512. RY (2) H 30	1.37	2.08	0.048
31. LP (1) O 6	78. BD*(1) O 1- C 12	0.13	0.97	0.010
31. LP (1) O 6	98. BD*(1) C 11- C 13	1.26	1.05	0.032
31. LP (1) O 6	101. BD*(1) C 13- H 26	2.98	1.08	0.051
31. LP (1) O 6	102. BD*(1) C 13- H 27	0.82	1.06	0.026
31. LP (1) O 6	323. RY (1) C 13	1.48	1.60	0.043
31. LP (1) O 6	324. RY (2) C 13	0.24	1.62	0.018
31. LP (1) O 6	325. RY (3) C 13	0.49	1.93	0.027
31. LP (1) O 6	326. RY (4) C 13	0.17	1.59	0.015
31. LP (1) O 6	327. RY (5) C 13	0.48	2.42	0.031
31. LP (1) O 6	336. RY (14) C 13	0.14	2.02	0.015
31. LP (1) O 6	337. RY (15) C 13	0.12	3.52	0.018
31. LP (1) O 6	518. RY (2) H 31	1.17	2.46	0.048
31. LP (1) O 6	520. RY (4) H 31	0.13	2.35	0.016
32. LP (2) O 6	77. BD*(1) O 1- C 11	0.28	0.73	0.013
32. LP (2) O 6	95. BD*(1) C 9- H 22	0.20	0.83	0.012
32. LP (2) O 6	98. BD*(1) C 11- C 13	6.38	0.81	0.064
32. LP (2) O 6	99. BD*(1) C 11- H 24	0.80	0.83	0.023
32. LP (2) O 6	102. BD*(1) C 13- H 27	8.30	0.83	0.074
32. LP (2) O 6	119. RY (1) O 1	0.11	1.08	0.010
32. LP (2) O 6	289. RY (1) C 11	0.15	1.33	0.013
32. LP (2) O 6	323. RY (1) C 13	0.24	1.36	0.016
32. LP (2) O 6	324. RY (2) C 13	0.77	1.39	0.029
32. LP (2) O 6	325. RY (3) C 13	1.05	1.69	0.038
32. LP (2) O 6	335. RY (13) C 13	0.10	1.96	0.013
32. LP (2) O 6	493. RY (1) H 27	0.13	0.93	0.010
32. LP (2) O 6	517. RY (1) H 31	1.88	2.00	0.055
33. LP (1) O 7	86. BD*(1) O 5- H 30	3.28	1.14	0.055
33. LP (1) O 7	107. BD*(2) C 15- C 17	0.33	0.68	0.013
33. LP (1) O 7	108. BD*(1) C 15- C 18	2.68	1.09	0.048
33. LP (1) O 7	114. BD*(1) C 18- H 35	2.60	1.08	0.047
33. LP (1) O 7	406. RY (1) C 18	1.07	1.57	0.037
33. LP (1) O 7	408. RY (3) C 18	0.90	1.72	0.035
33. LP (1) O 7	409. RY (4) C 18	0.31	2.75	0.026
33. LP (1) O 7	413. RY (8) C 18	0.17	2.55	0.019
33. LP (1) O 7	559. RY (1) H 38	0.43	2.28	0.028
33. LP (1) O 7	560. RY (2) H 38	0.86	2.58	0.042
34. LP (2) O 7	86. BD*(1) O 5- H 30	5.65	0.95	0.065
34. LP (2) O 7	107. BD*(2) C 15- C 17	0.80	0.48	0.018
34. LP (2) O 7	108. BD*(1) C 15- C 18	3.39	0.89	0.049
34. LP (2) O 7	113. BD*(1) C 18- H 34	7.57	0.87	0.073
34. LP (2) O 7	114. BD*(1) C 18- H 35	0.50	0.89	0.019
34. LP (2) O 7	229. RY (9) O 7	0.10	2.34	0.014
34. LP (2) O 7	407. RY (2) C 18	1.33	1.83	0.044
34. LP (2) O 7	409. RY (4) C 18	0.29	2.55	0.024
34. LP (2) O 7	511. RY (1) H 30	0.14	2.33	0.016
34. LP (2) O 7	535. RY (1) H 34	0.10	0.97	0.009
34. LP (2) O 7	559. RY (1) H 38	1.47	2.09	0.050
34. LP (2) O 7	560. RY (2) H 38	0.32	2.39	0.025

Salicin (Conformer II)

Summary of Natural Population Analysis:

Atom No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
O 1	-0.63805	2.00000	6.61562	0.02243	8.63805
O 2	-0.58502	2.00000	6.56101	0.02401	8.58502
O 3	-0.76206	2.00000	6.74825	0.01382	8.76206
O 4	-0.74956	2.00000	6.73607	0.01349	8.74956
O 5	-0.78515	2.00000	6.77023	0.01493	8.78515
O 6	-0.73712	2.00000	6.72370	0.01343	8.73712
O 7	-0.75884	2.00000	6.74471	0.01413	8.75884
C 8	0.09752	1.99999	3.87638	0.02610	5.90248
C 9	0.09600	1.99999	3.87820	0.02581	5.90400
C 10	0.07661	1.99999	3.89682	0.02658	5.92339
C 11	0.09333	1.99999	3.88165	0.02503	5.90667
C 12	0.44759	1.99999	3.51927	0.03315	5.55241
C 13	-0.03202	1.99999	4.00873	0.02330	6.03202
C 14	0.33624	1.99999	3.63974	0.02403	5.66376
C 15	-0.11607	1.99999	4.10029	0.01578	6.11607
C 16	-0.26497	1.99999	4.24836	0.01661	6.26497
C 17	-0.19028	1.99999	4.17351	0.01678	6.19028
C 18	-0.03476	1.99999	4.01192	0.02284	6.03476
C 19	-0.18847	1.99999	4.17157	0.01690	6.18847
C 20	-0.22760	1.99999	4.21085	0.01675	6.22760
H 21	0.17584	0.00000	0.82113	0.00303	0.82416
H 22	0.17590	0.00000	0.82099	0.00311	0.82410
H 23	0.18427	0.00000	0.81299	0.00275	0.81573
H 24	0.18290	0.00000	0.81439	0.00271	0.81710
H 25	0.15970	0.00000	0.83734	0.00296	0.84030
H 26	0.16345	0.00000	0.83422	0.00233	0.83655
H 27	0.20365	0.00000	0.79466	0.00170	0.79635
H 28	0.48628	0.00000	0.50972	0.00400	0.51372
H 29	0.48274	0.00000	0.51319	0.00407	0.51726
H 30	0.51416	0.00000	0.48159	0.00424	0.48584
H 31	0.46679	0.00000	0.52856	0.00465	0.53321
H 32	0.23204	0.00000	0.76447	0.00349	0.76796
H 33	0.21388	0.00000	0.78436	0.00175	0.78612
H 34	0.17252	0.00000	0.82535	0.00213	0.82748
H 35	0.20221	0.00000	0.79565	0.00214	0.79779
H 36	0.21711	0.00000	0.78120	0.00169	0.78289
H 37	0.21748	0.00000	0.78083	0.00168	0.78252
H 38	0.47177	0.00000	0.52438	0.00385	0.52823
* Total *	0.00000	39.99990	111.54192	0.45817	152.00000

(Occupancy) Bond orbital / Coefficients / Hybrids

Lewis

21. (1.95919) LP (1) O 1 — s(42.49%)p 1.35(57.47%)d 0.00(0.03%)
0.0000 0.6517 0.0154 0.0014 0.0000
0.2200 -0.0019 -0.0024 0.0015 0.4022
0.0064 0.0008 0.0009 0.6037 0.0016
0.0036 -0.0006 -0.0069 -0.0063 -0.0120
0.0041 -0.0085

22. (1.92734) LP (2) O 1 — s(0.05%)p99.99(99.91%)d 0.78(0.04%)
0.0000 0.0204 -0.0076 0.0032 0.0001
0.4336 0.0090 0.0019 0.0002 0.6560
0.0123 0.0018 -0.0018 -0.6169 -0.0025
-0.0031 0.0030 -0.0083 -0.0033 -0.0029
0.0050 0.0163

23. (1.95786) LP (1) O 2 — s(34.16%)p 1.93(65.81%)d 0.00(0.03%)
0.0000 0.5843 0.0124 0.0014 0.0001
0.0911 -0.0036 -0.0021 0.0006 -0.6190
-0.0078 -0.0015 0.0009 0.5162 0.0064
-0.0033 -0.0003 0.0023 -0.0012 0.0152

```
                                      0.0081 -0.0065
24. (1.86554) LP ( 2) O  2           s(  2.17%)p45.03( 97.78%)d 0.02(  0.05%)
                                      0.0000  0.1472  0.0031 -0.0050  0.0004
                                     -0.2388  0.0017  0.0026 -0.0016  0.6736
                                      0.0054  0.0026 -0.0032  0.6833  0.0045
                                     -0.0062 -0.0034 -0.0027  0.0049 -0.0049
                                     -0.0060 -0.0192
25. (1.98024) LP ( 1) O  3           s( 47.76%)p 1.09( 52.20%)d 0.00(  0.03%)
                                      0.0000  0.6911  0.0087  0.0023  0.0001
                                     -0.6526 -0.0052 -0.0012 -0.0014 -0.0495
                                      0.0069 -0.0016  0.0009  0.3060  0.0016
                                      0.0005  0.0001 -0.0019  0.0104  0.0011
                                     -0.0143  0.0018
26. (1.96028) LP ( 2) O  3           s(  0.04%)p99.99( 99.92%)d 1.31(  0.05%)
                                      0.0000  0.0184 -0.0023  0.0033  0.0000
                                     -0.4114 -0.0085  0.0022  0.0007  0.0639
                                     -0.0005 -0.0004 -0.0007 -0.9085 -0.0168
                                     -0.0021  0.0037  0.0008 -0.0146 -0.0005
                                     -0.0082  0.0134
27. (1.98042) LP ( 1) O  4           s( 48.07%)p 1.08( 51.90%)d 0.00(  0.03%)
                                      0.0000  0.6933 -0.0080  0.0024  0.0000
                                     -0.2846  0.0028 -0.0008  0.0004  0.6051
                                      0.0052 -0.0004  0.0023 -0.2680  0.0005
                                     -0.0008 -0.0001  0.0117 -0.0025  0.0102
                                      0.0094  0.0032
28. (1.95902) LP ( 2) O  4           s(  0.07%)p99.99( 99.88%)d 0.69(  0.05%)
                                      0.0000  0.0266 -0.0038 -0.0019  0.0000
                                      0.4561  0.0108  0.0005  0.0003 -0.1997
                                     -0.0030  0.0025  0.0009 -0.8663 -0.0161
                                     -0.0024  0.0034 -0.0104 -0.0023  0.0151
                                     -0.0002 -0.0125
29. (1.97891) LP ( 1) O  5           s( 44.98%)p 1.22( 54.99%)d 0.00(  0.03%)
                                      0.0000  0.6706  0.0095  0.0024  0.0002
                                     -0.2478 -0.0061  0.0034 -0.0012 -0.4129
                                     -0.0017 -0.0027 -0.0009 -0.5639 -0.0042
                                     -0.0013  0.0000 -0.0077 -0.0073 -0.0119
                                      0.0045 -0.0066
30. (1.95388) LP ( 2) O  5           s(  0.16%)p99.99( 99.79%)d 0.27(  0.04%)
                                      0.0000  0.0404 -0.0025  0.0036  0.0002
                                     -0.3220 -0.0050  0.0030  0.0005 -0.6625
                                     -0.0152 -0.0016  0.0013  0.6744  0.0134
                                      0.0047 -0.0021 -0.0092  0.0002 -0.0007
                                      0.0066  0.0176
31. (1.98165) LP ( 1) O  6           s( 48.99%)p 1.04( 50.97%)d 0.00(  0.04%)
                                      0.0000  0.6999  0.0119  0.0002  0.0000
                                     -0.1078 -0.0024 -0.0012 -0.0014  0.6119
                                      0.0052 -0.0044  0.0015 -0.3515 -0.0028
                                      0.0014 -0.0002  0.0067 -0.0011  0.0120
                                      0.0127  0.0011
32. (1.95760) LP ( 2) O  6           s(  0.06%)p99.99( 99.89%)d 0.84(  0.05%)
                                      0.0000  0.0245 -0.0004  0.0046  0.0002
                                     -0.3479 -0.0051  0.0025  0.0004  0.3978
                                      0.0075  0.0024 -0.0007  0.8480  0.0198
                                     -0.0031 -0.0027  0.0092  0.0017 -0.0125
                                      0.0060  0.0157
33. (1.97568) LP ( 1) O  7           s( 44.79%)p 1.23( 55.18%)d 0.00(  0.03%)
                                      0.0000  0.6692  0.0075 -0.0003  0.0000
                                     -0.3709  0.0004  0.0057 -0.0013 -0.5973
                                     -0.0091  0.0064  0.0008  0.2392  0.0040
                                      0.0030  0.0009 -0.0120  0.0054  0.0088
                                      0.0026  0.0070
34. (1.95834) LP ( 2) O  7           s(  3.88%)p24.76( 96.08%)d 0.01(  0.04%)
                                      0.0000  0.1967  0.0100 -0.0005 -0.0001
                                     -0.7464 -0.0192  0.0009 -0.0002  0.5943
                                      0.0120  0.0000 -0.0025 -0.2235 -0.0019
                                      0.0052  0.0004  0.0009  0.0019 -0.0072
                                     -0.0176  0.0049

82. (0.00721) BD*( 1) O  3- H 28
            ( 25.39%)   0.5039* O  3 s( 20.94%)p 3.77( 78.93%)d 0.01(  0.13%)
                                      0.0000 -0.4575  0.0084 -0.0006  0.0002
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                                    -0.4293 -0.0059  0.0023 -0.0001  0.7400
                                    -0.0315  0.0053  0.0023  0.2373 -0.0002
                                     0.0005 -0.0006  0.0274  0.0151 -0.0140
                                    -0.0005  0.0132
             ( 74.61%)  -0.8638* H 28 s( 99.88%)p 0.00(  0.12%)
                                    -0.9994  0.0034 -0.0006  0.0000  0.0135
                                    -0.0321 -0.0060
83. (0.01777) BD*( 1) O  4- C  9
             ( 33.87%)   0.5820* O  4 s( 31.07%)p 2.22( 68.84%)d 0.00(  0.08%)
                                     0.0000 -0.5573 -0.0088  0.0054  0.0001
                                    -0.7069  0.0085  0.0060  0.0023  0.1208
                                     0.0018 -0.0070 -0.0003 -0.4171  0.0059
                                     0.0036  0.0005  0.0126 -0.0207  0.0101
                                    -0.0103  0.0058
             ( 66.13%)  -0.8132* C  9 s( 21.38%)p 3.67( 78.41%)d 0.01(  0.21%)
                                     0.0000 -0.4603  0.0438  0.0016  0.0008
                                     0.7746  0.0431 -0.0006 -0.0052 -0.0967
                                     0.0168 -0.0001 -0.0024  0.4153 -0.0054
                                    -0.0076  0.0070  0.0060 -0.0359  0.0022
                                    -0.0272  0.0070
84. (0.00756) BD*( 1) O  4- H 29
             ( 25.56%)   0.5056* O  4 s( 20.76%)p 3.81( 79.10%)d 0.01(  0.14%)
                                     0.0000 -0.4556 -0.0076 -0.0014  0.0000
                                     0.4577 -0.0268  0.0062 -0.0010  0.7601
                                    -0.0104  0.0006  0.0008  0.0518 -0.0127
                                     0.0014 -0.0003 -0.0179  0.0002  0.0052
                                     0.0259  0.0189
             ( 74.44%)  -0.8628* H 29 s( 99.87%)p 0.00(  0.13%)
                                    -0.9993  0.0033 -0.0008  0.0000 -0.0226
                                    -0.0279 -0.0058
85. (0.01890) BD*( 1) O  5- C 10
             ( 34.15%)   0.5844* O  5 s( 30.98%)p 2.23( 68.94%)d 0.00(  0.08%)
                                     0.0000 -0.5565  0.0088  0.0042 -0.0003
                                     0.3991 -0.0122 -0.0010  0.0022 -0.6186
                                     0.0084  0.0055  0.0002 -0.3837  0.0045
                                     0.0026  0.0007  0.0112  0.0063 -0.0223
                                     0.0115  0.0020
             ( 65.85%)  -0.8115* C 10 s( 21.83%)p 3.57( 77.96%)d 0.01(  0.21%)
                                     0.0000 -0.4654  0.0413 -0.0021  0.0002
                                    -0.4544 -0.0087 -0.0022 -0.0026  0.6617
                                     0.0407  0.0019 -0.0053  0.3652 -0.0071
                                    -0.0063  0.0083  0.0283  0.0192 -0.0265
                                     0.0089  0.0106
86. (0.02165) BD*( 1) O  5- H 30
             ( 23.42%)   0.4839* O  5 s( 23.86%)p 3.19( 76.01%)d 0.01(  0.13%)
                                     0.0000 -0.4884  0.0085  0.0002  0.0007
                                    -0.8204  0.0263  0.0013 -0.0026  0.0831
                                    -0.0207  0.0051 -0.0001 -0.2810 -0.0067
                                     0.0025  0.0008 -0.0057 -0.0254 -0.0047
                                    -0.0228  0.0061
             ( 76.58%)  -0.8751* H 30 s( 99.84%)p 0.00(  0.16%)
                                    -0.9992  0.0061  0.0001  0.0004  0.0387
                                    -0.0077  0.0067
87. (0.00781) BD*( 1) O  6- C 13
             ( 33.70%)   0.5805* O  6 s( 30.25%)p 2.30( 69.66%)d 0.00(  0.09%)
                                     0.0000 -0.5498  0.0143  0.0030 -0.0001
                                     0.4978 -0.0153  0.0004  0.0015  0.6635
                                     0.0002  0.0080  0.0008 -0.0912 -0.0007
                                    -0.0038  0.0005 -0.0176  0.0022  0.0112
                                     0.0155  0.0140
             ( 66.30%)  -0.8142* C 13 s( 21.93%)p 3.55( 77.83%)d 0.01(  0.24%)
                                     0.0000 -0.4657  0.0497 -0.0013  0.0007
                                    -0.5335 -0.0042  0.0001  0.0034 -0.6969
                                    -0.0600  0.0009  0.0033  0.0653  0.0035
                                     0.0031 -0.0028 -0.0410  0.0065  0.0036
                                     0.0046  0.0248
88. (0.00910) BD*( 1) O  6- H 31
             ( 26.27%)   0.5125* O  6 s( 20.69%)p 3.83( 79.17%)d 0.01(  0.14%)
                                     0.0000 -0.4548  0.0094 -0.0027  0.0002
                                    -0.7853  0.0342  0.0001 -0.0017  0.1606
                                     0.0126  0.0043  0.0001 -0.3844  0.0075
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                                     0.0005  0.0010  0.0198 -0.0248  0.0140
                                    -0.0136  0.0071
               ( 73.73%)  -0.8587* H 31 s( 99.87%)p 0.00(  0.13%)
                                    -0.9993  0.0041 -0.0003 -0.0001  0.0341
                                    -0.0017  0.0129
107. (0.35153) BD*( 2) C 15- C 17
               ( 47.81%)   0.6915* C 15 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.03%)
                                     0.0000 -0.0014  0.0030 -0.0002  0.1379
                                    -0.0015  0.0022 -0.0009  0.3919  0.0029
                                     0.0155  0.0024  0.9091 -0.0139  0.0063
                                    -0.0099  0.0057  0.0058  0.0099 -0.0027
                                    -0.0132
               ( 52.19%)  -0.7224* C 17 s(  0.00%)p 1.00( 99.95%)d 0.00(  0.05%)
                                     0.0000 -0.0001 -0.0043  0.0004 -0.0017
                                     0.1397  0.0031  0.0030  0.0000  0.4067
                                     0.0068  0.0084 -0.0002  0.9023  0.0129
                                     0.0110 -0.0048 -0.0101 -0.0191  0.0004
                                    -0.0048  0.0060
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SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

Threshold for printing: 0.10 kcal/mol

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
within unit 1				
21. LP (1) O 1	79. BD*(1) O 2- C 12	5.40	0.97	0.065
21. LP (1) O 1	88. BD*(1) O 6- H 31	0.33	1.12	0.017
21. LP (1) O 1	94. BD*(1) C 9- C 11	0.57	1.03	0.022
21. LP (1) O 1	95. BD*(1) C 9- H 22	0.14	1.04	0.011
21. LP (1) O 1	96. BD*(1) C 10- C 12	0.57	1.03	0.022
21. LP (1) O 1	97. BD*(1) C 10- H 23	0.14	1.04	0.011
21. LP (1) O 1	98. BD*(1) C 11- C 13	1.70	1.05	0.038
21. LP (1) O 1	99. BD*(1) C 11- H 24	1.39	1.05	0.034
21. LP (1) O 1	100. BD*(1) C 12- H 25	1.34	1.02	0.033
21. LP (1) O 1	102. BD*(1) C 13- H 27	0.47	1.08	0.020
21. LP (1) O 1	124. RY (6) O 1	0.16	2.19	0.017
21. LP (1) O 1	125. RY (7) O 1	0.10	1.85	0.012
21. LP (1) O 1	289. RY (1) C 11	1.63	1.53	0.045
21. LP (1) O 1	290. RY (2) C 11	0.45	2.13	0.028
21. LP (1) O 1	291. RY (3) C 11	0.26	1.93	0.020
21. LP (1) O 1	292. RY (4) C 11	0.17	2.61	0.019
21. LP (1) O 1	295. RY (7) C 11	0.13	3.79	0.020
21. LP (1) O 1	303. RY (15) C 11	0.12	3.32	0.018
21. LP (1) O 1	306. RY (1) C 12	2.24	1.81	0.057
21. LP (1) O 1	307. RY (2) C 12	0.13	3.14	0.018
21. LP (1) O 1	308. RY (3) C 12	0.18	2.36	0.018
21. LP (1) O 1	309. RY (4) C 12	0.15	2.27	0.017
21. LP (1) O 1	310. RY (5) C 12	0.33	2.20	0.024
21. LP (1) O 1	316. RY (11) C 12	0.12	3.22	0.018
21. LP (1) O 1	322. RY (17) C 12	0.13	3.49	0.019
22. LP (2) O 1	83. BD*(1) O 4- C 9	1.15	0.77	0.027
22. LP (2) O 1	85. BD*(1) O 5- C 10	1.10	0.78	0.026
22. LP (2) O 1	88. BD*(1) O 6- H 31	0.21	0.91	0.013
22. LP (2) O 1	94. BD*(1) C 9- C 11	6.44	0.83	0.065
22. LP (2) O 1	96. BD*(1) C 10- C 12	6.95	0.82	0.068
22. LP (2) O 1	99. BD*(1) C 11- H 24	6.47	0.85	0.066
22. LP (2) O 1	100. BD*(1) C 12- H 25	7.39	0.82	0.070
22. LP (2) O 1	110. BD*(1) C 16- H 32	0.37	0.90	0.016
22. LP (2) O 1	272. RY (1) C 10	0.18	1.49	0.014
22. LP (2) O 1	289. RY (1) C 11	0.14	1.33	0.012
22. LP (2) O 1	292. RY (4) C 11	0.67	2.41	0.036
22. LP (2) O 1	294. RY (6) C 11	0.16	2.37	0.017
22. LP (2) O 1	306. RY (1) C 12	0.13	1.61	0.013
22. LP (2) O 1	308. RY (3) C 12	0.12	2.16	0.014
22. LP (2) O 1	309. RY (4) C 12	0.58	2.07	0.031
22. LP (2) O 1	310. RY (5) C 12	0.55	2.00	0.030

22. LP (2) O 1	311. RY (6) C 12	0.37	2.47	0.027
22. LP (2) O 1	475. RY (1) H 24	0.24	1.27	0.016
22. LP (2) O 1	481. RY (1) H 25	0.18	1.31	0.014
23. LP (1) O 2	78. BD*(1) O 1- C 12	0.49	0.94	0.019
23. LP (1) O 2	86. BD*(1) O 5- H 30	0.16	1.09	0.012
23. LP (1) O 2	92. BD*(1) C 8- C 10	0.55	1.01	0.021
23. LP (1) O 2	96. BD*(1) C 10- C 12	2.21	1.00	0.042
23. LP (1) O 2	100. BD*(1) C 12- H 25	2.64	1.00	0.046
23. LP (1) O 2	103. BD*(1) C 14- C 15	1.13	1.18	0.033
23. LP (1) O 2	104. BD*(1) C 14- C 16	6.40	1.19	0.078
23. LP (1) O 2	105. BD*(2) C 14- C 16	1.14	0.62	0.024
23. LP (1) O 2	106. BD*(1) C 15- C 17	0.22	1.20	0.015
23. LP (1) O 2	108. BD*(1) C 15- C 18	0.14	1.04	0.011
23. LP (1) O 2	109. BD*(1) C 16- C 19	0.22	1.19	0.014
23. LP (1) O 2	110. BD*(1) C 16- H 32	0.24	1.07	0.014
23. LP (1) O 2	113. BD*(1) C 18- H 34	0.41	1.02	0.018
23. LP (1) O 2	273. RY (2) C 10	0.15	1.89	0.015
23. LP (1) O 2	307. RY (2) C 12	1.63	3.11	0.064
23. LP (1) O 2	308. RY (3) C 12	0.25	2.33	0.021
23. LP (1) O 2	309. RY (4) C 12	0.11	2.24	0.014
23. LP (1) O 2	312. RY (7) C 12	0.17	2.40	0.018
23. LP (1) O 2	313. RY (8) C 12	0.15	2.44	0.017
23. LP (1) O 2	318. RY (13) C 12	0.18	4.60	0.025
23. LP (1) O 2	340. RY (1) C 14	1.96	1.76	0.052
23. LP (1) O 2	343. RY (4) C 14	0.39	2.36	0.027
23. LP (1) O 2	344. RY (5) C 14	0.21	1.50	0.016
23. LP (1) O 2	345. RY (6) C 14	0.12	2.29	0.015
23. LP (1) O 2	351. RY (12) C 14	0.14	2.77	0.017
24. LP (2) O 2	77. BD*(1) O 1- C 11	0.52	0.77	0.018
24. LP (2) O 2	78. BD*(1) O 1- C 12	15.58	0.78	0.098
24. LP (2) O 2	79. BD*(1) O 2- C 12	0.15	0.79	0.010
24. LP (2) O 2	86. BD*(1) O 5- H 30	0.22	0.93	0.013
24. LP (2) O 2	92. BD*(1) C 8- C 10	0.19	0.86	0.011
24. LP (2) O 2	96. BD*(1) C 10- C 12	0.82	0.84	0.023
24. LP (2) O 2	97. BD*(1) C 10- H 23	0.18	0.86	0.011
24. LP (2) O 2	100. BD*(1) C 12- H 25	3.60	0.84	0.049
24. LP (2) O 2	103. BD*(1) C 14- C 15	1.98	1.02	0.040
24. LP (2) O 2	104. BD*(1) C 14- C 16	1.24	1.03	0.032
24. LP (2) O 2	105. BD*(2) C 14- C 16	25.42	0.47	0.097
24. LP (2) O 2	106. BD*(1) C 15- C 17	0.13	1.04	0.010
24. LP (2) O 2	107. BD*(2) C 15- C 17	0.13	0.47	0.007
24. LP (2) O 2	121. RY (3) O 1	0.16	1.24	0.012
24. LP (2) O 2	306. RY (1) C 12	0.60	1.63	0.028
24. LP (2) O 2	308. RY (3) C 12	0.21	2.17	0.019
24. LP (2) O 2	310. RY (5) C 12	0.12	2.01	0.014
24. LP (2) O 2	311. RY (6) C 12	0.62	2.49	0.035
24. LP (2) O 2	316. RY (11) C 12	0.13	3.04	0.018
24. LP (2) O 2	341. RY (2) C 14	0.18	1.64	0.015
24. LP (2) O 2	342. RY (3) C 14	1.01	2.82	0.048
24. LP (2) O 2	343. RY (4) C 14	0.28	2.20	0.022
24. LP (2) O 2	344. RY (5) C 14	0.11	1.34	0.011
24. LP (2) O 2	345. RY (6) C 14	0.12	2.14	0.014
25. LP (1) O 3	84. BD*(1) O 4- H 29	0.20	1.13	0.013
25. LP (1) O 3	91. BD*(1) C 8- C 9	1.77	1.06	0.039
25. LP (1) O 3	92. BD*(1) C 8- C 10	1.24	1.07	0.032
25. LP (1) O 3	93. BD*(1) C 8- H 21	0.96	1.06	0.029
25. LP (1) O 3	94. BD*(1) C 9- C 11	0.37	1.06	0.018
25. LP (1) O 3	96. BD*(1) C 10- C 12	0.14	1.05	0.011
25. LP (1) O 3	97. BD*(1) C 10- H 23	0.20	1.07	0.013
25. LP (1) O 3	238. RY (1) C 8	1.82	1.56	0.048
25. LP (1) O 3	240. RY (3) C 8	0.80	1.58	0.032
25. LP (1) O 3	241. RY (4) C 8	0.17	2.17	0.017
25. LP (1) O 3	242. RY (5) C 8	0.38	2.25	0.026
25. LP (1) O 3	245. RY (8) C 8	0.16	2.96	0.019
25. LP (1) O 3	251. RY (14) C 8	0.11	2.91	0.016
25. LP (1) O 3	257. RY (3) C 9	0.13	1.45	0.012
25. LP (1) O 3	499. RY (1) H 28	0.11	2.28	0.014
25. LP (1) O 3	500. RY (2) H 28	1.09	2.56	0.047
26. LP (2) O 3	84. BD*(1) O 4- H 29	0.20	0.90	0.012
26. LP (2) O 3	85. BD*(1) O 5- C 10	0.18	0.77	0.011
26. LP (2) O 3	92. BD*(1) C 8- C 10	6.11	0.83	0.064

26. LP (2) O 3	93. BD*(1) C 8- H 21	8.71	0.83	0.076
26. LP (2) O 3	95. BD*(1) C 9- H 22	0.11	0.83	0.008
26. LP (2) O 3	96. BD*(1) C 10- C 12	0.73	0.82	0.022
26. LP (2) O 3	238. RY (1) C 8	0.15	1.32	0.013
26. LP (2) O 3	239. RY (2) C 8	0.43	1.50	0.023
26. LP (2) O 3	241. RY (4) C 8	1.08	1.94	0.041
26. LP (2) O 3	242. RY (5) C 8	0.15	2.02	0.015
26. LP (2) O 3	248. RY (11) C 8	0.10	1.70	0.012
26. LP (2) O 3	272. RY (1) C 10	0.13	1.49	0.012
26. LP (2) O 3	457. RY (1) H 21	0.19	1.18	0.013
26. LP (2) O 3	499. RY (1) H 28	1.66	2.05	0.052
27. LP (1) O 4	77. BD*(1) O 1- C 11	0.57	0.97	0.021
27. LP (1) O 4	91. BD*(1) C 8- C 9	1.78	1.06	0.039
27. LP (1) O 4	92. BD*(1) C 8- C 10	0.20	1.06	0.013
27. LP (1) O 4	93. BD*(1) C 8- H 21	0.20	1.06	0.013
27. LP (1) O 4	94. BD*(1) C 9- C 11	1.65	1.05	0.037
27. LP (1) O 4	95. BD*(1) C 9- H 22	0.49	1.06	0.020
27. LP (1) O 4	102. BD*(1) C 13- H 27	0.10	1.09	0.009
27. LP (1) O 4	255. RY (1) C 9	1.91	1.59	0.049
27. LP (1) O 4	257. RY (3) C 9	0.70	1.44	0.028
27. LP (1) O 4	258. RY (4) C 9	0.16	2.22	0.017
27. LP (1) O 4	259. RY (5) C 9	0.51	2.37	0.031
27. LP (1) O 4	269. RY (15) C 9	0.16	3.98	0.023
27. LP (1) O 4	289. RY (1) C 11	0.24	1.54	0.017
27. LP (1) O 4	506. RY (2) H 29	1.17	2.56	0.049
28. LP (2) O 4	77. BD*(1) O 1- C 11	0.10	0.74	0.008
28. LP (2) O 4	81. BD*(1) O 3- C 8	0.17	0.76	0.010
28. LP (2) O 4	91. BD*(1) C 8- C 9	4.95	0.83	0.057
28. LP (2) O 4	92. BD*(1) C 8- C 10	0.66	0.83	0.021
28. LP (2) O 4	94. BD*(1) C 9- C 11	0.32	0.82	0.015
28. LP (2) O 4	95. BD*(1) C 9- H 22	9.95	0.83	0.081
28. LP (2) O 4	99. BD*(1) C 11- H 24	0.10	0.84	0.008
28. LP (2) O 4	238. RY (1) C 8	0.21	1.32	0.015
28. LP (2) O 4	256. RY (2) C 9	0.44	1.52	0.023
28. LP (2) O 4	258. RY (4) C 9	1.19	1.99	0.043
28. LP (2) O 4	259. RY (5) C 9	0.11	2.14	0.013
28. LP (2) O 4	463. RY (1) H 22	0.20	1.18	0.014
28. LP (2) O 4	505. RY (1) H 29	1.78	2.05	0.054
29. LP (1) O 5	78. BD*(1) O 1- C 12	0.14	0.97	0.010
29. LP (1) O 5	82. BD*(1) O 3- H 28	0.15	1.11	0.011
29. LP (1) O 5	91. BD*(1) C 8- C 9	0.41	1.04	0.018
29. LP (1) O 5	92. BD*(1) C 8- C 10	2.03	1.04	0.041
29. LP (1) O 5	96. BD*(1) C 10- C 12	1.17	1.03	0.031
29. LP (1) O 5	97. BD*(1) C 10- H 23	1.48	1.05	0.035
29. LP (1) O 5	100. BD*(1) C 12- H 25	0.24	1.03	0.014
29. LP (1) O 5	272. RY (1) C 10	2.00	1.70	0.052
29. LP (1) O 5	273. RY (2) C 10	0.13	1.92	0.014
29. LP (1) O 5	274. RY (3) C 10	0.65	1.86	0.031
29. LP (1) O 5	276. RY (5) C 10	0.40	2.44	0.028
29. LP (1) O 5	285. RY (14) C 10	0.21	3.56	0.024
29. LP (1) O 5	511. RY (1) H 30	1.02	2.50	0.045
29. LP (1) O 5	513. RY (3) H 30	0.15	2.18	0.016
30. LP (2) O 5	78. BD*(1) O 1- C 12	1.28	0.75	0.028
30. LP (2) O 5	79. BD*(1) O 2- C 12	0.20	0.76	0.011
30. LP (2) O 5	82. BD*(1) O 3- H 28	0.16	0.89	0.011
30. LP (2) O 5	93. BD*(1) C 8- H 21	0.12	0.82	0.009
30. LP (2) O 5	96. BD*(1) C 10- C 12	7.42	0.81	0.069
30. LP (2) O 5	97. BD*(1) C 10- H 23	8.54	0.83	0.075
30. LP (2) O 5	272. RY (1) C 10	0.28	1.48	0.018
30. LP (2) O 5	273. RY (2) C 10	0.14	1.71	0.014
30. LP (2) O 5	274. RY (3) C 10	0.39	1.64	0.023
30. LP (2) O 5	275. RY (4) C 10	0.95	1.78	0.037
30. LP (2) O 5	277. RY (6) C 10	0.16	2.50	0.018
30. LP (2) O 5	306. RY (1) C 12	0.24	1.60	0.017
30. LP (2) O 5	469. RY (1) H 23	0.19	1.28	0.014
30. LP (2) O 5	512. RY (2) H 30	1.37	2.08	0.048
31. LP (1) O 6	78. BD*(1) O 1- C 12	0.10	0.97	0.009
31. LP (1) O 6	98. BD*(1) C 11- C 13	0.95	1.06	0.028
31. LP (1) O 6	99. BD*(1) C 11- H 24	0.16	1.06	0.011
31. LP (1) O 6	101. BD*(1) C 13- H 26	1.04	1.06	0.030
31. LP (1) O 6	102. BD*(1) C 13- H 27	3.02	1.09	0.051

31. LP (1) O 6	323. RY (1) C 13	1.60	1.56	0.045
31. LP (1) O 6	325. RY (3) C 13	0.60	2.03	0.031
31. LP (1) O 6	326. RY (4) C 13	0.44	2.19	0.028
31. LP (1) O 6	335. RY (13) C 13	0.12	3.43	0.018
31. LP (1) O 6	518. RY (2) H 31	1.19	2.44	0.048
31. LP (1) O 6	520. RY (4) H 31	0.11	2.47	0.014
32. LP (2) O 6	77. BD*(1) O 1- C 11	0.33	0.73	0.014
32. LP (2) O 6	94. BD*(1) C 9- C 11	0.97	0.81	0.025
32. LP (2) O 6	98. BD*(1) C 11- C 13	6.53	0.82	0.065
32. LP (2) O 6	101. BD*(1) C 13- H 26	7.67	0.82	0.071
32. LP (2) O 6	289. RY (1) C 11	0.21	1.30	0.015
32. LP (2) O 6	323. RY (1) C 13	0.23	1.32	0.016
32. LP (2) O 6	324. RY (2) C 13	0.85	1.45	0.031
32. LP (2) O 6	325. RY (3) C 13	0.79	1.79	0.034
32. LP (2) O 6	327. RY (5) C 13	0.18	1.59	0.015
32. LP (2) O 6	487. RY (1) H 26	0.13	1.02	0.010
32. LP (2) O 6	517. RY (1) H 31	1.89	1.91	0.054
33. LP (1) O 7	86. BD*(1) O 5- H 30	3.24	1.14	0.054
33. LP (1) O 7	107. BD*(2) C 15- C 17	0.32	0.68	0.013
33. LP (1) O 7	108. BD*(1) C 15- C 18	2.58	1.09	0.047
33. LP (1) O 7	114. BD*(1) C 18- H 35	2.63	1.08	0.048
33. LP (1) O 7	406. RY (1) C 18	1.08	1.58	0.037
33. LP (1) O 7	408. RY (3) C 18	0.87	1.72	0.035
33. LP (1) O 7	409. RY (4) C 18	0.32	2.74	0.027
33. LP (1) O 7	413. RY (8) C 18	0.14	2.12	0.016
33. LP (1) O 7	559. RY (1) H 38	0.40	2.28	0.027
33. LP (1) O 7	560. RY (2) H 38	0.89	2.59	0.043
34. LP (2) O 7	86. BD*(1) O 5- H 30	5.35	0.95	0.063
34. LP (2) O 7	107. BD*(2) C 15- C 17	0.83	0.48	0.018
34. LP (2) O 7	108. BD*(1) C 15- C 18	3.53	0.89	0.050
34. LP (2) O 7	113. BD*(1) C 18- H 34	7.54	0.87	0.072
34. LP (2) O 7	114. BD*(1) C 18- H 35	0.44	0.88	0.018
34. LP (2) O 7	229. RY (9) O 7	0.10	2.34	0.014
34. LP (2) O 7	407. RY (2) C 18	1.33	1.83	0.044
34. LP (2) O 7	409. RY (4) C 18	0.28	2.54	0.024
34. LP (2) O 7	511. RY (1) H 30	0.13	2.32	0.015
34. LP (2) O 7	535. RY (1) H 34	0.11	0.97	0.009
34. LP (2) O 7	559. RY (1) H 38	1.52	2.08	0.050
34. LP (2) O 7	560. RY (2) H 38	0.30	2.39	0.024

Salicin (Conformer III)

Summary of Natural Population Analysis:

Atom No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
O 1	-0.62162	2.00000	6.59967	0.02195	8.62162
O 2	-0.58609	2.00000	6.56204	0.02405	8.58609
O 3	-0.76356	2.00000	6.74990	0.01367	8.76356
O 4	-0.77215	2.00000	6.75879	0.01336	8.77215
O 5	-0.78595	2.00000	6.77089	0.01506	8.78595
O 6	-0.75071	2.00000	6.73698	0.01374	8.75071
O 7	-0.75957	2.00000	6.74536	0.01421	8.75957
C 8	0.09525	1.99999	3.87891	0.02585	5.90475
C 9	0.09693	1.99999	3.87793	0.02514	5.90307
C 10	0.07707	1.99999	3.89628	0.02665	5.92293
C 11	0.09307	1.99999	3.88312	0.02382	5.90693
C 12	0.44737	1.99999	3.51961	0.03303	5.55263
C 13	-0.02765	1.99999	4.00277	0.02488	6.02765
C 14	0.33509	1.99999	3.64069	0.02423	5.66491
C 15	-0.11668	1.99999	4.10088	0.01580	6.11668
C 16	-0.26186	1.99999	4.24525	0.01662	6.26186
C 17	-0.19167	1.99999	4.17484	0.01684	6.19167
C 18	-0.03417	1.99999	4.01142	0.02276	6.03417
C 19	-0.18909	1.99999	4.17238	0.01672	6.18909
C 20	-0.22766	1.99999	4.21088	0.01679	6.22766
H 21	0.17706	0.00000	0.81992	0.00302	0.82294
H 22	0.17830	0.00000	0.81864	0.00306	0.82170
H 23	0.18442	0.00000	0.81277	0.00282	0.81558
H 24	0.18081	0.00000	0.81617	0.00302	0.81919
H 25	0.15875	0.00000	0.83833	0.00292	0.84125
H 26	0.18835	0.00000	0.80931	0.00235	0.81165
H 27	0.16180	0.00000	0.83597	0.00224	0.83820
H 28	0.48728	0.00000	0.50871	0.00400	0.51272
H 29	0.49205	0.00000	0.50406	0.00390	0.50795
H 30	0.51486	0.00000	0.48089	0.00425	0.48514
H 31	0.48885	0.00000	0.50707	0.00408	0.51115
H 32	0.23700	0.00000	0.76019	0.00281	0.76300
H 33	0.21363	0.00000	0.78461	0.00176	0.78637
H 34	0.17246	0.00000	0.82542	0.00212	0.82754
H 35	0.20217	0.00000	0.79569	0.00214	0.79783
H 36	0.21644	0.00000	0.78187	0.00168	0.78356
H 37	0.21725	0.00000	0.78107	0.00167	0.78275
H 38	0.47217	0.00000	0.52400	0.00383	0.52783
* Total *	0.00000	39.99990	111.54328	0.45682	152.00000

(Occupancy) Bond orbital / Coefficients / Hybrids

---------- Lewis ----------

21. (1.95858) LP (1) O 1 s(42.83%)p 1.33(57.13%)d 0.00(0.03%)
0.0000 0.6543 0.0148 0.0019 0.0000
-0.2305 0.0029 0.0033 -0.0013 -0.4152
-0.0048 0.0018 -0.0008 0.5880 0.0023
-0.0034 -0.0003 -0.0073 0.0068 0.0126
0.0049 -0.0083

22. (1.92576) LP (2) O 1 s(0.01%)p 1.00(99.95%)d 0.00(0.04%)
0.0000 -0.0034 0.0072 -0.0029 -0.0001
0.3862 0.0073 0.0004 0.0002 0.6729
0.0137 -0.0031 -0.0020 0.6303 0.0036
-0.0025 -0.0030 0.0082 -0.0024 -0.0030
-0.0057 -0.0172

23. (1.95742) LP (1) O 2 s(34.13%)p 1.93(65.84%)d 0.00(0.03%)
0.0000 0.5840 0.0128 0.0014 0.0001
-0.1190 0.0031 0.0019 -0.0007 0.6436
0.0086 0.0011 -0.0008 0.4795 0.0060
-0.0035 -0.0003 0.0032 0.0017 -0.0152
0.0086 -0.0050

24. (1.86737) LP (2) O 2 s(2.27%)p42.98(97.68%)d 0.02(0.05%)

```
                                     0.0000  0.1506  0.0032 -0.0049  0.0004
                                     0.2652 -0.0014 -0.0026  0.0016 -0.6236
                                    -0.0049 -0.0027  0.0029  0.7194  0.0044
                                    -0.0058 -0.0037 -0.0034 -0.0048  0.0027
                                    -0.0057 -0.0195
25. (1.98022) LP ( 1) O  3           s( 47.73%)p 1.09( 52.23%)d 0.00(  0.03%)
                                     0.0000  0.6908  0.0086  0.0023  0.0001
                                     0.6390  0.0055  0.0009  0.0014  0.0848
                                    -0.0069  0.0019 -0.0007  0.3267  0.0021
                                     0.0004  0.0002 -0.0033 -0.0107 -0.0020
                                    -0.0136  0.0012
26. (1.96066) LP ( 2) O  3           s(  0.04%)p99.99( 99.91%)d 1.16(  0.05%)
                                     0.0000  0.0195 -0.0023  0.0033  0.0001
                                     0.4449  0.0091 -0.0021 -0.0008 -0.0769
                                     0.0003  0.0002  0.0007 -0.8916 -0.0162
                                    -0.0022  0.0035  0.0006  0.0134  0.0016
                                    -0.0087  0.0141
27. (1.97723) LP ( 1) O  4           s( 46.90%)p 1.13( 53.07%)d 0.00(  0.03%)
                                     0.0000  0.6848  0.0080  0.0023  0.0000
                                     0.2815 -0.0037  0.0004  0.0007 -0.5779
                                    -0.0082  0.0030 -0.0024 -0.3426  0.0006
                                    -0.0012  0.0005  0.0107  0.0033 -0.0105
                                     0.0073  0.0018
28. (1.96116) LP ( 2) O  4           s(  0.37%)p99.99( 99.58%)d 0.11(  0.04%)
                                     0.0000  0.0610 -0.0008  0.0031 -0.0001
                                     0.4392  0.0088  0.0000  0.0001 -0.2275
                                    -0.0052  0.0026  0.0005  0.8665  0.0130
                                     0.0027 -0.0037  0.0098 -0.0038  0.0138
                                    -0.0001  0.0113
29. (1.97872) LP ( 1) O  5           s( 44.86%)p 1.23( 55.11%)d 0.00(  0.03%)
                                     0.0000  0.6697  0.0097  0.0024  0.0002
                                     0.2460  0.0062 -0.0033  0.0012  0.3948
                                     0.0016  0.0023  0.0008 -0.5784 -0.0042
                                    -0.0016 -0.0001 -0.0072  0.0076  0.0117
                                     0.0044 -0.0072
30. (1.95378) LP ( 2) O  5           s(  0.18%)p99.99( 99.77%)d 0.24(  0.04%)
                                     0.0000  0.0424 -0.0025  0.0036  0.0002
                                     0.2752  0.0041 -0.0032 -0.0005  0.7073
                                     0.0162  0.0018 -0.0016  0.6490  0.0129
                                     0.0046 -0.0020 -0.0086 -0.0004  0.0022
                                     0.0073  0.0174
31. (1.97936) LP ( 1) O  6           s( 47.65%)p 1.10( 52.31%)d 0.00(  0.04%)
                                     0.0000  0.6902  0.0114  0.0006  0.0000
                                     0.1211  0.0000  0.0014  0.0003 -0.6538
                                    -0.0055  0.0019 -0.0021 -0.2845 -0.0014
                                     0.0009  0.0001  0.0061 -0.0004 -0.0105
                                     0.0138  0.0046
32. (1.95744) LP ( 2) O  6           s(  0.05%)p99.99( 99.90%)d 1.02(  0.05%)
                                     0.0000  0.0223 -0.0015  0.0046  0.0002
                                     0.5047  0.0123  0.0025 -0.0002 -0.2431
                                    -0.0046 -0.0039  0.0006  0.8274  0.0184
                                    -0.0031 -0.0026  0.0121  0.0005  0.0159
                                     0.0035  0.0108
33. (1.97540) LP ( 1) O  7           s( 43.99%)p 1.27( 55.98%)d 0.00(  0.03%)
                                     0.0000  0.6632  0.0073 -0.0002  0.0000
                                     0.3187 -0.0014 -0.0062  0.0013  0.6443
                                     0.0096 -0.0063 -0.0009  0.2071  0.0036
                                     0.0023  0.0009 -0.0118 -0.0042 -0.0082
                                     0.0049  0.0077
34. (1.95797) LP ( 2) O  7           s(  4.65%)p20.49( 95.31%)d 0.01(  0.04%)
                                     0.0000  0.2154  0.0103 -0.0005 -0.0001
                                     0.7845  0.0199 -0.0013  0.0002 -0.5572
                                    -0.0109 -0.0004  0.0026 -0.1631 -0.0008
                                     0.0051  0.0003 -0.0013 -0.0028  0.0062
                                    -0.0178  0.0042
82. (0.00714) BD*( 1) O  3- H 28
            ( 25.34%)   0.5034* O  3 s( 21.00%)p 3.76( 78.86%)d 0.01(  0.13%)
                                     0.0000 -0.4582  0.0083 -0.0006  0.0001
                                     0.4491  0.0049 -0.0021  0.0000 -0.7140
                                     0.0314 -0.0055 -0.0021  0.2758 -0.0010
                                     0.0006 -0.0006  0.0262 -0.0173  0.0149
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                                    -0.0025  0.0114
             ( 74.66%)  -0.8640* H 28 s( 99.88%)p 0.00(  0.12%)
                                    -0.9994  0.0034 -0.0007  0.0000 -0.0146
                                     0.0313 -0.0076
83. (0.01938) BD*( 1) O  4- C  9
             ( 33.28%)   0.5769* O  4 s( 31.41%)p 2.18( 68.52%)d 0.00(  0.08%)
                                     0.0000 -0.5603  0.0078  0.0058  0.0001
                                     0.7401 -0.0094 -0.0059  0.0019 -0.0898
                                    -0.0009  0.0069  0.0006 -0.3594  0.0064
                                     0.0029  0.0006  0.0118  0.0186 -0.0075
                                    -0.0123  0.0083
             ( 66.72%)  -0.8168* C  9 s( 20.96%)p 3.76( 78.82%)d 0.01(  0.22%)
                                     0.0000 -0.4557  0.0450  0.0017  0.0008
                                    -0.8070 -0.0435  0.0018  0.0050  0.0688
                                    -0.0129 -0.0002  0.0021  0.3605 -0.0029
                                    -0.0075  0.0064  0.0042  0.0328 -0.0005
                                    -0.0309  0.0112
84. (0.00865) BD*( 1) O  4- H 29
             ( 25.05%)   0.5005* O  4 s( 21.29%)p 3.69( 78.58%)d 0.01(  0.13%)
                                     0.0000 -0.4614  0.0078 -0.0016 -0.0001
                                    -0.4223  0.0286 -0.0078 -0.0007 -0.7775
                                     0.0063 -0.0020 -0.0016  0.0424 -0.0108
                                     0.0014 -0.0002 -0.0153  0.0001 -0.0047
                                     0.0265  0.0188
             ( 74.95%)  -0.8657* H 29 s( 99.88%)p 0.00(  0.12%)
                                    -0.9994  0.0038  0.0009 -0.0001  0.0195
                                     0.0285 -0.0055
85. (0.01880) BD*( 1) O  5- C 10
             ( 34.18%)   0.5846* O  5 s( 30.97%)p 2.23( 68.95%)d 0.00(  0.08%)
                                     0.0000 -0.5564  0.0090  0.0042 -0.0003
                                    -0.4144  0.0128  0.0013 -0.0024  0.5822
                                    -0.0079 -0.0054 -0.0004 -0.4225  0.0051
                                     0.0029  0.0007  0.0112 -0.0077  0.0228
                                     0.0097 -0.0001
             ( 65.82%)  -0.8113* C 10 s( 21.86%)p 3.57( 77.93%)d 0.01(  0.21%)
                                     0.0000 -0.4657  0.0416 -0.0022  0.0005
                                     0.4737  0.0104 -0.0026  0.0029 -0.6223
                                    -0.0396 -0.0022  0.0050  0.4071 -0.0095
                                    -0.0061  0.0091  0.0273 -0.0219  0.0275
                                     0.0060  0.0075
86. (0.02251) BD*( 1) O  5- H 30
             ( 23.35%)   0.4832* O  5 s( 23.97%)p 3.17( 75.90%)d 0.01(  0.12%)
                                     0.0000 -0.4895  0.0085  0.0002  0.0007
                                     0.8303 -0.0272 -0.0013  0.0028 -0.0602
                                     0.0193 -0.0051  0.0001 -0.2545 -0.0084
                                     0.0027  0.0008 -0.0066  0.0245  0.0050
                                    -0.0231  0.0069
             ( 76.65%)  -0.8755* H 30 s( 99.84%)p 0.00(  0.16%)
                                    -0.9992  0.0062  0.0002  0.0004 -0.0393
                                     0.0064  0.0052
87. (0.00596) BD*( 1) O  6- C 13
             ( 34.07%)   0.5837* O  6 s( 29.98%)p 2.33( 69.93%)d 0.00(  0.09%)
                                     0.0000 -0.5473  0.0146  0.0039 -0.0002
                                     0.6504 -0.0117 -0.0033  0.0020 -0.2575
                                    -0.0080 -0.0098 -0.0001 -0.4578  0.0087
                                    -0.0032  0.0006  0.0169  0.0201 -0.0147
                                    -0.0038  0.0049
             ( 65.93%)  -0.8120* C 13 s( 22.28%)p 3.48( 77.49%)d 0.01(  0.23%)
                                     0.0000 -0.4695  0.0490 -0.0008  0.0003
                                    -0.7078 -0.0419 -0.0013  0.0049  0.2500
                                     0.0467 -0.0003 -0.0015  0.4551  0.0184
                                     0.0040 -0.0066  0.0146  0.0382 -0.0069
                                    -0.0238  0.0016
88. (0.01203) BD*( 1) O  6- H 31
             ( 25.08%)   0.5008* O  6 s( 22.32%)p 3.47( 77.54%)d 0.01(  0.14%)
                                     0.0000 -0.4723  0.0072 -0.0027  0.0002
                                    -0.5524  0.0302 -0.0030 -0.0011 -0.6674
                                     0.0104 -0.0035  0.0002  0.1535 -0.0166
                                    -0.0015 -0.0003 -0.0256  0.0028  0.0016
                                     0.0199  0.0195
             ( 74.92%)  -0.8656* H 31 s( 99.85%)p 0.00(  0.15%)
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                                     -0.9992  0.0032  0.0004  0.0005  0.0260
                                      0.0261 -0.0121
107. (0.35276) BD*( 2) C 15- C 17
               ( 47.86%)   0.6918* C 15 s(  0.00%)p 1.00( 99.96%)d 0.00(  0.03%)
                                      0.0000 -0.0019  0.0032 -0.0002 -0.1397
                                      0.0013 -0.0018  0.0009 -0.3329 -0.0022
                                     -0.0148 -0.0022  0.9320 -0.0140  0.0064
                                     -0.0109  0.0055 -0.0056 -0.0117 -0.0022
                                     -0.0121
               ( 52.14%)  -0.7221* C 17 s(  0.00%)p 1.00( 99.95%)d 0.00(  0.05%)
                                      0.0000  0.0000 -0.0043  0.0005 -0.0015
                                     -0.1417 -0.0031 -0.0030  0.0000 -0.3469
                                     -0.0060 -0.0076  0.0001  0.9266  0.0132
                                      0.0111 -0.0053 -0.0091  0.0195  0.0005
                                     -0.0045  0.0066
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SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

Threshold for printing: 0.10 kcal/mol

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
within unit 1				
21. LP (1) O 1	79. BD*(1) O 2- C 12	5.53	0.97	0.065
21. LP (1) O 1	85. BD*(1) O 5- C 10	0.12	0.98	0.010
21. LP (1) O 1	87. BD*(1) O 6- C 13	0.50	0.99	0.020
21. LP (1) O 1	94. BD*(1) C 9- C 11	0.68	1.02	0.024
21. LP (1) O 1	95. BD*(1) C 9- H 22	0.16	1.04	0.011
21. LP (1) O 1	96. BD*(1) C 10- C 12	0.79	1.02	0.025
21. LP (1) O 1	97. BD*(1) C 10- H 23	0.13	1.04	0.011
21. LP (1) O 1	98. BD*(1) C 11- C 13	1.90	1.04	0.040
21. LP (1) O 1	99. BD*(1) C 11- H 24	1.38	1.04	0.034
21. LP (1) O 1	100. BD*(1) C 12- H 25	1.08	1.02	0.030
21. LP (1) O 1	110. BD*(1) C 16- H 32	0.11	1.10	0.010
21. LP (1) O 1	126. RY (8) O 1	0.18	2.29	0.018
21. LP (1) O 1	289. RY (1) C 11	0.91	1.63	0.034
21. LP (1) O 1	290. RY (2) C 11	1.31	2.19	0.048
21. LP (1) O 1	306. RY (1) C 12	2.25	1.81	0.057
21. LP (1) O 1	307. RY (2) C 12	0.18	3.27	0.021
21. LP (1) O 1	308. RY (3) C 12	0.16	2.39	0.018
21. LP (1) O 1	309. RY (4) C 12	0.15	2.14	0.016
21. LP (1) O 1	310. RY (5) C 12	0.34	2.25	0.025
21. LP (1) O 1	313. RY (8) C 12	0.11	2.40	0.015
21. LP (1) O 1	316. RY (11) C 12	0.14	3.18	0.019
21. LP (1) O 1	322. RY (17) C 12	0.12	3.46	0.018
21. LP (1) O 1	323. RY (1) C 13	0.24	1.54	0.017
22. LP (2) O 1	83. BD*(1) O 4- C 9	1.28	0.76	0.028
22. LP (2) O 1	85. BD*(1) O 5- C 10	0.98	0.78	0.025
22. LP (2) O 1	94. BD*(1) C 9- C 11	6.45	0.82	0.065
22. LP (2) O 1	96. BD*(1) C 10- C 12	6.86	0.82	0.067
22. LP (2) O 1	99. BD*(1) C 11- H 24	6.82	0.84	0.068
22. LP (2) O 1	100. BD*(1) C 12- H 25	7.81	0.82	0.071
22. LP (2) O 1	101. BD*(1) C 13- H 26	0.12	0.86	0.009
22. LP (2) O 1	110. BD*(1) C 16- H 32	0.39	0.90	0.017
22. LP (2) O 1	122. RY (4) O 1	0.11	1.94	0.013
22. LP (2) O 1	272. RY (1) C 10	0.18	1.49	0.015
22. LP (2) O 1	289. RY (1) C 11	0.21	1.43	0.015
22. LP (2) O 1	292. RY (4) C 11	0.90	2.19	0.040
22. LP (2) O 1	294. RY (6) C 11	0.11	2.17	0.014
22. LP (2) O 1	296. RY (8) C 11	0.10	2.64	0.015
22. LP (2) O 1	306. RY (1) C 12	0.11	1.61	0.012
22. LP (2) O 1	307. RY (2) C 12	0.10	3.07	0.016
22. LP (2) O 1	308. RY (3) C 12	0.14	2.19	0.016
22. LP (2) O 1	309. RY (4) C 12	0.66	1.94	0.032
22. LP (2) O 1	310. RY (5) C 12	0.45	2.05	0.027
22. LP (2) O 1	311. RY (6) C 12	0.40	2.40	0.028
22. LP (2) O 1	475. RY (1) H 24	0.25	1.18	0.015

22. LP (2) O 1	481. RY (1) H 25	0.19	1.31	0.014
23. LP (1) O 2	77. BD*(1) O 1- C 11	0.11	0.93	0.009
23. LP (1) O 2	78. BD*(1) O 1- C 12	0.56	0.94	0.020
23. LP (1) O 2	85. BD*(1) O 5- C 10	0.10	0.95	0.009
23. LP (1) O 2	86. BD*(1) O 5- H 30	0.15	1.09	0.012
23. LP (1) O 2	92. BD*(1) C 8- C 10	0.59	1.01	0.022
23. LP (1) O 2	96. BD*(1) C 10- C 12	2.21	0.99	0.042
23. LP (1) O 2	100. BD*(1) C 12- H 25	2.51	1.00	0.045
23. LP (1) O 2	103. BD*(1) C 14- C 15	1.11	1.18	0.032
23. LP (1) O 2	104. BD*(1) C 14- C 16	6.34	1.19	0.077
23. LP (1) O 2	105. BD*(2) C 14- C 16	1.27	0.62	0.025
23. LP (1) O 2	106. BD*(1) C 15- C 17	0.22	1.20	0.014
23. LP (1) O 2	108. BD*(1) C 15- C 18	0.13	1.04	0.011
23. LP (1) O 2	109. BD*(1) C 16- C 19	0.21	1.19	0.014
23. LP (1) O 2	110. BD*(1) C 16- H 32	0.23	1.08	0.014
23. LP (1) O 2	113. BD*(1) C 18- H 34	0.40	1.02	0.018
23. LP (1) O 2	273. RY (2) C 10	0.15	1.92	0.015
23. LP (1) O 2	307. RY (2) C 12	1.54	3.25	0.063
23. LP (1) O 2	308. RY (3) C 12	0.27	2.36	0.023
23. LP (1) O 2	309. RY (4) C 12	0.14	2.12	0.016
23. LP (1) O 2	312. RY (7) C 12	0.23	2.39	0.021
23. LP (1) O 2	313. RY (8) C 12	0.13	2.38	0.016
23. LP (1) O 2	318. RY (13) C 12	0.19	4.21	0.025
23. LP (1) O 2	340. RY (1) C 14	1.97	1.76	0.053
23. LP (1) O 2	342. RY (3) C 14	0.10	2.98	0.015
23. LP (1) O 2	343. RY (4) C 14	0.37	2.35	0.026
23. LP (1) O 2	344. RY (5) C 14	0.20	1.52	0.015
23. LP (1) O 2	345. RY (6) C 14	0.15	2.24	0.017
23. LP (1) O 2	351. RY (12) C 14	0.14	2.94	0.018
24. LP (2) O 2	77. BD*(1) O 1- C 11	0.50	0.77	0.018
24. LP (2) O 2	78. BD*(1) O 1- C 12	15.44	0.78	0.098
24. LP (2) O 2	79. BD*(1) O 2- C 12	0.16	0.79	0.010
24. LP (2) O 2	86. BD*(1) O 5- H 30	0.22	0.93	0.013
24. LP (2) O 2	92. BD*(1) C 8- C 10	0.18	0.85	0.011
24. LP (2) O 2	96. BD*(1) C 10- C 12	0.72	0.84	0.022
24. LP (2) O 2	97. BD*(1) C 10- H 23	0.19	0.86	0.011
24. LP (2) O 2	100. BD*(1) C 12- H 25	3.79	0.84	0.050
24. LP (2) O 2	103. BD*(1) C 14- C 15	2.17	1.02	0.042
24. LP (2) O 2	104. BD*(1) C 14- C 16	1.35	1.03	0.033
24. LP (2) O 2	105. BD*(2) C 14- C 16	24.40	0.47	0.095
24. LP (2) O 2	106. BD*(1) C 15- C 17	0.14	1.04	0.011
24. LP (2) O 2	107. BD*(2) C 15- C 17	0.13	0.47	0.007
24. LP (2) O 2	113. BD*(1) C 18- H 34	0.10	0.86	0.008
24. LP (2) O 2	121. RY (3) O 1	0.16	1.26	0.013
24. LP (2) O 2	306. RY (1) C 12	0.61	1.63	0.028
24. LP (2) O 2	308. RY (3) C 12	0.20	2.21	0.019
24. LP (2) O 2	310. RY (5) C 12	0.17	2.07	0.017
24. LP (2) O 2	311. RY (6) C 12	0.59	2.42	0.034
24. LP (2) O 2	316. RY (11) C 12	0.14	3.00	0.018
24. LP (2) O 2	341. RY (2) C 14	0.17	1.62	0.015
24. LP (2) O 2	342. RY (3) C 14	0.96	2.82	0.047
24. LP (2) O 2	343. RY (4) C 14	0.32	2.19	0.024
24. LP (2) O 2	345. RY (6) C 14	0.15	2.09	0.016
25. LP (1) O 3	84. BD*(1) O 4- H 29	0.24	1.13	0.015
25. LP (1) O 3	91. BD*(1) C 8- C 9	1.77	1.07	0.039
25. LP (1) O 3	92. BD*(1) C 8- C 10	1.24	1.07	0.032
25. LP (1) O 3	93. BD*(1) C 8- H 21	0.95	1.07	0.028
25. LP (1) O 3	94. BD*(1) C 9- C 11	0.37	1.06	0.018
25. LP (1) O 3	96. BD*(1) C 10- C 12	0.14	1.05	0.011
25. LP (1) O 3	97. BD*(1) C 10- H 23	0.20	1.07	0.013
25. LP (1) O 3	238. RY (1) C 8	1.78	1.60	0.048
25. LP (1) O 3	240. RY (3) C 8	0.84	1.58	0.033
25. LP (1) O 3	241. RY (4) C 8	0.17	2.20	0.017
25. LP (1) O 3	242. RY (5) C 8	0.34	2.26	0.025
25. LP (1) O 3	245. RY (8) C 8	0.13	3.08	0.018
25. LP (1) O 3	257. RY (3) C 9	0.20	1.40	0.015
25. LP (1) O 3	499. RY (1) H 28	0.12	2.28	0.015
25. LP (1) O 3	500. RY (2) H 28	1.08	2.56	0.047
26. LP (2) O 3	84. BD*(1) O 4- H 29	0.20	0.90	0.012
26. LP (2) O 3	85. BD*(1) O 5- C 10	0.18	0.78	0.010
26. LP (2) O 3	92. BD*(1) C 8- C 10	6.05	0.84	0.063

26. LP (2) O 3	93. BD*(1) C 8- H 21	8.69	0.83	0.076
26. LP (2) O 3	96. BD*(1) C 10- C 12	0.72	0.82	0.022
26. LP (2) O 3	238. RY (1) C 8	0.17	1.37	0.013
26. LP (2) O 3	239. RY (2) C 8	0.38	1.51	0.021
26. LP (2) O 3	241. RY (4) C 8	1.09	1.96	0.041
26. LP (2) O 3	242. RY (5) C 8	0.13	2.03	0.015
26. LP (2) O 3	248. RY (11) C 8	0.18	1.49	0.015
26. LP (2) O 3	272. RY (1) C 10	0.12	1.49	0.012
26. LP (2) O 3	457. RY (1) H 21	0.19	1.18	0.013
26. LP (2) O 3	499. RY (1) H 28	1.65	2.05	0.052
27. LP (1) O 4	77. BD*(1) O 1- C 11	0.48	0.99	0.019
27. LP (1) O 4	88. BD*(1) O 6- H 31	2.60	1.17	0.049
27. LP (1) O 4	91. BD*(1) C 8- C 9	1.13	1.07	0.031
27. LP (1) O 4	92. BD*(1) C 8- C 10	0.12	1.07	0.010
27. LP (1) O 4	93. BD*(1) C 8- H 21	0.18	1.07	0.012
27. LP (1) O 4	94. BD*(1) C 9- C 11	1.75	1.06	0.038
27. LP (1) O 4	95. BD*(1) C 9- H 22	1.00	1.07	0.029
27. LP (1) O 4	255. RY (1) C 9	1.81	1.60	0.048
27. LP (1) O 4	256. RY (2) C 9	0.14	1.81	0.014
27. LP (1) O 4	257. RY (3) C 9	0.46	1.41	0.023
27. LP (1) O 4	258. RY (4) C 9	0.23	2.26	0.020
27. LP (1) O 4	259. RY (5) C 9	0.41	2.34	0.028
27. LP (1) O 4	269. RY (15) C 9	0.13	3.35	0.019
27. LP (1) O 4	289. RY (1) C 11	0.14	1.66	0.014
27. LP (1) O 4	505. RY (1) H 29	0.30	2.31	0.024
27. LP (1) O 4	506. RY (2) H 29	0.89	2.58	0.043
28. LP (2) O 4	81. BD*(1) O 3- C 8	0.21	0.77	0.011
28. LP (2) O 4	88. BD*(1) O 6- H 31	0.69	0.94	0.023
28. LP (2) O 4	91. BD*(1) C 8- C 9	5.42	0.84	0.060
28. LP (2) O 4	92. BD*(1) C 8- C 10	0.71	0.84	0.022
28. LP (2) O 4	94. BD*(1) C 9- C 11	0.14	0.83	0.010
28. LP (2) O 4	95. BD*(1) C 9- H 22	8.73	0.85	0.077
28. LP (2) O 4	238. RY (1) C 8	0.16	1.38	0.013
28. LP (2) O 4	255. RY (1) C 9	0.17	1.37	0.014
28. LP (2) O 4	256. RY (2) C 9	0.44	1.58	0.023
28. LP (2) O 4	258. RY (4) C 9	0.89	2.03	0.038
28. LP (2) O 4	259. RY (5) C 9	0.16	2.11	0.016
28. LP (2) O 4	463. RY (1) H 22	0.22	1.25	0.015
28. LP (2) O 4	505. RY (1) H 29	1.36	2.08	0.048
28. LP (2) O 4	506. RY (2) H 29	0.25	2.35	0.021
29. LP (1) O 5	78. BD*(1) O 1- C 12	0.14	0.97	0.011
29. LP (1) O 5	82. BD*(1) O 3- H 28	0.14	1.11	0.011
29. LP (1) O 5	91. BD*(1) C 8- C 9	0.42	1.04	0.019
29. LP (1) O 5	92. BD*(1) C 8- C 10	2.06	1.04	0.041
29. LP (1) O 5	96. BD*(1) C 10- C 12	1.17	1.02	0.031
29. LP (1) O 5	97. BD*(1) C 10- H 23	1.50	1.04	0.035
29. LP (1) O 5	100. BD*(1) C 12- H 25	0.25	1.03	0.014
29. LP (1) O 5	272. RY (1) C 10	1.98	1.69	0.052
29. LP (1) O 5	273. RY (2) C 10	0.16	1.95	0.016
29. LP (1) O 5	274. RY (3) C 10	0.65	1.86	0.031
29. LP (1) O 5	276. RY (5) C 10	0.39	2.39	0.027
29. LP (1) O 5	285. RY (14) C 10	0.22	3.46	0.025
29. LP (1) O 5	511. RY (1) H 30	1.03	2.50	0.045
29. LP (1) O 5	513. RY (3) H 30	0.16	2.19	0.017
30. LP (2) O 5	78. BD*(1) O 1- C 12	1.27	0.75	0.028
30. LP (2) O 5	79. BD*(1) O 2- C 12	0.19	0.76	0.011
30. LP (2) O 5	82. BD*(1) O 3- H 28	0.16	0.89	0.011
30. LP (2) O 5	93. BD*(1) C 8- H 21	0.12	0.82	0.009
30. LP (2) O 5	96. BD*(1) C 10- C 12	7.48	0.81	0.069
30. LP (2) O 5	97. BD*(1) C 10- H 23	8.54	0.83	0.075
30. LP (2) O 5	272. RY (1) C 10	0.30	1.48	0.019
30. LP (2) O 5	273. RY (2) C 10	0.13	1.73	0.013
30. LP (2) O 5	274. RY (3) C 10	0.35	1.65	0.021
30. LP (2) O 5	275. RY (4) C 10	0.97	1.79	0.037
30. LP (2) O 5	276. RY (5) C 10	0.11	2.18	0.014
30. LP (2) O 5	277. RY (6) C 10	0.18	2.38	0.018
30. LP (2) O 5	306. RY (1) C 12	0.25	1.60	0.018
30. LP (2) O 5	469. RY (1) H 23	0.19	1.26	0.014
30. LP (2) O 5	512. RY (2) H 30	1.36	2.08	0.047
31. LP (1) O 6	77. BD*(1) O 1- C 11	0.13	0.95	0.010
31. LP (1) O 6	98. BD*(1) C 11- C 13	1.26	1.03	0.032

31. LP (1) O 6	99. BD*(1) C 11- H 24	0.25	1.04	0.015
31. LP (1) O 6	101. BD*(1) C 13- H 26	3.32	1.06	0.053
31. LP (1) O 6	102. BD*(1) C 13- H 27	0.85	1.05	0.027
31. LP (1) O 6	323. RY (1) C 13	1.94	1.54	0.049
31. LP (1) O 6	325. RY (3) C 13	0.47	2.13	0.028
31. LP (1) O 6	326. RY (4) C 13	0.38	2.38	0.027
31. LP (1) O 6	330. RY (8) C 13	0.10	3.75	0.017
31. LP (1) O 6	335. RY (13) C 13	0.13	1.90	0.014
31. LP (1) O 6	518. RY (2) H 31	1.15	2.51	0.048
31. LP (1) O 6	520. RY (4) H 31	0.10	1.66	0.012
32. LP (2) O 6	77. BD*(1) O 1- C 11	1.19	0.73	0.026
32. LP (2) O 6	98. BD*(1) C 11- C 13	6.08	0.81	0.062
32. LP (2) O 6	101. BD*(1) C 13- H 26	0.14	0.84	0.010
32. LP (2) O 6	102. BD*(1) C 13- H 27	8.90	0.82	0.076
32. LP (2) O 6	323. RY (1) C 13	0.34	1.31	0.019
32. LP (2) O 6	324. RY (2) C 13	0.74	1.37	0.028
32. LP (2) O 6	325. RY (3) C 13	0.94	1.91	0.038
32. LP (2) O 6	493. RY (1) H 27	0.15	1.00	0.011
32. LP (2) O 6	517. RY (1) H 31	1.84	1.99	0.054
33. LP (1) O 7	86. BD*(1) O 5- H 30	3.27	1.14	0.054
33. LP (1) O 7	107. BD*(2) C 15- C 17	0.35	0.68	0.014
33. LP (1) O 7	108. BD*(1) C 15- C 18	2.76	1.09	0.049
33. LP (1) O 7	114. BD*(1) C 18- H 35	2.56	1.08	0.047
33. LP (1) O 7	406. RY (1) C 18	1.09	1.58	0.037
33. LP (1) O 7	408. RY (3) C 18	0.85	1.75	0.034
33. LP (1) O 7	409. RY (4) C 18	0.31	2.73	0.026
33. LP (1) O 7	559. RY (1) H 38	0.46	2.28	0.029
33. LP (1) O 7	560. RY (2) H 38	0.84	2.58	0.042
34. LP (2) O 7	86. BD*(1) O 5- H 30	5.90	0.95	0.067
34. LP (2) O 7	107. BD*(2) C 15- C 17	0.78	0.49	0.017
34. LP (2) O 7	108. BD*(1) C 15- C 18	3.26	0.90	0.048
34. LP (2) O 7	113. BD*(1) C 18- H 34	7.53	0.88	0.072
34. LP (2) O 7	114. BD*(1) C 18- H 35	0.54	0.89	0.020
34. LP (2) O 7	407. RY (2) C 18	1.32	1.79	0.043
34. LP (2) O 7	409. RY (4) C 18	0.30	2.54	0.025
34. LP (2) O 7	511. RY (1) H 30	0.14	2.33	0.016
34. LP (2) O 7	535. RY (1) H 34	0.10	0.97	0.009
34. LP (2) O 7	559. RY (1) H 38	1.44	2.09	0.049
34. LP (2) O 7	560. RY (2) H 38	0.34	2.39	0.026

Salicin (Conformer V)

Summary of Natural Population Analysis:

Atom No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
O 1	-0.63730	2.00000	6.61496	0.02234	8.63730
O 2	-0.58554	2.00000	6.56203	0.02352	8.58554
O 3	-0.76219	2.00000	6.74843	0.01376	8.76219
O 4	-0.74948	2.00000	6.73598	0.01351	8.74948
O 5	-0.78590	2.00000	6.77077	0.01514	8.78590
O 6	-0.73737	2.00000	6.72394	0.01344	8.73737
O 7	-0.76549	2.00000	6.75111	0.01439	8.76549
C 8	0.09708	1.99999	3.87690	0.02603	5.90292
C 9	0.09603	1.99999	3.87821	0.02576	5.90397
C 10	0.07726	1.99999	3.89611	0.02664	5.92274
C 11	0.09310	1.99999	3.88190	0.02500	5.90690
C 12	0.44660	1.99999	3.52040	0.03301	5.55340
C 13	-0.03196	1.99999	4.00865	0.02331	6.03196
C 14	0.33617	1.99999	3.64024	0.02360	5.66383
C 15	-0.09827	1.99999	4.08081	0.01747	6.09827
C 16	-0.26573	1.99999	4.24929	0.01645	6.26573
C 17	-0.18168	1.99999	4.16521	0.01648	6.18168
C 18	-0.03068	1.99999	4.01071	0.01998	6.03068
C 19	-0.18868	1.99999	4.17176	0.01693	6.18868
C 20	-0.22725	1.99999	4.21065	0.01661	6.22725
H 21	0.17673	0.00000	0.82024	0.00303	0.82327
H 22	0.17550	0.00000	0.82139	0.00312	0.82450
H 23	0.18227	0.00000	0.81494	0.00279	0.81773
H 24	0.18320	0.00000	0.81409	0.00271	0.81680
H 25	0.16223	0.00000	0.83478	0.00299	0.83777
H 26	0.16308	0.00000	0.83459	0.00234	0.83692
H 27	0.20344	0.00000	0.79485	0.00171	0.79656
H 28	0.48537	0.00000	0.51064	0.00400	0.51463
H 29	0.48254	0.00000	0.51338	0.00408	0.51746
H 30	0.51305	0.00000	0.48268	0.00428	0.48695
H 31	0.46721	0.00000	0.52815	0.00464	0.53279
H 32	0.23040	0.00000	0.76619	0.00341	0.76960
H 33	0.21306	0.00000	0.78523	0.00171	0.78694
H 34	0.17283	0.00000	0.82511	0.00206	0.82717
H 35	0.18371	0.00000	0.81403	0.00226	0.81629
H 36	0.21627	0.00000	0.78203	0.00170	0.78373
H 37	0.21680	0.00000	0.78152	0.00168	0.78320
H 38	0.47359	0.00000	0.52255	0.00386	0.52641
* Total *	0.00000	39.99990	111.54440	0.45570	152.00000

(Occupancy) Bond orbital / Coefficients / Hybrids

---------- Lewis ----------

21. (1.95921) LP (1) O 1 s(42.51%)p 1.35(57.46%)d 0.00(0.03%)
0.0000 0.6518 0.0154 0.0015 0.0000
0.2148 -0.0019 -0.0022 0.0016 0.3923
0.0062 0.0007 0.0008 0.6120 0.0017
0.0035 -0.0006 -0.0067 -0.0063 -0.0118
0.0040 -0.0090

22. (1.92735) LP (2) O 1 s(0.05%)p99.99(99.91%)d 0.78(0.04%)
0.0000 0.0205 -0.0074 0.0031 0.0001
0.4216 0.0091 0.0021 0.0002 0.6762
0.0127 0.0021 -0.0020 -0.6032 -0.0025
-0.0030 0.0029 -0.0081 -0.0034 -0.0036
0.0052 0.0162

23. (1.95835) LP (1) O 2 s(34.33%)p 1.91(65.63%)d 0.00(0.03%)
0.0000 0.5858 0.0124 0.0015 0.0001
0.0911 -0.0037 -0.0020 0.0007 -0.6131
-0.0077 -0.0013 0.0009 0.5215 0.0064
-0.0035 -0.0002 0.0024 -0.0012 0.0152
0.0079 -0.0067

24. (1.86578) LP (2) O 2 s(2.06%)p47.48(97.89%)d 0.02(0.05%)

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                                     0.0000  0.1435  0.0026 -0.0045  0.0004
                                    -0.2348  0.0010  0.0022 -0.0016  0.6799
                                     0.0053  0.0027 -0.0032  0.6792  0.0045
                                    -0.0059 -0.0034 -0.0027  0.0047 -0.0053
                                    -0.0059 -0.0192
25. (1.98035) LP ( 1) O  3           s( 47.80%)p 1.09( 52.17%)d 0.00(  0.03%)
                                     0.0000  0.6913  0.0086  0.0023  0.0001
                                    -0.6429 -0.0051 -0.0012 -0.0014 -0.0701
                                     0.0068 -0.0016  0.0008  0.3214  0.0020
                                     0.0005  0.0001 -0.0026  0.0107  0.0018
                                    -0.0140  0.0014
26. (1.96058) LP ( 2) O  3           s(  0.05%)p99.99( 99.90%)d 0.91(  0.05%)
                                     0.0000  0.0222 -0.0021  0.0033  0.0000
                                    -0.4340 -0.0090  0.0022  0.0007  0.0948
                                     0.0002 -0.0002 -0.0007 -0.8951 -0.0166
                                    -0.0021  0.0035  0.0012 -0.0138 -0.0013
                                    -0.0086  0.0139
27. (1.98044) LP ( 1) O  4           s( 48.06%)p 1.08( 51.90%)d 0.00(  0.03%)
                                     0.0000  0.6932 -0.0080  0.0023  0.0000
                                    -0.2972  0.0027 -0.0008  0.0004  0.6072
                                     0.0051 -0.0005  0.0024 -0.2490  0.0006
                                    -0.0008 -0.0001  0.0121 -0.0024  0.0097
                                     0.0093  0.0038
28. (1.95902) LP ( 2) O  4           s(  0.08%)p99.99( 99.87%)d 0.65(  0.05%)
                                     0.0000  0.0274 -0.0039 -0.0019  0.0000
                                     0.4563  0.0109  0.0005  0.0003 -0.1660
                                    -0.0023  0.0026  0.0009 -0.8732 -0.0162
                                    -0.0024  0.0034 -0.0103 -0.0030  0.0157
                                     0.0006 -0.0117
29. (1.97876) LP ( 1) O  5           s( 44.93%)p 1.23( 55.04%)d 0.00(  0.03%)
                                     0.0000  0.6702  0.0094  0.0023  0.0004
                                    -0.2600 -0.0063  0.0038 -0.0010 -0.4474
                                    -0.0031 -0.0027 -0.0010 -0.5315 -0.0032
                                    -0.0010  0.0000 -0.0080 -0.0073 -0.0120
                                     0.0053 -0.0052
30. (1.95437) LP ( 2) O  5           s(  0.13%)p99.99( 99.83%)d 0.34(  0.04%)
                                     0.0000  0.0357 -0.0018  0.0038 -0.0001
                                    -0.2219 -0.0023  0.0012  0.0003 -0.6640
                                    -0.0160 -0.0013  0.0013  0.7125  0.0139
                                     0.0046 -0.0023 -0.0081  0.0023  0.0009
                                     0.0081  0.0175
31. (1.98161) LP ( 1) O  6           s( 48.98%)p 1.04( 50.99%)d 0.00(  0.04%)
                                     0.0000  0.6997  0.0119  0.0002  0.0000
                                    -0.1237 -0.0025 -0.0012 -0.0014  0.6205
                                     0.0053 -0.0043  0.0016 -0.3309 -0.0026
                                     0.0013 -0.0002  0.0073 -0.0012  0.0114
                                     0.0128  0.0017
32. (1.95761) LP ( 2) O  6           s(  0.06%)p99.99( 99.89%)d 0.94(  0.05%)
                                     0.0000  0.0232 -0.0004  0.0047  0.0002
                                    -0.3407 -0.0050  0.0024  0.0004  0.3670
                                     0.0068  0.0025 -0.0006  0.8646  0.0201
                                    -0.0030 -0.0028  0.0091  0.0025 -0.0136
                                     0.0053  0.0150
33. (1.98087) LP ( 1) O  7           s( 42.51%)p 1.35( 57.45%)d 0.00(  0.03%)
                                     0.0000  0.6520  0.0068 -0.0025  0.0000
                                    -0.0973  0.0055  0.0070 -0.0014  0.1066
                                     0.0039 -0.0005  0.0013 -0.7440 -0.0047
                                     0.0013  0.0008  0.0014 -0.0075  0.0066
                                    -0.0026 -0.0149
34. (1.96022) LP ( 2) O  7           s(  7.04%)p13.19( 92.92%)d 0.01(  0.04%)
                                     0.0000  0.2652  0.0108  0.0033  0.0000
                                    -0.8883 -0.0215  0.0025  0.0006  0.0932
                                     0.0018  0.0030  0.0002  0.3617  0.0064
                                    -0.0030 -0.0027  0.0072 -0.0096 -0.0018
                                    -0.0094  0.0118

82. (0.00699) BD*( 1) O  3- H 28
              ( 25.45%)   0.5045* O  3 s( 20.89%)p 3.78( 78.98%)d 0.01(  0.14%)
                                     0.0000 -0.4569  0.0084 -0.0007  0.0002
                                    -0.4328 -0.0056  0.0022 -0.0001  0.7250
                                    -0.0315  0.0053  0.0022  0.2753 -0.0016
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                                    0.0006 -0.0007  0.0265  0.0168 -0.0152
                                   -0.0013  0.0116
            ( 74.55%)  -0.8634* H 28 s( 99.88%)p 0.00(  0.12%)
                                   -0.9994  0.0032  0.0006  0.0000  0.0136
                                   -0.0315 -0.0076
83. (0.01771) BD*( 1) O  4- C  9
            ( 33.87%)   0.5819* O  4 s( 31.08%)p 2.22( 68.84%)d 0.00(  0.08%)
                                    0.0000 -0.5574 -0.0088  0.0055  0.0001
                                   -0.7104  0.0084  0.0061  0.0022  0.1193
                                    0.0018 -0.0070 -0.0003 -0.4114  0.0060
                                    0.0033  0.0004  0.0128 -0.0204  0.0097
                                   -0.0105  0.0064
            ( 66.13%)  -0.8132* C  9 s( 21.38%)p 3.67( 78.41%)d 0.01(  0.21%)
                                    0.0000 -0.4603  0.0439  0.0016  0.0008
                                    0.7776  0.0434 -0.0005 -0.0052 -0.0945
                                    0.0162  0.0000 -0.0024  0.4101 -0.0048
                                   -0.0073  0.0069  0.0060 -0.0356  0.0019
                                   -0.0275  0.0073
84. (0.00762) BD*( 1) O  4- H 29
            ( 25.57%)   0.5057* O  4 s( 20.76%)p 3.81( 79.10%)d 0.01(  0.14%)
                                    0.0000 -0.4556 -0.0076 -0.0015  0.0000
                                    0.4438 -0.0266  0.0063 -0.0010  0.7667
                                   -0.0106  0.0006  0.0009  0.0718 -0.0130
                                    0.0014 -0.0003 -0.0169 -0.0003  0.0036
                                    0.0267  0.0191
            ( 74.43%)  -0.8627* H 29 s( 99.87%)p 0.00(  0.13%)
                                   -0.9993  0.0033 -0.0008  0.0000 -0.0220
                                   -0.0281 -0.0066
85. (0.01886) BD*( 1) O  5- C 10
            ( 34.16%)   0.5845* O  5 s( 30.88%)p 2.24( 69.04%)d 0.00(  0.08%)
                                    0.0000 -0.5556  0.0090  0.0040 -0.0002
                                    0.4154 -0.0132 -0.0011  0.0025 -0.5980
                                    0.0071  0.0056  0.0004 -0.4000  0.0053
                                    0.0024  0.0007  0.0113  0.0071 -0.0224
                                    0.0110  0.0019
            ( 65.84%)  -0.8114* C 10 s( 21.82%)p 3.57( 77.98%)d 0.01(  0.21%)
                                    0.0000 -0.4652  0.0412 -0.0023  0.0001
                                   -0.4667 -0.0093 -0.0022 -0.0025  0.6429
                                    0.0411  0.0018 -0.0052  0.3830 -0.0073
                                   -0.0065  0.0084  0.0280  0.0208 -0.0269
                                    0.0067  0.0095
86. (0.02326) BD*( 1) O  5- H 30
            ( 23.41%)   0.4838* O  5 s( 24.04%)p 3.15( 75.83%)d 0.01(  0.13%)
                                    0.0000 -0.4903  0.0081  0.0000  0.0009
                                   -0.8413  0.0280  0.0015 -0.0026  0.0176
                                   -0.0190  0.0050  0.0000 -0.2212 -0.0083
                                    0.0031  0.0007 -0.0099 -0.0223 -0.0060
                                   -0.0231  0.0092
            ( 76.59%)  -0.8752* H 30 s( 99.84%)p 0.00(  0.16%)
                                   -0.9992  0.0066  0.0002 -0.0001  0.0397
                                   -0.0050  0.0047
87. (0.00781) BD*( 1) O  6- C 13
            ( 33.71%)   0.5806* O  6 s( 30.25%)p 2.30( 69.66%)d 0.00(  0.09%)
                                    0.0000 -0.5498  0.0144  0.0030 -0.0001
                                    0.4859 -0.0153  0.0006  0.0015  0.6737
                                   -0.0002  0.0081  0.0009 -0.0798 -0.0006
                                   -0.0035  0.0005 -0.0170  0.0016  0.0103
                                    0.0164  0.0145
            ( 66.29%)  -0.8142* C 13 s( 21.95%)p 3.55( 77.82%)d 0.01(  0.24%)
                                    0.0000 -0.4658  0.0498 -0.0013  0.0007
                                   -0.5211 -0.0032  0.0002  0.0033 -0.7072
                                   -0.0601  0.0010  0.0033  0.0533  0.0021
                                    0.0031 -0.0026 -0.0409  0.0058  0.0029
                                    0.0060  0.0249
88. (0.00917) BD*( 1) O  6- H 31
            ( 26.25%)   0.5123* O  6 s( 20.71%)p 3.82( 79.14%)d 0.01(  0.14%)
                                    0.0000 -0.4550  0.0094 -0.0026  0.0002
                                   -0.7935  0.0341  0.0002 -0.0017  0.1584
                                    0.0130  0.0043  0.0001 -0.3678  0.0073
                                    0.0006  0.0010  0.0202 -0.0241  0.0133
                                   -0.0142  0.0084
```

(73.75%) -0.8588* H 31 s(99.87%)p 0.00(0.13%)
                                -0.9993 0.0042 -0.0002 -0.0001 0.0344
                                -0.0015 0.0123

SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

Threshold for printing: 0.10 kcal/mol

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
within unit 1				
21. LP (1) O 1	79. BD*(1) O 2- C 12	5.40	0.97	0.065
21. LP (1) O 1	88. BD*(1) O 6- H 31	0.34	1.12	0.017
21. LP (1) O 1	94. BD*(1) C 9- C 11	0.58	1.03	0.022
21. LP (1) O 1	95. BD*(1) C 9- H 22	0.14	1.04	0.011
21. LP (1) O 1	96. BD*(1) C 10- C 12	0.58	1.03	0.022
21. LP (1) O 1	97. BD*(1) C 10- H 23	0.14	1.04	0.011
21. LP (1) O 1	98. BD*(1) C 11- C 13	1.70	1.05	0.038
21. LP (1) O 1	99. BD*(1) C 11- H 24	1.39	1.05	0.034
21. LP (1) O 1	100. BD*(1) C 12- H 25	1.33	1.03	0.033
21. LP (1) O 1	102. BD*(1) C 13- H 27	0.47	1.08	0.020
21. LP (1) O 1	124. RY (6) O 1	0.16	2.17	0.016
21. LP (1) O 1	125. RY (7) O 1	0.11	1.86	0.013
21. LP (1) O 1	289. RY (1) C 11	1.64	1.53	0.045
21. LP (1) O 1	290. RY (2) C 11	0.43	2.14	0.027
21. LP (1) O 1	291. RY (3) C 11	0.25	1.94	0.020
21. LP (1) O 1	292. RY (4) C 11	0.18	2.61	0.019
21. LP (1) O 1	295. RY (7) C 11	0.12	3.88	0.019
21. LP (1) O 1	303. RY (15) C 11	0.12	3.23	0.018
21. LP (1) O 1	306. RY (1) C 12	2.26	1.86	0.058
21. LP (1) O 1	308. RY (3) C 12	0.18	2.41	0.018
21. LP (1) O 1	309. RY (4) C 12	0.18	2.21	0.018
21. LP (1) O 1	310. RY (5) C 12	0.30	2.21	0.023
21. LP (1) O 1	316. RY (11) C 12	0.13	3.22	0.018
21. LP (1) O 1	322. RY (17) C 12	0.13	3.52	0.019
22. LP (2) O 1	83. BD*(1) O 4- C 9	1.15	0.77	0.027
22. LP (2) O 1	85. BD*(1) O 5- C 10	1.08	0.78	0.026
22. LP (2) O 1	88. BD*(1) O 6- H 31	0.23	0.91	0.013
22. LP (2) O 1	94. BD*(1) C 9- C 11	6.46	0.83	0.065
22. LP (2) O 1	96. BD*(1) C 10- C 12	6.97	0.82	0.068
22. LP (2) O 1	99. BD*(1) C 11- H 24	6.49	0.85	0.066
22. LP (2) O 1	100. BD*(1) C 12- H 25	7.40	0.82	0.070
22. LP (2) O 1	110. BD*(1) C 16- H 32	0.33	0.90	0.015
22. LP (2) O 1	272. RY (1) C 10	0.18	1.50	0.015
22. LP (2) O 1	289. RY (1) C 11	0.14	1.33	0.012
22. LP (2) O 1	292. RY (4) C 11	0.67	2.41	0.036
22. LP (2) O 1	294. RY (6) C 11	0.17	2.34	0.018
22. LP (2) O 1	306. RY (1) C 12	0.11	1.66	0.012
22. LP (2) O 1	307. RY (2) C 12	0.10	2.81	0.015
22. LP (2) O 1	308. RY (3) C 12	0.14	2.21	0.016
22. LP (2) O 1	309. RY (4) C 12	0.52	2.01	0.029
22. LP (2) O 1	310. RY (5) C 12	0.67	2.01	0.033
22. LP (2) O 1	311. RY (6) C 12	0.33	2.47	0.025
22. LP (2) O 1	475. RY (1) H 24	0.25	1.27	0.016
22. LP (2) O 1	481. RY (1) H 25	0.18	1.31	0.014
23. LP (1) O 2	78. BD*(1) O 1- C 12	0.36	0.94	0.016
23. LP (1) O 2	86. BD*(1) O 5- H 30	0.18	1.09	0.012
23. LP (1) O 2	89. BD*(1) O 7- C 18	0.11	0.91	0.009
23. LP (1) O 2	92. BD*(1) C 8- C 10	0.54	1.02	0.021
23. LP (1) O 2	96. BD*(1) C 10- C 12	2.16	1.00	0.041
23. LP (1) O 2	100. BD*(1) C 12- H 25	2.80	1.00	0.047
23. LP (1) O 2	103. BD*(1) C 14- C 15	1.13	1.18	0.033
23. LP (1) O 2	104. BD*(1) C 14- C 16	6.35	1.19	0.078
23. LP (1) O 2	105. BD*(2) C 14- C 16	1.03	0.63	0.023
23. LP (1) O 2	106. BD*(1) C 15- C 17	0.21	1.20	0.014

23. LP (1) O 2	108. BD*(1) C 15- C 18	0.14	1.04	0.011
23. LP (1) O 2	109. BD*(1) C 16- C 19	0.22	1.19	0.014
23. LP (1) O 2	110. BD*(1) C 16- H 32	0.25	1.08	0.015
23. LP (1) O 2	113. BD*(1) C 18- H 34	0.42	1.01	0.018
23. LP (1) O 2	273. RY (2) C 10	0.14	1.91	0.015
23. LP (1) O 2	307. RY (2) C 12	1.77	2.98	0.065
23. LP (1) O 2	308. RY (3) C 12	0.17	2.38	0.018
23. LP (1) O 2	312. RY (7) C 12	0.16	2.38	0.017
23. LP (1) O 2	313. RY (8) C 12	0.13	2.52	0.016
23. LP (1) O 2	319. RY (14) C 12	0.17	4.58	0.025
23. LP (1) O 2	340. RY (1) C 14	1.98	1.75	0.053
23. LP (1) O 2	343. RY (4) C 14	0.45	2.43	0.030
23. LP (1) O 2	344. RY (5) C 14	0.13	1.62	0.013
24. LP (2) O 2	77. BD*(1) O 1- C 11	0.53	0.77	0.018
24. LP (2) O 2	78. BD*(1) O 1- C 12	15.66	0.78	0.099
24. LP (2) O 2	79. BD*(1) O 2- C 12	0.15	0.79	0.010
24. LP (2) O 2	86. BD*(1) O 5- H 30	0.33	0.93	0.016
24. LP (2) O 2	92. BD*(1) C 8- C 10	0.22	0.86	0.012
24. LP (2) O 2	96. BD*(1) C 10- C 12	0.98	0.84	0.026
24. LP (2) O 2	97. BD*(1) C 10- H 23	0.19	0.86	0.011
24. LP (2) O 2	100. BD*(1) C 12- H 25	3.26	0.84	0.047
24. LP (2) O 2	103. BD*(1) C 14- C 15	1.87	1.02	0.039
24. LP (2) O 2	104. BD*(1) C 14- C 16	1.18	1.03	0.031
24. LP (2) O 2	105. BD*(2) C 14- C 16	25.56	0.47	0.097
24. LP (2) O 2	106. BD*(1) C 15- C 17	0.12	1.04	0.010
24. LP (2) O 2	107. BD*(2) C 15- C 17	0.12	0.48	0.007
24. LP (2) O 2	121. RY (3) O 1	0.16	1.25	0.012
24. LP (2) O 2	306. RY (1) C 12	0.62	1.67	0.029
24. LP (2) O 2	308. RY (3) C 12	0.21	2.22	0.019
24. LP (2) O 2	310. RY (5) C 12	0.11	2.03	0.013
24. LP (2) O 2	311. RY (6) C 12	0.63	2.49	0.035
24. LP (2) O 2	316. RY (11) C 12	0.13	3.03	0.018
24. LP (2) O 2	341. RY (2) C 14	0.20	1.67	0.016
24. LP (2) O 2	342. RY (3) C 14	0.98	2.96	0.048
24. LP (2) O 2	343. RY (4) C 14	0.17	2.27	0.018
24. LP (2) O 2	344. RY (5) C 14	0.17	1.46	0.014
25. LP (1) O 3	84. BD*(1) O 4- H 29	0.20	1.14	0.013
25. LP (1) O 3	91. BD*(1) C 8- C 9	1.77	1.07	0.039
25. LP (1) O 3	92. BD*(1) C 8- C 10	1.14	1.07	0.031
25. LP (1) O 3	93. BD*(1) C 8- H 21	1.05	1.07	0.030
25. LP (1) O 3	94. BD*(1) C 9- C 11	0.37	1.06	0.018
25. LP (1) O 3	96. BD*(1) C 10- C 12	0.13	1.05	0.010
25. LP (1) O 3	97. BD*(1) C 10- H 23	0.20	1.07	0.013
25. LP (1) O 3	238. RY (1) C 8	1.80	1.56	0.047
25. LP (1) O 3	240. RY (3) C 8	0.78	1.57	0.031
25. LP (1) O 3	241. RY (4) C 8	0.18	2.19	0.018
25. LP (1) O 3	242. RY (5) C 8	0.38	2.26	0.026
25. LP (1) O 3	245. RY (8) C 8	0.16	2.99	0.019
25. LP (1) O 3	257. RY (3) C 9	0.13	1.45	0.012
25. LP (1) O 3	499. RY (1) H 28	0.11	2.28	0.014
25. LP (1) O 3	500. RY (2) H 28	1.09	2.56	0.047
26. LP (2) O 3	84. BD*(1) O 4- H 29	0.23	0.90	0.013
26. LP (2) O 3	85. BD*(1) O 5- C 10	0.18	0.78	0.011
26. LP (2) O 3	92. BD*(1) C 8- C 10	6.30	0.83	0.065
26. LP (2) O 3	93. BD*(1) C 8- H 21	8.43	0.83	0.075
26. LP (2) O 3	95. BD*(1) C 9- H 22	0.11	0.83	0.009
26. LP (2) O 3	96. BD*(1) C 10- C 12	0.75	0.82	0.022
26. LP (2) O 3	238. RY (1) C 8	0.16	1.33	0.013
26. LP (2) O 3	239. RY (2) C 8	0.39	1.51	0.022
26. LP (2) O 3	241. RY (4) C 8	1.09	1.96	0.041
26. LP (2) O 3	242. RY (5) C 8	0.15	2.03	0.015
26. LP (2) O 3	248. RY (11) C 8	0.12	1.65	0.013
26. LP (2) O 3	272. RY (1) C 10	0.12	1.49	0.012
26. LP (2) O 3	457. RY (1) H 21	0.18	1.19	0.013
26. LP (2) O 3	499. RY (1) H 28	1.67	2.05	0.052
27. LP (1) O 4	77. BD*(1) O 1- C 11	0.57	0.97	0.021
27. LP (1) O 4	91. BD*(1) C 8- C 9	1.79	1.06	0.039
27. LP (1) O 4	92. BD*(1) C 8- C 10	0.21	1.06	0.013
27. LP (1) O 4	93. BD*(1) C 8- H 21	0.20	1.06	0.013
27. LP (1) O 4	94. BD*(1) C 9- C 11	1.65	1.05	0.037
27. LP (1) O 4	95. BD*(1) C 9- H 22	0.47	1.06	0.020

27. LP (1) O 4	102. BD*(1) C 13- H 27	0.10	1.09	0.009
27. LP (1) O 4	255. RY (1) C 9	1.91	1.60	0.049
27. LP (1) O 4	257. RY (3) C 9	0.71	1.44	0.028
27. LP (1) O 4	258. RY (4) C 9	0.17	2.22	0.017
27. LP (1) O 4	259. RY (5) C 9	0.51	2.37	0.031
27. LP (1) O 4	269. RY (15) C 9	0.17	3.88	0.023
27. LP (1) O 4	289. RY (1) C 11	0.23	1.55	0.017
27. LP (1) O 4	506. RY (2) H 29	1.16	2.56	0.049
28. LP (2) O 4	77. BD*(1) O 1- C 11	0.11	0.74	0.008
28. LP (2) O 4	81. BD*(1) O 3- C 8	0.17	0.75	0.010
28. LP (2) O 4	91. BD*(1) C 8- C 9	4.90	0.83	0.057
28. LP (2) O 4	92. BD*(1) C 8- C 10	0.65	0.83	0.021
28. LP (2) O 4	94. BD*(1) C 9- C 11	0.34	0.82	0.015
28. LP (2) O 4	95. BD*(1) C 9- H 22	9.99	0.83	0.081
28. LP (2) O 4	99. BD*(1) C 11- H 24	0.10	0.84	0.008
28. LP (2) O 4	238. RY (1) C 8	0.21	1.32	0.015
28. LP (2) O 4	256. RY (2) C 9	0.45	1.53	0.023
28. LP (2) O 4	258. RY (4) C 9	1.19	1.99	0.043
28. LP (2) O 4	259. RY (5) C 9	0.10	2.14	0.013
28. LP (2) O 4	463. RY (1) H 22	0.20	1.18	0.014
28. LP (2) O 4	505. RY (1) H 29	1.78	2.05	0.054
29. LP (1) O 5	78. BD*(1) O 1- C 12	0.21	0.97	0.013
29. LP (1) O 5	82. BD*(1) O 3- H 28	0.15	1.11	0.012
29. LP (1) O 5	91. BD*(1) C 8- C 9	0.39	1.04	0.018
29. LP (1) O 5	92. BD*(1) C 8- C 10	2.02	1.04	0.041
29. LP (1) O 5	96. BD*(1) C 10- C 12	1.49	1.03	0.035
29. LP (1) O 5	97. BD*(1) C 10- H 23	1.10	1.04	0.030
29. LP (1) O 5	100. BD*(1) C 12- H 25	0.24	1.03	0.014
29. LP (1) O 5	198. RY (12) O 5	0.11	14.53	0.036
29. LP (1) O 5	201. RY (15) O 5	0.11	19.54	0.041
29. LP (1) O 5	272. RY (1) C 10	2.11	1.70	0.053
29. LP (1) O 5	273. RY (2) C 10	0.15	1.94	0.015
29. LP (1) O 5	274. RY (3) C 10	0.52	1.71	0.027
29. LP (1) O 5	275. RY (4) C 10	0.13	2.17	0.015
29. LP (1) O 5	276. RY (5) C 10	0.41	2.47	0.029
29. LP (1) O 5	285. RY (14) C 10	0.16	3.61	0.021
29. LP (1) O 5	511. RY (1) H 30	1.08	2.51	0.047
29. LP (1) O 5	513. RY (3) H 30	0.14	2.16	0.016
30. LP (2) O 5	78. BD*(1) O 1- C 12	1.15	0.75	0.026
30. LP (2) O 5	79. BD*(1) O 2- C 12	0.20	0.76	0.011
30. LP (2) O 5	92. BD*(1) C 8- C 10	0.15	0.83	0.010
30. LP (2) O 5	93. BD*(1) C 8- H 21	0.10	0.82	0.008
30. LP (2) O 5	96. BD*(1) C 10- C 12	6.33	0.81	0.064
30. LP (2) O 5	97. BD*(1) C 10- H 23	9.46	0.83	0.079
30. LP (2) O 5	221. RY (1) O 7	0.10	1.02	0.009
30. LP (2) O 5	272. RY (1) C 10	0.28	1.48	0.018
30. LP (2) O 5	273. RY (2) C 10	0.20	1.72	0.016
30. LP (2) O 5	275. RY (4) C 10	1.12	1.95	0.042
30. LP (2) O 5	277. RY (6) C 10	0.20	2.39	0.020
30. LP (2) O 5	306. RY (1) C 12	0.22	1.64	0.017
30. LP (2) O 5	469. RY (1) H 23	0.20	1.27	0.014
30. LP (2) O 5	512. RY (2) H 30	1.45	2.06	0.049
31. LP (1) O 6	78. BD*(1) O 1- C 12	0.10	0.98	0.009
31. LP (1) O 6	98. BD*(1) C 11- C 13	0.99	1.06	0.029
31. LP (1) O 6	99. BD*(1) C 11- H 24	0.16	1.06	0.012
31. LP (1) O 6	101. BD*(1) C 13- H 26	1.00	1.06	0.029
31. LP (1) O 6	102. BD*(1) C 13- H 27	3.02	1.09	0.051
31. LP (1) O 6	323. RY (1) C 13	1.61	1.56	0.045
31. LP (1) O 6	325. RY (3) C 13	0.60	2.04	0.031
31. LP (1) O 6	326. RY (4) C 13	0.44	2.18	0.028
31. LP (1) O 6	337. RY (15) C 13	0.11	3.88	0.018
31. LP (1) O 6	518. RY (2) H 31	1.19	2.44	0.048
31. LP (1) O 6	520. RY (4) H 31	0.11	2.46	0.015
32. LP (2) O 6	77. BD*(1) O 1- C 11	0.33	0.73	0.014
32. LP (2) O 6	94. BD*(1) C 9- C 11	0.96	0.81	0.025
32. LP (2) O 6	98. BD*(1) C 11- C 13	6.43	0.82	0.065
32. LP (2) O 6	101. BD*(1) C 13- H 26	7.80	0.82	0.072
32. LP (2) O 6	289. RY (1) C 11	0.22	1.31	0.015
32. LP (2) O 6	323. RY (1) C 13	0.23	1.32	0.016
32. LP (2) O 6	324. RY (2) C 13	0.83	1.45	0.031
32. LP (2) O 6	325. RY (3) C 13	0.81	1.80	0.034

32. LP (2) O 6	327. RY (5) C 13	0.18	1.58	0.015
32. LP (2) O 6	487. RY (1) H 26	0.13	1.02	0.010
32. LP (2) O 6	517. RY (1) H 31	1.89	1.91	0.054
33. LP (1) O 7	86. BD*(1) O 5- H 30	2.39	1.13	0.046
33. LP (1) O 7	106. BD*(1) C 15- C 17	0.12	1.24	0.011
33. LP (1) O 7	107. BD*(2) C 15- C 17	0.31	0.68	0.013
33. LP (1) O 7	108. BD*(1) C 15- C 18	1.51	1.08	0.036
33. LP (1) O 7	114. BD*(1) C 18- H 35	1.94	1.06	0.041
33. LP (1) O 7	406. RY (1) C 18	0.56	1.56	0.026
33. LP (1) O 7	407. RY (2) C 18	1.44	2.02	0.048
33. LP (1) O 7	411. RY (6) C 18	0.35	2.34	0.026
33. LP (1) O 7	419. RY (14) C 18	0.22	2.78	0.022
33. LP (1) O 7	559. RY (1) H 38	0.86	2.23	0.039
33. LP (1) O 7	560. RY (2) H 38	0.65	2.50	0.036
34. LP (2) O 7	86. BD*(1) O 5- H 30	7.07	0.96	0.074
34. LP (2) O 7	113. BD*(1) C 18- H 34	5.82	0.89	0.064
34. LP (2) O 7	114. BD*(1) C 18- H 35	5.35	0.89	0.062
34. LP (2) O 7	190. RY (4) O 5	0.11	1.70	0.012
34. LP (2) O 7	407. RY (2) C 18	0.13	1.85	0.014
34. LP (2) O 7	408. RY (3) C 18	1.05	1.65	0.037
34. LP (2) O 7	409. RY (4) C 18	0.31	1.84	0.021
34. LP (2) O 7	410. RY (5) C 18	0.28	1.77	0.020
34. LP (2) O 7	511. RY (1) H 30	0.16	2.36	0.018
34. LP (2) O 7	541. RY (1) H 35	0.19	1.03	0.013
34. LP (2) O 7	559. RY (1) H 38	1.17	2.06	0.044
34. LP (2) O 7	560. RY (2) H 38	0.66	2.33	0.035

Salicin (Conformer VIII)

Summary of Natural Population Analysis:

		Natural Population			
Atom No	Natural Charge	Core	Valence	Rydberg	Total
O 1	-0.62051	2.00000	6.59868	0.02183	8.62051
O 2	-0.58635	2.00000	6.56280	0.02355	8.58635
O 3	-0.76372	2.00000	6.75010	0.01362	8.76372
O 4	-0.77213	2.00000	6.75876	0.01337	8.77213
O 5	-0.78671	2.00000	6.77148	0.01524	8.78671
O 6	-0.75081	2.00000	6.73707	0.01374	8.75081
O 7	-0.76587	2.00000	6.75146	0.01441	8.76587
C 8	0.09472	1.99999	3.87951	0.02578	5.90528
C 9	0.09703	1.99999	3.87788	0.02509	5.90297
C 10	0.07773	1.99999	3.89559	0.02669	5.92227
C 11	0.09292	1.99999	3.88327	0.02382	5.90708
C 12	0.44620	1.99999	3.52091	0.03290	5.55380
C 13	-0.02784	1.99999	4.00294	0.02490	6.02784
C 14	0.33540	1.99999	3.64083	0.02378	5.66460
C 15	-0.09883	1.99999	4.08132	0.01752	6.09883
C 16	-0.26287	1.99999	4.24645	0.01642	6.26287
C 17	-0.18299	1.99999	4.16648	0.01651	6.18299
C 18	-0.03018	1.99999	4.01024	0.01994	6.03018
C 19	-0.18931	1.99999	4.17257	0.01674	6.18931
C 20	-0.22745	1.99999	4.21081	0.01665	6.22745
H 21	0.17794	0.00000	0.81905	0.00302	0.82206
H 22	0.17785	0.00000	0.81909	0.00306	0.82215
H 23	0.18241	0.00000	0.81473	0.00286	0.81759
H 24	0.18110	0.00000	0.81589	0.00301	0.81890
H 25	0.16148	0.00000	0.83557	0.00295	0.83852

H 26	0.18880	0.00000	0.80885	0.00235	0.81120
H 27	0.16140	0.00000	0.83636	0.00224	0.83860
H 28	0.48636	0.00000	0.50964	0.00400	0.51364
H 29	0.49185	0.00000	0.50425	0.00391	0.50815
H 30	0.51368	0.00000	0.48203	0.00429	0.48632
H 31	0.48870	0.00000	0.50722	0.00408	0.51130
H 32	0.23472	0.00000	0.76249	0.00280	0.76528
H 33	0.21276	0.00000	0.78553	0.00171	0.78724
H 34	0.17278	0.00000	0.82517	0.00205	0.82722
H 35	0.18382	0.00000	0.81392	0.00226	0.81618
H 36	0.21563	0.00000	0.78268	0.00170	0.78437
H 37	0.21655	0.00000	0.78178	0.00167	0.78345
H 38	0.47375	0.00000	0.52240	0.00385	0.52625
* Total *	0.00000	39.99990	111.54580	0.45430	152.00000

(Occupancy) Bond orbital / Coefficients / Hybrids

---------- Lewis ----------

21. (1.95863) LP (1) O 1 s(42.86%)p 1.33(57.10%)d 0.00(0.04%)
0.0000 0.6545 0.0149 0.0020 0.0000
-0.2255 0.0028 0.0031 -0.0013 -0.4029
-0.0046 0.0017 -0.0007 0.5982 0.0024
-0.0034 -0.0003 -0.0070 0.0069 0.0124
0.0048 -0.0088

22. (1.92572) LP (2) O 1 s(0.01%)p 1.00(99.95%)d 0.00(0.04%)
0.0000 -0.0030 0.0072 -0.0028 -0.0001
0.3756 0.0074 0.0006 0.0002 0.6948
0.0141 -0.0035 -0.0021 0.6127 0.0033
-0.0023 -0.0028 0.0080 -0.0026 -0.0039
-0.0059 -0.0171

23. (1.95802) LP (1) O 2 s(34.30%)p 1.91(65.66%)d 0.00(0.03%)
0.0000 0.5856 0.0128 0.0014 0.0001
-0.1176 0.0033 0.0018 -0.0008 0.6384
0.0085 0.0009 -0.0008 0.4849 0.0061
-0.0038 -0.0002 0.0031 0.0017 -0.0152
0.0085 -0.0052

24. (1.86715) LP (2) O 2 s(2.14%)p45.75(97.82%)d 0.02(0.05%)
0.0000 0.1461 0.0025 -0.0045 0.0005
0.2596 -0.0008 -0.0022 0.0016 -0.6304
-0.0048 -0.0029 0.0029 0.7164 0.0044
-0.0055 -0.0037 -0.0034 -0.0046 0.0030
-0.0057 -0.0195

25. (1.98033) LP (1) O 3 s(47.77%)p 1.09(52.20%)d 0.00(0.03%)
0.0000 0.6911 0.0085 0.0023 0.0000
0.6307 0.0054 0.0009 0.0014 0.1055
-0.0067 0.0019 -0.0006 0.3362 0.0024
0.0004 0.0002 -0.0040 -0.0109 -0.0027
-0.0133 0.0010

26. (1.96095) LP (2) O 3 s(0.05%)p99.99(99.90%)d 0.87(0.05%)
0.0000 0.0226 -0.0022 0.0034 0.0000
0.4621 0.0094 -0.0021 -0.0009 -0.1080
-0.0004 0.0000 0.0007 -0.8795 -0.0161
-0.0022 0.0034 0.0009 0.0128 0.0024
-0.0091 0.0144

27. (1.97722) LP (1) O 4 s(46.90%)p 1.13(53.07%)d 0.00(0.03%)
0.0000 0.6848 0.0080 0.0023 0.0000
0.2919 -0.0035 0.0004 0.0008 -0.5844
-0.0082 0.0030 -0.0025 -0.3222 0.0008
-0.0013 0.0005 0.0111 0.0031 -0.0101
0.0073 0.0024

28. (1.96117) LP (2) O 4 s(0.36%)p99.99(99.60%)d 0.12(0.04%)
0.0000 0.0598 -0.0008 0.0031 -0.0001
0.4413 0.0089 0.0000 0.0000 -0.1916
-0.0045 0.0028 0.0004 0.8742 0.0131
0.0026 -0.0038 0.0097 -0.0043 0.0144
-0.0008 0.0104

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29. (1.97859) LP ( 1) O  5           s( 44.83%)p 1.23( 55.14%)d 0.00(  0.03%)
                                      0.0000  0.6695  0.0096  0.0022  0.0004
                                      0.2537  0.0064 -0.0037  0.0010  0.4281
                                      0.0031  0.0024  0.0009 -0.5511 -0.0033
                                     -0.0012  0.0000 -0.0074  0.0076  0.0119
                                      0.0052 -0.0060
30. (1.95428) LP ( 2) O  5           s(  0.15%)p99.99( 99.81%)d 0.30(  0.04%)
                                      0.0000  0.0379 -0.0018  0.0039 -0.0001
                                      0.1810  0.0015 -0.0014 -0.0003  0.7088
                                      0.0170  0.0015 -0.0015  0.6800  0.0132
                                      0.0047 -0.0022 -0.0075 -0.0022  0.0009
                                      0.0088  0.0174
31. (1.97939) LP ( 1) O  6           s( 47.65%)p 1.10( 52.31%)d 0.00(  0.04%)
                                      0.0000  0.6902  0.0114  0.0006  0.0000
                                      0.1315  0.0002  0.0014  0.0003 -0.6603
                                     -0.0056  0.0019 -0.0021 -0.2642 -0.0012
                                      0.0008  0.0001  0.0065 -0.0004 -0.0098
                                      0.0139  0.0052
32. (1.95748) LP ( 2) O  6           s(  0.05%)p99.99( 99.90%)d 1.07(  0.05%)
                                      0.0000  0.0217 -0.0014  0.0046  0.0002
                                      0.5074  0.0124  0.0025 -0.0002 -0.2103
                                     -0.0039 -0.0041  0.0005  0.8347  0.0186
                                     -0.0030 -0.0026  0.0122 -0.0001  0.0165
                                      0.0026  0.0099
33. (1.98071) LP ( 1) O  7           s( 41.84%)p 1.39( 58.13%)d 0.00(  0.03%)
                                      0.0000  0.6468  0.0065 -0.0026  0.0000
                                      0.1012 -0.0055 -0.0070  0.0014 -0.1547
                                     -0.0044  0.0000 -0.0013 -0.7396 -0.0047
                                      0.0016  0.0009  0.0018  0.0080 -0.0083
                                     -0.0021 -0.0139
34. (1.95970) LP ( 2) O  7           s(  7.69%)p12.00( 92.27%)d 0.00(  0.04%)
                                      0.0000  0.2771  0.0112  0.0031  0.0000
                                      0.8860  0.0215 -0.0027 -0.0005 -0.0284
                                     -0.0006 -0.0030 -0.0003  0.3693  0.0068
                                     -0.0032 -0.0027  0.0068  0.0085  0.0030
                                     -0.0104  0.0115

82. (0.00694) BD*( 1) O  3- H 28
              ( 25.40%)   0.5040* O  3 s( 20.96%)p 3.77( 78.91%)d 0.01(  0.13%)
                                      0.0000 -0.4577  0.0083 -0.0007  0.0001
                                      0.4522  0.0047 -0.0020  0.0000 -0.6975
                                      0.0313 -0.0055 -0.0020  0.3115 -0.0024
                                      0.0007 -0.0007  0.0252 -0.0188  0.0158
                                     -0.0033  0.0099
              ( 74.60%)  -0.8637* H 28 s( 99.88%)p 0.00(  0.12%)
                                     -0.9994  0.0032  0.0008  0.0000 -0.0147
                                      0.0306 -0.0091
83. (0.01931) BD*( 1) O  4- C  9
              ( 33.27%)   0.5768* O  4 s( 31.42%)p 2.18( 68.51%)d 0.00(  0.08%)
                                      0.0000 -0.5604  0.0078  0.0058  0.0001
                                      0.7418 -0.0094 -0.0060  0.0019 -0.0895
                                     -0.0008  0.0069  0.0006 -0.3558  0.0064
                                      0.0026  0.0006  0.0120  0.0183 -0.0071
                                     -0.0125  0.0087
              ( 66.73%)  -0.8169* C  9 s( 20.97%)p 3.76( 78.82%)d 0.01(  0.22%)
                                      0.0000 -0.4557  0.0450  0.0017  0.0008
                                     -0.8084 -0.0437  0.0016  0.0050  0.0678
                                     -0.0123 -0.0003  0.0021  0.3576 -0.0025
                                     -0.0071  0.0065  0.0043  0.0326 -0.0003
                                     -0.0311  0.0113
84. (0.00870) BD*( 1) O  4- H 29
              ( 25.06%)   0.5006* O  4 s( 21.29%)p 3.69( 78.58%)d 0.01(  0.13%)
                                      0.0000 -0.4614  0.0079 -0.0016 -0.0001
                                     -0.4100  0.0284 -0.0078 -0.0007 -0.7824
                                      0.0065 -0.0020 -0.0016  0.0670 -0.0111
                                      0.0014 -0.0003 -0.0144  0.0006 -0.0028
                                      0.0271  0.0191
              ( 74.94%)  -0.8657* H 29 s( 99.88%)p 0.00(  0.12%)
                                     -0.9994  0.0038  0.0008 -0.0001  0.0190
                                      0.0286 -0.0065
85. (0.01880) BD*( 1) O  5- C 10
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              ( 34.18%)   0.5847* O  5 s( 30.87%)p 2.24( 69.05%)d 0.00(  0.08%)
                                        0.0000 -0.5556  0.0093  0.0039 -0.0002
                                       -0.4304  0.0137  0.0015 -0.0025  0.5596
                                       -0.0065 -0.0055 -0.0005 -0.4378  0.0058
                                        0.0027  0.0007  0.0113 -0.0085  0.0229
                                        0.0091 -0.0003
              ( 65.82%)  -0.8113* C 10 s( 21.85%)p 3.57( 77.95%)d 0.01(  0.21%)
                                        0.0000 -0.4655  0.0415 -0.0024  0.0004
                                        0.4854  0.0109 -0.0026  0.0028 -0.6018
                                       -0.0399 -0.0021  0.0049  0.4240 -0.0099
                                       -0.0063  0.0093  0.0267 -0.0235  0.0275
                                        0.0038  0.0062
  86. (0.02411) BD*( 1) O  5- H 30
              ( 23.34%)   0.4831* O  5 s( 24.13%)p 3.14( 75.74%)d 0.01(  0.12%)
                                        0.0000 -0.4912  0.0081  0.0000  0.0009
                                        0.8455 -0.0287 -0.0014  0.0027  0.0052
                                        0.0175 -0.0048  0.0000 -0.2032 -0.0098
                                        0.0033  0.0007 -0.0107  0.0218  0.0063
                                       -0.0230  0.0094
              ( 76.66%)  -0.8755* H 30 s( 99.84%)p 0.00(  0.16%)
                                       -0.9992  0.0068  0.0002 -0.0001 -0.0400
                                        0.0036  0.0036
  87. (0.00598) BD*( 1) O  6- C 13
              ( 34.06%)   0.5836* O  6 s( 29.98%)p 2.33( 69.92%)d 0.00(  0.09%)
                                        0.0000 -0.5473  0.0146  0.0039 -0.0002
                                        0.6546 -0.0116 -0.0035  0.0020 -0.2612
                                       -0.0079 -0.0099 -0.0001 -0.4496  0.0089
                                       -0.0029  0.0006  0.0174  0.0198 -0.0142
                                       -0.0039  0.0057
              ( 65.94%)  -0.8120* C 13 s( 22.28%)p 3.48( 77.49%)d 0.01(  0.23%)
                                        0.0000 -0.4694  0.0491 -0.0007  0.0003
                                       -0.7119 -0.0425 -0.0013  0.0050  0.2528
                                        0.0465 -0.0002 -0.0015  0.4471  0.0170
                                        0.0040 -0.0063  0.0150  0.0378 -0.0069
                                       -0.0241  0.0020
  88. (0.01203) BD*( 1) O  6- H 31
              ( 25.09%)   0.5009* O  6 s( 22.31%)p 3.47( 77.54%)d 0.01(  0.14%)
                                        0.0000 -0.4723  0.0072 -0.0027  0.0002
                                       -0.5425  0.0300 -0.0031 -0.0011 -0.6707
                                        0.0104 -0.0036  0.0002  0.1731 -0.0169
                                       -0.0013 -0.0003 -0.0249  0.0035  0.0033
                                        0.0205  0.0194
              ( 74.91%)  -0.8655* H 31 s( 99.85%)p 0.00(  0.15%)
                                       -0.9992  0.0032  0.0004  0.0005  0.0255
                                        0.0261 -0.0129

 107. (0.34844) BD*( 2) C 15- C 17
              ( 47.87%)   0.6919* C 15 s(  0.01%)p99.99( 99.95%)d 2.81(  0.03%)
                                        0.0000  0.0105 -0.0033  0.0002  0.1406
                                       -0.0036  0.0037 -0.0015  0.3671 -0.0007
                                        0.0137  0.0045 -0.9190  0.0112 -0.0022
                                        0.0111 -0.0058  0.0054  0.0129  0.0028
                                        0.0104
              ( 52.13%)  -0.7220* C 17 s(  0.00%)p 1.00( 99.94%)d 0.00(  0.05%)
                                        0.0000  0.0025 -0.0018  0.0009  0.0011
                                        0.1493  0.0012  0.0019 -0.0004  0.3713
                                        0.0030  0.0071 -0.0002 -0.9159 -0.0135
                                       -0.0116  0.0051  0.0097 -0.0192  0.0006
                                        0.0046 -0.0077



SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

     Threshold for printing:   0.10 kcal/mol
                                                          E(2) E(NL)-E(L) F(L,NL)
      Donor (L) NBO              Acceptor (NL) NBO      kcal/mol   a.u.    a.u.
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within unit  1
  21. LP ( 1) O  1           79. BD*( 1) O  2- C 12      5.52    0.97   0.065
  21. LP ( 1) O  1           85. BD*( 1) O  5- C 10      0.12    0.98   0.010
  21. LP ( 1) O  1           87. BD*( 1) O  6- C 13      0.50    0.99   0.020
  21. LP ( 1) O  1           94. BD*( 1) C  9- C 11      0.69    1.02   0.024
  21. LP ( 1) O  1           95. BD*( 1) C  9- H 22      0.16    1.04   0.011
  21. LP ( 1) O  1           96. BD*( 1) C 10- C 12      0.81    1.02   0.026
  21. LP ( 1) O  1           97. BD*( 1) C 10- H 23      0.14    1.04   0.011
  21. LP ( 1) O  1           98. BD*( 1) C 11- C 13      1.90    1.03   0.040
  21. LP ( 1) O  1           99. BD*( 1) C 11- H 24      1.37    1.04   0.034
  21. LP ( 1) O  1          100. BD*( 1) C 12- H 25      1.08    1.02   0.030
  21. LP ( 1) O  1          126. RY ( 8) O  1            0.19    2.30   0.019
  21. LP ( 1) O  1          289. RY ( 1) C 11            0.92    1.63   0.035
  21. LP ( 1) O  1          290. RY ( 2) C 11            1.29    2.21   0.048
  21. LP ( 1) O  1          306. RY ( 1) C 12            2.28    1.87   0.058
  21. LP ( 1) O  1          307. RY ( 2) C 12            0.12    3.13   0.017
  21. LP ( 1) O  1          308. RY ( 3) C 12            0.16    2.45   0.018
  21. LP ( 1) O  1          309. RY ( 4) C 12            0.16    2.10   0.017
  21. LP ( 1) O  1          310. RY ( 5) C 12            0.33    2.24   0.024
  21. LP ( 1) O  1          313. RY ( 8) C 12            0.12    2.46   0.015
  21. LP ( 1) O  1          316. RY (11) C 12            0.16    3.21   0.020
  21. LP ( 1) O  1          322. RY (17) C 12            0.12    3.46   0.018
  21. LP ( 1) O  1          323. RY ( 1) C 13            0.25    1.54   0.017
  22. LP ( 2) O  1           83. BD*( 1) O  4- C  9      1.28    0.75   0.028
  22. LP ( 2) O  1           85. BD*( 1) O  5- C 10      0.97    0.78   0.025
  22. LP ( 2) O  1           94. BD*( 1) C  9- C 11      6.46    0.82   0.065
  22. LP ( 2) O  1           96. BD*( 1) C 10- C 12      6.89    0.82   0.067
  22. LP ( 2) O  1           99. BD*( 1) C 11- H 24      6.86    0.84   0.068
  22. LP ( 2) O  1          100. BD*( 1) C 12- H 25      7.81    0.82   0.072
  22. LP ( 2) O  1          101. BD*( 1) C 13- H 26      0.12    0.86   0.009
  22. LP ( 2) O  1          110. BD*( 1) C 16- H 32      0.35    0.90   0.016
  22. LP ( 2) O  1          122. RY ( 4) O  1            0.11    1.96   0.013
  22. LP ( 2) O  1          272. RY ( 1) C 10            0.19    1.49   0.015
  22. LP ( 2) O  1          289. RY ( 1) C 11            0.21    1.43   0.015
  22. LP ( 2) O  1          292. RY ( 4) C 11            0.92    2.18   0.040
  22. LP ( 2) O  1          294. RY ( 6) C 11            0.11    2.15   0.014
  22. LP ( 2) O  1          296. RY ( 8) C 11            0.11    2.53   0.015
  22. LP ( 2) O  1          307. RY ( 2) C 12            0.11    2.93   0.016
  22. LP ( 2) O  1          308. RY ( 3) C 12            0.16    2.25   0.017
  22. LP ( 2) O  1          309. RY ( 4) C 12            0.60    1.89   0.030
  22. LP ( 2) O  1          310. RY ( 5) C 12            0.57    2.04   0.030
  22. LP ( 2) O  1          311. RY ( 6) C 12            0.34    2.41   0.026
  22. LP ( 2) O  1          475. RY ( 1) H 24            0.26    1.17   0.015
  22. LP ( 2) O  1          481. RY ( 1) H 25            0.19    1.31   0.014
  23. LP ( 1) O  2           78. BD*( 1) O  1- C 12      0.41    0.94   0.018
  23. LP ( 1) O  2           85. BD*( 1) O  5- C 10      0.10    0.95   0.009
  23. LP ( 1) O  2           86. BD*( 1) O  5- H 30      0.18    1.09   0.012
  23. LP ( 1) O  2           89. BD*( 1) O  7- C 18      0.11    0.91   0.009
  23. LP ( 1) O  2           92. BD*( 1) C  8- C 10      0.58    1.01   0.022
  23. LP ( 1) O  2           96. BD*( 1) C 10- C 12      2.15    0.99   0.041
  23. LP ( 1) O  2          100. BD*( 1) C 12- H 25      2.69    1.00   0.046
  23. LP ( 1) O  2          103. BD*( 1) C 14- C 15      1.11    1.18   0.032
  23. LP ( 1) O  2          104. BD*( 1) C 14- C 16      6.29    1.19   0.077
  23. LP ( 1) O  2          105. BD*( 2) C 14- C 16      1.13    0.63   0.024
  23. LP ( 1) O  2          106. BD*( 1) C 15- C 17      0.21    1.20   0.014
  23. LP ( 1) O  2          108. BD*( 1) C 15- C 18      0.13    1.04   0.011
  23. LP ( 1) O  2          109. BD*( 1) C 16- C 19      0.21    1.19   0.014
  23. LP ( 1) O  2          110. BD*( 1) C 16- H 32      0.24    1.08   0.014
  23. LP ( 1) O  2          113. BD*( 1) C 18- H 34      0.41    1.01   0.018
  23. LP ( 1) O  2          273. RY ( 2) C 10            0.15    1.93   0.015
  23. LP ( 1) O  2          307. RY ( 2) C 12            1.69    3.11   0.065
  23. LP ( 1) O  2          308. RY ( 3) C 12            0.19    2.43   0.019
  23. LP ( 1) O  2          309. RY ( 4) C 12            0.13    2.07   0.015
  23. LP ( 1) O  2          312. RY ( 7) C 12            0.21    2.37   0.020
  23. LP ( 1) O  2          313. RY ( 8) C 12            0.11    2.44   0.015
  23. LP ( 1) O  2          318. RY (13) C 12            0.20    3.94   0.025
  23. LP ( 1) O  2          340. RY ( 1) C 14            2.00    1.76   0.053
  23. LP ( 1) O  2          343. RY ( 4) C 14            0.43    2.41   0.029
  23. LP ( 1) O  2          344. RY ( 5) C 14            0.13    1.64   0.013
  23. LP ( 1) O  2          351. RY (12) C 14            0.11    2.97   0.016
  24. LP ( 2) O  2           77. BD*( 1) O  1- C 11      0.51    0.77   0.018
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24. LP (2) O 2	78. BD*(1) O 1- C 12	15.56	0.78	0.098
24. LP (2) O 2	79. BD*(1) O 2- C 12	0.15	0.79	0.010
24. LP (2) O 2	86. BD*(1) O 5- H 30	0.32	0.93	0.015
24. LP (2) O 2	92. BD*(1) C 8- C 10	0.22	0.85	0.012
24. LP (2) O 2	96. BD*(1) C 10- C 12	0.89	0.84	0.024
24. LP (2) O 2	97. BD*(1) C 10- H 23	0.20	0.86	0.012
24. LP (2) O 2	100. BD*(1) C 12- H 25	3.41	0.84	0.048
24. LP (2) O 2	103. BD*(1) C 14- C 15	2.02	1.02	0.041
24. LP (2) O 2	104. BD*(1) C 14- C 16	1.27	1.03	0.032
24. LP (2) O 2	105. BD*(2) C 14- C 16	24.73	0.47	0.096
24. LP (2) O 2	106. BD*(1) C 15- C 17	0.13	1.04	0.010
24. LP (2) O 2	107. BD*(2) C 15- C 17	0.12	0.47	0.007
24. LP (2) O 2	121. RY (3) O 1	0.15	1.27	0.013
24. LP (2) O 2	306. RY (1) C 12	0.63	1.68	0.029
24. LP (2) O 2	308. RY (3) C 12	0.20	2.27	0.019
24. LP (2) O 2	310. RY (5) C 12	0.14	2.06	0.015
24. LP (2) O 2	311. RY (6) C 12	0.63	2.43	0.035
24. LP (2) O 2	316. RY (11) C 12	0.14	3.02	0.018
24. LP (2) O 2	341. RY (2) C 14	0.20	1.65	0.016
24. LP (2) O 2	342. RY (3) C 14	0.94	2.99	0.047
24. LP (2) O 2	343. RY (4) C 14	0.21	2.25	0.019
24. LP (2) O 2	344. RY (5) C 14	0.13	1.48	0.012
24. LP (2) O 2	345. RY (6) C 14	0.11	2.10	0.014
25. LP (1) O 3	84. BD*(1) O 4- H 29	0.24	1.13	0.015
25. LP (1) O 3	91. BD*(1) C 8- C 9	1.77	1.07	0.039
25. LP (1) O 3	92. BD*(1) C 8- C 10	1.16	1.07	0.031
25. LP (1) O 3	93. BD*(1) C 8- H 21	1.02	1.07	0.029
25. LP (1) O 3	94. BD*(1) C 9- C 11	0.37	1.06	0.018
25. LP (1) O 3	96. BD*(1) C 10- C 12	0.13	1.05	0.010
25. LP (1) O 3	97. BD*(1) C 10- H 23	0.20	1.07	0.013
25. LP (1) O 3	238. RY (1) C 8	1.76	1.60	0.047
25. LP (1) O 3	240. RY (3) C 8	0.83	1.57	0.032
25. LP (1) O 3	241. RY (4) C 8	0.17	2.21	0.018
25. LP (1) O 3	242. RY (5) C 8	0.34	2.28	0.025
25. LP (1) O 3	245. RY (8) C 8	0.13	3.12	0.018
25. LP (1) O 3	257. RY (3) C 9	0.20	1.41	0.015
25. LP (1) O 3	499. RY (1) H 28	0.12	2.28	0.015
25. LP (1) O 3	500. RY (2) H 28	1.08	2.56	0.047
26. LP (2) O 3	84. BD*(1) O 4- H 29	0.22	0.90	0.012
26. LP (2) O 3	85. BD*(1) O 5- C 10	0.18	0.78	0.010
26. LP (2) O 3	92. BD*(1) C 8- C 10	6.22	0.84	0.064
26. LP (2) O 3	93. BD*(1) C 8- H 21	8.46	0.83	0.075
26. LP (2) O 3	96. BD*(1) C 10- C 12	0.74	0.82	0.022
26. LP (2) O 3	238. RY (1) C 8	0.17	1.37	0.014
26. LP (2) O 3	239. RY (2) C 8	0.35	1.52	0.021
26. LP (2) O 3	241. RY (4) C 8	1.10	1.98	0.042
26. LP (2) O 3	242. RY (5) C 8	0.13	2.05	0.015
26. LP (2) O 3	248. RY (11) C 8	0.17	1.55	0.015
26. LP (2) O 3	272. RY (1) C 10	0.11	1.49	0.011
26. LP (2) O 3	457. RY (1) H 21	0.19	1.18	0.013
26. LP (2) O 3	499. RY (1) H 28	1.66	2.05	0.052
27. LP (1) O 4	77. BD*(1) O 1- C 11	0.47	0.99	0.019
27. LP (1) O 4	88. BD*(1) O 6- H 31	2.61	1.17	0.049
27. LP (1) O 4	91. BD*(1) C 8- C 9	1.14	1.07	0.031
27. LP (1) O 4	92. BD*(1) C 8- C 10	0.12	1.07	0.010
27. LP (1) O 4	93. BD*(1) C 8- H 21	0.18	1.07	0.012
27. LP (1) O 4	94. BD*(1) C 9- C 11	1.75	1.06	0.038
27. LP (1) O 4	95. BD*(1) C 9- H 22	0.99	1.07	0.029
27. LP (1) O 4	255. RY (1) C 9	1.81	1.60	0.048
27. LP (1) O 4	256. RY (2) C 9	0.16	1.81	0.015
27. LP (1) O 4	257. RY (3) C 9	0.43	1.41	0.022
27. LP (1) O 4	258. RY (4) C 9	0.23	2.26	0.020
27. LP (1) O 4	259. RY (5) C 9	0.41	2.34	0.028
27. LP (1) O 4	269. RY (15) C 9	0.13	3.31	0.018
27. LP (1) O 4	289. RY (1) C 11	0.14	1.67	0.014
27. LP (1) O 4	505. RY (1) H 29	0.30	2.31	0.023
27. LP (1) O 4	506. RY (2) H 29	0.89	2.58	0.043
28. LP (2) O 4	81. BD*(1) O 3- C 8	0.21	0.77	0.011
28. LP (2) O 4	88. BD*(1) O 6- H 31	0.68	0.94	0.022
28. LP (2) O 4	91. BD*(1) C 8- C 9	5.38	0.84	0.060
28. LP (2) O 4	92. BD*(1) C 8- C 10	0.71	0.84	0.022

28. LP (2) O 4	94. BD*(1) C 9- C 11	0.15	0.83	0.010
28. LP (2) O 4	95. BD*(1) C 9- H 22	8.77	0.85	0.077
28. LP (2) O 4	238. RY (1) C 8	0.16	1.38	0.013
28. LP (2) O 4	255. RY (1) C 9	0.18	1.37	0.014
28. LP (2) O 4	256. RY (2) C 9	0.42	1.58	0.023
28. LP (2) O 4	257. RY (3) C 9	0.11	1.18	0.010
28. LP (2) O 4	258. RY (4) C 9	0.88	2.03	0.038
28. LP (2) O 4	259. RY (5) C 9	0.16	2.11	0.016
28. LP (2) O 4	463. RY (1) H 22	0.22	1.25	0.015
28. LP (2) O 4	505. RY (1) H 29	1.37	2.08	0.048
28. LP (2) O 4	506. RY (2) H 29	0.24	2.35	0.021
29. LP (1) O 5	78. BD*(1) O 1- C 12	0.21	0.97	0.013
29. LP (1) O 5	82. BD*(1) O 3- H 28	0.14	1.11	0.011
29. LP (1) O 5	91. BD*(1) C 8- C 9	0.40	1.04	0.018
29. LP (1) O 5	92. BD*(1) C 8- C 10	2.06	1.04	0.041
29. LP (1) O 5	96. BD*(1) C 10- C 12	1.48	1.02	0.035
29. LP (1) O 5	97. BD*(1) C 10- H 23	1.14	1.04	0.031
29. LP (1) O 5	100. BD*(1) C 12- H 25	0.25	1.03	0.014
29. LP (1) O 5	197. RY (11) O 5	0.12	15.49	0.039
29. LP (1) O 5	201. RY (15) O 5	0.11	22.78	0.045
29. LP (1) O 5	272. RY (1) C 10	2.09	1.70	0.053
29. LP (1) O 5	273. RY (2) C 10	0.18	1.96	0.017
29. LP (1) O 5	274. RY (3) C 10	0.52	1.74	0.027
29. LP (1) O 5	275. RY (4) C 10	0.14	2.17	0.015
29. LP (1) O 5	276. RY (5) C 10	0.41	2.43	0.028
29. LP (1) O 5	285. RY (14) C 10	0.17	3.52	0.022
29. LP (1) O 5	511. RY (1) H 30	1.09	2.51	0.047
29. LP (1) O 5	513. RY (3) H 30	0.15	2.17	0.016
30. LP (2) O 5	78. BD*(1) O 1- C 12	1.15	0.75	0.026
30. LP (2) O 5	79. BD*(1) O 2- C 12	0.19	0.76	0.011
30. LP (2) O 5	82. BD*(1) O 3- H 28	0.10	0.89	0.008
30. LP (2) O 5	92. BD*(1) C 8- C 10	0.13	0.82	0.009
30. LP (2) O 5	93. BD*(1) C 8- H 21	0.11	0.82	0.008
30. LP (2) O 5	96. BD*(1) C 10- C 12	6.44	0.81	0.064
30. LP (2) O 5	97. BD*(1) C 10- H 23	9.43	0.83	0.079
30. LP (2) O 5	221. RY (1) O 7	0.10	1.02	0.009
30. LP (2) O 5	272. RY (1) C 10	0.30	1.48	0.019
30. LP (2) O 5	273. RY (2) C 10	0.18	1.75	0.016
30. LP (2) O 5	275. RY (4) C 10	1.12	1.95	0.042
30. LP (2) O 5	277. RY (6) C 10	0.20	2.36	0.019
30. LP (2) O 5	306. RY (1) C 12	0.22	1.66	0.017
30. LP (2) O 5	469. RY (1) H 23	0.20	1.26	0.014
30. LP (2) O 5	512. RY (2) H 30	1.45	2.06	0.049
31. LP (1) O 6	77. BD*(1) O 1- C 11	0.13	0.96	0.010
31. LP (1) O 6	98. BD*(1) C 11- C 13	1.26	1.03	0.032
31. LP (1) O 6	99. BD*(1) C 11- H 24	0.25	1.04	0.015
31. LP (1) O 6	101. BD*(1) C 13- H 26	3.32	1.06	0.053
31. LP (1) O 6	102. BD*(1) C 13- H 27	0.84	1.05	0.026
31. LP (1) O 6	323. RY (1) C 13	1.93	1.54	0.049
31. LP (1) O 6	325. RY (3) C 13	0.47	2.14	0.028
31. LP (1) O 6	326. RY (4) C 13	0.39	2.38	0.027
31. LP (1) O 6	330. RY (8) C 13	0.10	3.83	0.018
31. LP (1) O 6	335. RY (13) C 13	0.12	1.85	0.013
31. LP (1) O 6	518. RY (2) H 31	1.15	2.50	0.048
31. LP (1) O 6	520. RY (4) H 31	0.10	1.65	0.011
32. LP (2) O 6	77. BD*(1) O 1- C 11	1.19	0.73	0.026
32. LP (2) O 6	98. BD*(1) C 11- C 13	6.06	0.81	0.062
32. LP (2) O 6	101. BD*(1) C 13- H 26	0.14	0.84	0.010
32. LP (2) O 6	102. BD*(1) C 13- H 27	8.91	0.82	0.076
32. LP (2) O 6	323. RY (1) C 13	0.35	1.31	0.019
32. LP (2) O 6	324. RY (2) C 13	0.73	1.37	0.028
32. LP (2) O 6	325. RY (3) C 13	0.94	1.91	0.038
32. LP (2) O 6	493. RY (1) H 27	0.15	1.00	0.011
32. LP (2) O 6	517. RY (1) H 31	1.84	1.99	0.054
33. LP (1) O 7	86. BD*(1) O 5- H 30	2.40	1.13	0.047
33. LP (1) O 7	106. BD*(1) C 15- C 17	0.12	1.24	0.011
33. LP (1) O 7	107. BD*(2) C 15- C 17	0.31	0.67	0.013
33. LP (1) O 7	108. BD*(1) C 15- C 18	1.53	1.08	0.036
33. LP (1) O 7	114. BD*(1) C 18- H 35	2.01	1.06	0.041
33. LP (1) O 7	406. RY (1) C 18	0.55	1.56	0.026
33. LP (1) O 7	407. RY (2) C 18	1.43	2.02	0.048

33. LP (1) O 7	411. RY (6) C 18	0.34	2.42	0.026
33. LP (1) O 7	419. RY (14) C 18	0.18	2.86	0.020
33. LP (1) O 7	559. RY (1) H 38	0.91	2.23	0.040
33. LP (1) O 7	560. RY (2) H 38	0.61	2.50	0.035
34. LP (2) O 7	86. BD*(1) O 5- H 30	7.61	0.97	0.077
34. LP (2) O 7	113. BD*(1) C 18- H 34	5.72	0.89	0.064
34. LP (2) O 7	114. BD*(1) C 18- H 35	5.27	0.90	0.061
34. LP (2) O 7	190. RY (4) O 5	0.11	1.74	0.013
34. LP (2) O 7	407. RY (2) C 18	0.13	1.86	0.014
34. LP (2) O 7	408. RY (3) C 18	1.03	1.65	0.037
34. LP (2) O 7	409. RY (4) C 18	0.31	1.84	0.021
34. LP (2) O 7	410. RY (5) C 18	0.28	1.78	0.020
34. LP (2) O 7	511. RY (1) H 30	0.17	2.36	0.018
34. LP (2) O 7	541. RY (1) H 35	0.19	1.04	0.012
34. LP (2) O 7	559. RY (1) H 38	1.10	2.07	0.043
34. LP (2) O 7	560. RY (2) H 38	0.69	2.33	0.036

Salicin VII

Summary of Natural Population Analysis:

		Natural Population			
Atom No	Natural Charge	Core	Valence	Rydberg	Total
O 1	-0.63990	2.00000	6.61625	0.02365	8.63990
O 2	-0.59808	2.00000	6.57434	0.02375	8.59808
O 3	-0.76213	2.00000	6.74820	0.01393	8.76213
O 4	-0.74944	2.00000	6.73588	0.01356	8.74944
O 5	-0.78379	2.00000	6.76887	0.01493	8.78379
O 6	-0.73735	2.00000	6.72367	0.01368	8.73735
O 7	-0.75503	2.00000	6.74168	0.01335	8.75503
C 8	0.09852	1.99999	3.87543	0.02605	5.90148
C 9	0.09596	1.99999	3.87815	0.02590	5.90404
C 10	0.07309	1.99999	3.90003	0.02688	5.92691
C 11	0.09232	1.99999	3.88240	0.02528	5.90768
C 12	0.45235	1.99999	3.51392	0.03374	5.54765
C 13	-0.03107	1.99999	4.00785	0.02323	6.03107
C 14	0.32200	1.99999	3.65444	0.02357	5.67800
C 15	-0.12719	1.99999	4.11162	0.01558	6.12719
C 16	-0.22683	1.99999	4.20856	0.01827	6.22683
C 17	-0.19051	1.99999	4.17364	0.01687	6.19051
C 18	-0.04179	1.99999	4.01801	0.02378	6.04179
C 19	-0.19504	1.99999	4.17872	0.01633	6.19504
C 20	-0.21431	1.99999	4.19764	0.01668	6.21431
H 21	0.17523	0.00000	0.82170	0.00307	0.82477

H 22	0.17607	0.00000	0.82087	0.00306	0.82393
H 23	0.18617	0.00000	0.81100	0.00283	0.81383
H 24	0.18386	0.00000	0.81333	0.00281	0.81614
H 25	0.15212	0.00000	0.84492	0.00296	0.84788
H 26	0.16247	0.00000	0.83517	0.00236	0.83753
H 27	0.20351	0.00000	0.79477	0.00171	0.79649
H 28	0.48626	0.00000	0.50977	0.00397	0.51374
H 29	0.48261	0.00000	0.51333	0.00407	0.51739
H 30	0.51275	0.00000	0.48303	0.00422	0.48725
H 31	0.46611	0.00000	0.52914	0.00475	0.53389
H 32	0.23116	0.00000	0.76631	0.00253	0.76884
H 33	0.21391	0.00000	0.78422	0.00187	0.78609
H 34	0.20069	0.00000	0.79678	0.00254	0.79931
H 35	0.17498	0.00000	0.82286	0.00216	0.82502
H 36	0.21782	0.00000	0.78048	0.00170	0.78218
H 37	0.21725	0.00000	0.78107	0.00168	0.78275
H 38	0.47522	0.00000	0.52090	0.00388	0.52478
* Total *	0.00000	39.99990	111.53896	0.46113	152.00000

SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

Threshold for printing: 0.10 kcal/mol

Donor (L) NBO	Acceptor (NL) NBO	E(2) kcal/mol	E(NL)-E(L) a.u.	F(L,NL) a.u.
within unit 1				
21. LP (1) O 1	79. BD*(1) O 2- C 12	5.25	0.97	0.064
21. LP (1) O 1	88. BD*(1) O 6- H 31	0.33	1.12	0.017
21. LP (1) O 1	94. BD*(1) C 9- C 11	0.51	1.03	0.020
21. LP (1) O 1	95. BD*(1) C 9- H 22	0.14	1.04	0.011
21. LP (1) O 1	96. BD*(1) C 10- C 12	0.57	1.02	0.022
21. LP (1) O 1	97. BD*(1) C 10- H 23	0.13	1.04	0.010
21. LP (1) O 1	98. BD*(1) C 11- C 13	1.69	1.05	0.038
21. LP (1) O 1	99. BD*(1) C 11- H 24	1.50	1.05	0.035
21. LP (1) O 1	100. BD*(1) C 12- H 25	1.40	1.02	0.034
21. LP (1) O 1	102. BD*(1) C 13- H 27	0.47	1.08	0.020
21. LP (1) O 1	124. RY (6) O 1	0.21	1.99	0.018
21. LP (1) O 1	289. RY (1) C 11	1.54	1.55	0.044
21. LP (1) O 1	290. RY (2) C 11	0.58	2.19	0.032
21. LP (1) O 1	291. RY (3) C 11	0.18	2.00	0.017
21. LP (1) O 1	292. RY (4) C 11	0.18	2.49	0.019
21. LP (1) O 1	295. RY (7) C 11	0.11	3.99	0.019
21. LP (1) O 1	306. RY (1) C 12	2.30	1.75	0.057
21. LP (1) O 1	307. RY (2) C 12	0.20	2.71	0.021
21. LP (1) O 1	308. RY (3) C 12	0.21	2.47	0.020
21. LP (1) O 1	310. RY (5) C 12	0.28	2.49	0.023
21. LP (1) O 1	316. RY (11) C 12	0.15	4.58	0.024
21. LP (1) O 1	322. RY (17) C 12	0.12	3.21	0.017
22. LP (2) O 1	83. BD*(1) O 4- C 9	1.19	0.77	0.027
22. LP (2) O 1	85. BD*(1) O 5- C 10	1.11	0.78	0.026
22. LP (2) O 1	88. BD*(1) O 6- H 31	0.38	0.91	0.017
22. LP (2) O 1	94. BD*(1) C 9- C 11	6.53	0.83	0.066
22. LP (2) O 1	96. BD*(1) C 10- C 12	6.97	0.82	0.068
22. LP (2) O 1	99. BD*(1) C 11- H 24	6.23	0.85	0.065
22. LP (2) O 1	100. BD*(1) C 12- H 25	7.15	0.82	0.068
22. LP (2) O 1	272. RY (1) C 10	0.15	1.47	0.013
22. LP (2) O 1	289. RY (1) C 11	0.16	1.35	0.013
22. LP (2) O 1	292. RY (4) C 11	0.70	2.29	0.036
22. LP (2) O 1	294. RY (6) C 11	0.15	2.42	0.017
22. LP (2) O 1	306. RY (1) C 12	0.25	1.55	0.017
22. LP (2) O 1	308. RY (3) C 12	0.18	2.26	0.018
22. LP (2) O 1	309. RY (4) C 12	0.88	1.85	0.036
22. LP (2) O 1	311. RY (6) C 12	0.41	2.07	0.026
22. LP (2) O 1	313. RY (8) C 12	0.12	1.99	0.014
22. LP (2) O 1	475. RY (1) H 24	0.19	1.24	0.014
22. LP (2) O 1	481. RY (1) H 25	0.18	1.31	0.014

23. LP (1) O 2	79. BD*(1) O 2- C 12	0.18	0.96	0.012
23. LP (1) O 2	92. BD*(1) C 8- C 10	0.39	1.03	0.018
23. LP (1) O 2	96. BD*(1) C 10- C 12	1.55	1.01	0.035
23. LP (1) O 2	100. BD*(1) C 12- H 25	3.77	1.01	0.055
23. LP (1) O 2	103. BD*(1) C 14- C 15	0.59	1.19	0.024
23. LP (1) O 2	104. BD*(1) C 14- C 16	0.45	1.20	0.021
23. LP (1) O 2	105. BD*(2) C 14- C 16	9.57	0.64	0.070
23. LP (1) O 2	108. BD*(1) C 15- C 18	0.11	1.04	0.010
23. LP (1) O 2	110. BD*(1) C 16- H 32	0.13	1.09	0.011
23. LP (1) O 2	147. RY (12) O 2	0.11	3.75	0.018
23. LP (1) O 2	273. RY (2) C 10	0.15	1.77	0.014
23. LP (1) O 2	307. RY (2) C 12	2.01	2.69	0.066
23. LP (1) O 2	311. RY (6) C 12	0.29	2.25	0.023
23. LP (1) O 2	312. RY (7) C 12	0.20	2.35	0.019
23. LP (1) O 2	318. RY (13) C 12	0.13	3.44	0.019
23. LP (1) O 2	320. RY (15) C 12	0.10	2.73	0.015
23. LP (1) O 2	340. RY (1) C 14	1.78	1.92	0.052
23. LP (1) O 2	341. RY (2) C 14	0.16	1.67	0.014
23. LP (1) O 2	344. RY (5) C 14	0.62	2.25	0.033
23. LP (1) O 2	347. RY (8) C 14	0.12	1.88	0.013
23. LP (1) O 2	348. RY (9) C 14	0.21	2.24	0.020
24. LP (2) O 2	77. BD*(1) O 1- C 11	0.65	0.76	0.020
24. LP (2) O 2	78. BD*(1) O 1- C 12	16.47	0.77	0.101
24. LP (2) O 2	86. BD*(1) O 5- H 30	0.24	0.92	0.013
24. LP (2) O 2	89. BD*(1) O 7- C 18	0.13	0.75	0.009
24. LP (2) O 2	92. BD*(1) C 8- C 10	0.29	0.85	0.014
24. LP (2) O 2	96. BD*(1) C 10- C 12	1.17	0.83	0.028
24. LP (2) O 2	97. BD*(1) C 10- H 23	0.17	0.85	0.011
24. LP (2) O 2	100. BD*(1) C 12- H 25	2.86	0.83	0.043
24. LP (2) O 2	103. BD*(1) C 14- C 15	7.51	1.01	0.078
24. LP (2) O 2	104. BD*(1) C 14- C 16	7.66	1.02	0.079
24. LP (2) O 2	106. BD*(1) C 15- C 17	0.46	1.03	0.019
24. LP (2) O 2	109. BD*(1) C 16- C 19	0.39	1.02	0.018
24. LP (2) O 2	114. BD*(1) C 18- H 35	0.27	0.85	0.013
24. LP (2) O 2	306. RY (1) C 12	0.79	1.56	0.031
24. LP (2) O 2	308. RY (3) C 12	0.31	2.27	0.024
24. LP (2) O 2	310. RY (5) C 12	0.42	2.29	0.028
24. LP (2) O 2	311. RY (6) C 12	0.24	2.07	0.020
24. LP (2) O 2	342. RY (3) C 14	1.31	2.51	0.051
24. LP (2) O 2	345. RY (6) C 14	0.22	2.16	0.019
24. LP (2) O 2	374. RY (2) C 16	0.13	1.46	0.012
24. LP (2) O 2	481. RY (1) H 25	0.11	1.32	0.011
25. LP (1) O 3	84. BD*(1) O 4- H 29	0.20	1.14	0.014
25. LP (1) O 3	91. BD*(1) C 8- C 9	1.78	1.06	0.039
25. LP (1) O 3	92. BD*(1) C 8- C 10	1.24	1.07	0.032
25. LP (1) O 3	93. BD*(1) C 8- H 21	0.97	1.06	0.029
25. LP (1) O 3	94. BD*(1) C 9- C 11	0.36	1.06	0.017
25. LP (1) O 3	96. BD*(1) C 10- C 12	0.14	1.05	0.011
25. LP (1) O 3	97. BD*(1) C 10- H 23	0.20	1.07	0.013
25. LP (1) O 3	238. RY (1) C 8	1.82	1.56	0.048
25. LP (1) O 3	240. RY (3) C 8	0.80	1.57	0.032
25. LP (1) O 3	241. RY (4) C 8	0.15	2.18	0.016
25. LP (1) O 3	242. RY (5) C 8	0.40	2.24	0.027
25. LP (1) O 3	245. RY (8) C 8	0.16	2.99	0.020
25. LP (1) O 3	251. RY (14) C 8	0.15	2.67	0.018
25. LP (1) O 3	257. RY (3) C 9	0.13	1.45	0.012
25. LP (1) O 3	499. RY (1) H 28	0.10	2.28	0.014
25. LP (1) O 3	500. RY (2) H 28	1.06	2.57	0.047
26. LP (2) O 3	84. BD*(1) O 4- H 29	0.21	0.90	0.012
26. LP (2) O 3	85. BD*(1) O 5- C 10	0.18	0.77	0.011
26. LP (2) O 3	92. BD*(1) C 8- C 10	6.11	0.83	0.064
26. LP (2) O 3	93. BD*(1) C 8- H 21	8.70	0.83	0.076
26. LP (2) O 3	95. BD*(1) C 9- H 22	0.11	0.83	0.008
26. LP (2) O 3	96. BD*(1) C 10- C 12	0.73	0.82	0.022
26. LP (2) O 3	238. RY (1) C 8	0.15	1.33	0.013
26. LP (2) O 3	239. RY (2) C 8	0.44	1.51	0.023
26. LP (2) O 3	241. RY (4) C 8	1.08	1.95	0.041
26. LP (2) O 3	242. RY (5) C 8	0.13	2.01	0.014
26. LP (2) O 3	272. RY (1) C 10	0.14	1.46	0.013
26. LP (2) O 3	457. RY (1) H 21	0.18	1.18	0.013
26. LP (2) O 3	499. RY (1) H 28	1.66	2.04	0.052

27. LP (1) O 4	77. BD*(1) O 1- C 11	0.56	0.97	0.021
27. LP (1) O 4	91. BD*(1) C 8- C 9	1.78	1.06	0.039
27. LP (1) O 4	92. BD*(1) C 8- C 10	0.20	1.06	0.013
27. LP (1) O 4	93. BD*(1) C 8- H 21	0.20	1.06	0.013
27. LP (1) O 4	94. BD*(1) C 9- C 11	1.65	1.05	0.037
27. LP (1) O 4	95. BD*(1) C 9- H 22	0.48	1.06	0.020
27. LP (1) O 4	102. BD*(1) C 13- H 27	0.12	1.09	0.010
27. LP (1) O 4	255. RY (1) C 9	1.96	1.60	0.050
27. LP (1) O 4	257. RY (3) C 9	0.65	1.45	0.027
27. LP (1) O 4	258. RY (4) C 9	0.15	2.21	0.016
27. LP (1) O 4	259. RY (5) C 9	0.51	2.35	0.031
27. LP (1) O 4	269. RY (15) C 9	0.16	3.55	0.021
27. LP (1) O 4	289. RY (1) C 11	0.22	1.57	0.017
27. LP (1) O 4	506. RY (2) H 29	1.17	2.55	0.049
28. LP (2) O 4	77. BD*(1) O 1- C 11	0.11	0.74	0.008
28. LP (2) O 4	81. BD*(1) O 3- C 8	0.17	0.76	0.010
28. LP (2) O 4	91. BD*(1) C 8- C 9	4.93	0.83	0.057
28. LP (2) O 4	92. BD*(1) C 8- C 10	0.66	0.83	0.021
28. LP (2) O 4	94. BD*(1) C 9- C 11	0.33	0.82	0.015
28. LP (2) O 4	95. BD*(1) C 9- H 22	9.96	0.83	0.081
28. LP (2) O 4	238. RY (1) C 8	0.21	1.32	0.015
28. LP (2) O 4	256. RY (2) C 9	0.44	1.53	0.023
28. LP (2) O 4	258. RY (4) C 9	1.22	1.98	0.044
28. LP (2) O 4	463. RY (1) H 22	0.21	1.19	0.014
28. LP (2) O 4	505. RY (1) H 29	1.78	2.05	0.054
29. LP (1) O 5	78. BD*(1) O 1- C 12	0.13	0.97	0.010
29. LP (1) O 5	82. BD*(1) O 3- H 28	0.15	1.11	0.012
29. LP (1) O 5	91. BD*(1) C 8- C 9	0.42	1.05	0.019
29. LP (1) O 5	92. BD*(1) C 8- C 10	1.98	1.05	0.041
29. LP (1) O 5	96. BD*(1) C 10- C 12	1.08	1.03	0.030
29. LP (1) O 5	97. BD*(1) C 10- H 23	1.53	1.05	0.036
29. LP (1) O 5	100. BD*(1) C 12- H 25	0.25	1.03	0.014
29. LP (1) O 5	272. RY (1) C 10	1.90	1.68	0.050
29. LP (1) O 5	274. RY (3) C 10	0.85	1.86	0.035
29. LP (1) O 5	276. RY (5) C 10	0.36	2.38	0.026
29. LP (1) O 5	285. RY (14) C 10	0.19	3.72	0.024
29. LP (1) O 5	511. RY (1) H 30	1.03	2.65	0.047
29. LP (1) O 5	513. RY (3) H 30	0.13	2.22	0.015
30. LP (2) O 5	78. BD*(1) O 1- C 12	1.26	0.75	0.027
30. LP (2) O 5	79. BD*(1) O 2- C 12	0.18	0.76	0.010
30. LP (2) O 5	82. BD*(1) O 3- H 28	0.17	0.89	0.011
30. LP (2) O 5	93. BD*(1) C 8- H 21	0.12	0.83	0.009
30. LP (2) O 5	96. BD*(1) C 10- C 12	7.58	0.81	0.070
30. LP (2) O 5	97. BD*(1) C 10- H 23	8.16	0.83	0.074
30. LP (2) O 5	113. BD*(1) C 18- H 34	0.26	0.84	0.013
30. LP (2) O 5	272. RY (1) C 10	0.23	1.46	0.016
30. LP (2) O 5	274. RY (3) C 10	0.47	1.64	0.025
30. LP (2) O 5	275. RY (4) C 10	0.96	1.74	0.037
30. LP (2) O 5	276. RY (5) C 10	0.13	2.16	0.015
30. LP (2) O 5	277. RY (6) C 10	0.15	2.31	0.016
30. LP (2) O 5	306. RY (1) C 12	0.22	1.54	0.017
30. LP (2) O 5	406. RY (1) C 18	0.11	1.29	0.011
30. LP (2) O 5	469. RY (1) H 23	0.16	1.25	0.013
30. LP (2) O 5	512. RY (2) H 30	1.38	2.10	0.048
31. LP (1) O 6	78. BD*(1) O 1- C 12	0.10	0.97	0.009
31. LP (1) O 6	98. BD*(1) C 11- C 13	1.26	1.06	0.033
31. LP (1) O 6	99. BD*(1) C 11- H 24	0.18	1.06	0.012
31. LP (1) O 6	101. BD*(1) C 13- H 26	0.72	1.06	0.025
31. LP (1) O 6	102. BD*(1) C 13- H 27	2.99	1.08	0.051
31. LP (1) O 6	323. RY (1) C 13	1.72	1.58	0.047
31. LP (1) O 6	325. RY (3) C 13	0.60	2.13	0.032
31. LP (1) O 6	326. RY (4) C 13	0.31	2.15	0.023
31. LP (1) O 6	327. RY (5) C 13	0.11	1.80	0.012
31. LP (1) O 6	335. RY (13) C 13	0.11	3.05	0.017
31. LP (1) O 6	337. RY (15) C 13	0.21	3.09	0.023
31. LP (1) O 6	518. RY (2) H 31	1.14	2.38	0.046
31. LP (1) O 6	520. RY (4) H 31	0.17	2.44	0.018
32. LP (2) O 6	77. BD*(1) O 1- C 11	0.30	0.73	0.013
32. LP (2) O 6	94. BD*(1) C 9- C 11	0.88	0.81	0.024
32. LP (2) O 6	98. BD*(1) C 11- C 13	5.64	0.82	0.061
32. LP (2) O 6	101. BD*(1) C 13- H 26	8.65	0.82	0.075

32. LP (2) O 6	102. BD*(1) C 13- H 27	0.15	0.85	0.010
32. LP (2) O 6	289. RY (1) C 11	0.23	1.32	0.015
32. LP (2) O 6	323. RY (1) C 13	0.24	1.34	0.016
32. LP (2) O 6	324. RY (2) C 13	0.75	1.44	0.029
32. LP (2) O 6	325. RY (3) C 13	0.94	1.89	0.038
32. LP (2) O 6	327. RY (5) C 13	0.13	1.56	0.013
32. LP (2) O 6	487. RY (1) H 26	0.13	1.02	0.010
32. LP (2) O 6	517. RY (1) H 31	1.92	1.90	0.054
33. LP (1) O 7	86. BD*(1) O 5- H 30	3.06	1.14	0.053
33. LP (1) O 7	107. BD*(2) C 15- C 17	0.34	0.68	0.013
33. LP (1) O 7	108. BD*(1) C 15- C 18	3.30	1.08	0.053
33. LP (1) O 7	113. BD*(1) C 18- H 34	2.20	1.07	0.043
33. LP (1) O 7	406. RY (1) C 18	1.29	1.53	0.040
33. LP (1) O 7	407. RY (2) C 18	0.10	1.73	0.012
33. LP (1) O 7	408. RY (3) C 18	0.64	1.89	0.031
33. LP (1) O 7	409. RY (4) C 18	0.32	2.66	0.026
33. LP (1) O 7	413. RY (8) C 18	0.14	3.09	0.019
33. LP (1) O 7	559. RY (1) H 38	0.25	2.34	0.022
33. LP (1) O 7	560. RY (2) H 38	1.10	2.52	0.047
34. LP (2) O 7	86. BD*(1) O 5- H 30	4.22	0.93	0.056
34. LP (2) O 7	107. BD*(2) C 15- C 17	0.43	0.47	0.013
34. LP (2) O 7	108. BD*(1) C 15- C 18	2.51	0.88	0.042
34. LP (2) O 7	113. BD*(1) C 18- H 34	1.50	0.87	0.032
34. LP (2) O 7	114. BD*(1) C 18- H 35	8.61	0.86	0.077
34. LP (2) O 7	407. RY (2) C 18	1.56	1.53	0.044
34. LP (2) O 7	408. RY (3) C 18	0.30	1.69	0.020
34. LP (2) O 7	409. RY (4) C 18	0.27	2.45	0.023
34. LP (2) O 7	541. RY (1) H 35	0.12	0.98	0.010
34. LP (2) O 7	559. RY (1) H 38	1.58	2.13	0.052
34. LP (2) O 7	560. RY (2) H 38	0.20	2.32	0.019

Salicin (Conformer X)

Summary of Natural Population Analysis:

		Natural Population			
Atom No	Natural Charge	Core	Valence	Rydberg	Total
O 1	-0.62248	2.00000	6.59929	0.02319	8.62248
O 2	-0.59740	2.00000	6.57458	0.02282	8.59740
O 3	-0.76371	2.00000	6.74992	0.01379	8.76371
O 4	-0.77212	2.00000	6.75871	0.01341	8.77212
O 5	-0.78444	2.00000	6.76940	0.01504	8.78444
O 6	-0.75083	2.00000	6.73707	0.01377	8.75083
O 7	-0.75553	2.00000	6.74219	0.01334	8.75553
C 8	0.09624	1.99999	3.87804	0.02573	5.90376
C 9	0.09715	1.99999	3.87762	0.02524	5.90285
C 10	0.07383	1.99999	3.89926	0.02691	5.92617
C 11	0.09259	1.99999	3.88323	0.02419	5.90741
C 12	0.45214	1.99999	3.51434	0.03353	5.54786
C 13	-0.02709	1.99999	4.00222	0.02487	6.02709
C 14	0.32355	1.99999	3.65284	0.02362	5.67645
C 15	-0.13220	1.99999	4.11604	0.01616	6.13220
C 16	-0.23502	1.99999	4.21663	0.01840	6.23502
C 17	-0.18042	1.99999	4.16314	0.01729	6.18042
C 18	-0.04142	1.99999	4.01765	0.02377	6.04142
C 19	-0.19119	1.99999	4.17564	0.01555	6.19119
C 20	-0.22003	1.99999	4.20266	0.01738	6.22003
H 21	0.17642	0.00000	0.82053	0.00305	0.82358

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   H 22    0.17780      0.00000     0.81919    0.00301     0.82220
   H 23    0.18581      0.00000     0.81131    0.00288     0.81419
   H 24    0.18166      0.00000     0.81527    0.00307     0.81834
   H 25    0.15132      0.00000     0.84577    0.00291     0.84868
   H 26    0.18922      0.00000     0.80847    0.00231     0.81078
   H 27    0.16039      0.00000     0.83739    0.00222     0.83961
   H 28    0.48723      0.00000     0.50881    0.00397     0.51277
   H 29    0.49174      0.00000     0.50436    0.00389     0.50826
   H 30    0.51344      0.00000     0.48233    0.00422     0.48656
   H 31    0.48864      0.00000     0.50728    0.00409     0.51136
   H 32    0.23762      0.00000     0.76040    0.00197     0.76238
   H 33    0.21274      0.00000     0.78506    0.00220     0.78726
   H 34    0.20004      0.00000     0.79743    0.00254     0.79996
   H 35    0.17481      0.00000     0.82301    0.00218     0.82519
   H 36    0.21719      0.00000     0.78112    0.00169     0.78281
   H 37    0.21668      0.00000     0.78161    0.00171     0.78332
   H 38    0.47561      0.00000     0.52053    0.00386     0.52439
==========================================================================
* Total *  0.00000     39.99990   111.54034    0.45976   152.00000


 21. (1.95817) LP ( 1) O  1           s( 42.77%)p 1.34( 57.19%)d 0.00(  0.03%)
                                       0.0000  0.6538  0.0156  0.0024  0.0000
                                      -0.2256  0.0039  0.0035 -0.0013  0.4787
                                       0.0056 -0.0020  0.0011 -0.5402  0.0000
                                       0.0004  0.0006  0.0081 -0.0053  0.0135
                                       0.0060 -0.0055
 22. (1.92628) LP ( 2) O  1           s(  0.01%)p99.99( 99.95%)d 4.06(  0.04%)
                                       0.0000  0.0070 -0.0056  0.0046  0.0001
                                      -0.4744 -0.0103 -0.0033 -0.0003  0.5457
                                       0.0125 -0.0029 -0.0015  0.6901  0.0072
                                      -0.0050 -0.0030  0.0096 -0.0025 -0.0019
                                       0.0047  0.0169
 23. (1.94268) LP ( 1) O  2           s( 38.79%)p 1.58( 61.17%)d 0.00(  0.04%)
                                       0.0000  0.6227  0.0143  0.0013  0.0001
                                      -0.0139  0.0003 -0.0013  0.0002 -0.4281
                                      -0.0060  0.0010  0.0001 -0.6542 -0.0097
                                       0.0072  0.0003 -0.0015  0.0006 -0.0136
                                       0.0067 -0.0115
 24. (1.91148) LP ( 2) O  2           s(  0.03%)p99.99( 99.92%)d 1.56(  0.05%)
                                       0.0000  0.0170  0.0020 -0.0014  0.0003
                                       0.2911  0.0000 -0.0022  0.0008  0.8047
                                       0.0081  0.0012 -0.0030 -0.5165 -0.0042
                                       0.0011  0.0026  0.0038  0.0056  0.0103
                                      -0.0071 -0.0161
 25. (1.98022) LP ( 1) O  3           s( 47.72%)p 1.09( 52.25%)d 0.00(  0.03%)
                                       0.0000  0.6907  0.0087  0.0022  0.0001
                                       0.6604  0.0051  0.0010  0.0014  0.0141
                                       0.0074 -0.0017  0.0012 -0.2933 -0.0008
                                      -0.0008  0.0002 -0.0005  0.0100  0.0007
                                      -0.0146  0.0021
 26. (1.96065) LP ( 2) O  3           s(  0.04%)p99.99( 99.92%)d 1.29(  0.05%)
                                       0.0000  0.0185 -0.0022  0.0031  0.0000
                                       0.3899  0.0082 -0.0025 -0.0006 -0.0367
                                      -0.0021 -0.0011 -0.0007  0.9195  0.0167
                                       0.0021 -0.0038  0.0006 -0.0153 -0.0019
                                      -0.0079  0.0126
 27. (1.97723) LP ( 1) O  4           s( 46.86%)p 1.13( 53.12%)d 0.00(  0.03%)
                                       0.0000  0.6845  0.0080  0.0022  0.0000
                                       0.2119 -0.0045  0.0005  0.0005  0.5294
                                       0.0078 -0.0030  0.0022  0.4537  0.0003
                                       0.0006 -0.0003 -0.0084 -0.0035 -0.0126
                                       0.0070 -0.0020
 28. (1.96105) LP ( 2) O  4           s(  0.43%)p99.99( 99.53%)d 0.10(  0.04%)
                                       0.0000  0.0652 -0.0007  0.0031 -0.0001
                                       0.4677  0.0089  0.0004  0.0001  0.4008
                                       0.0086 -0.0017 -0.0006 -0.7846 -0.0115
                                      -0.0030  0.0033 -0.0105 -0.0001  0.0092
                                       0.0034  0.0148
 29. (1.97929) LP ( 1) O  5           s( 45.12%)p 1.22( 54.85%)d 0.00(  0.03%)
                                       0.0000  0.6716 -0.0095  0.0027 -0.0001
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                                     0.2378  0.0073 -0.0013  0.0015 -0.4549
                                    -0.0021 -0.0038  0.0007  0.5338  0.0041
                                     0.0007  0.0000  0.0081 -0.0063  0.0126
                                     0.0053 -0.0052
30. (1.95309) LP ( 2) O  5           s(  0.12%)p99.99( 99.83%)d 0.35(  0.04%)
                                     0.0000  0.0350  0.0017  0.0037  0.0004
                                     0.3976  0.0044 -0.0060 -0.0004 -0.5764
                                    -0.0125 -0.0003 -0.0013 -0.7124 -0.0140
                                    -0.0032  0.0026  0.0098 -0.0004 -0.0023
                                     0.0053  0.0174
31. (1.97940) LP ( 1) O  6           s( 47.64%)p 1.10( 52.33%)d 0.00(  0.04%)
                                     0.0000  0.6901  0.0114  0.0006  0.0000
                                     0.0579 -0.0003  0.0012  0.0000  0.6080
                                     0.0053 -0.0018  0.0019  0.3876  0.0022
                                    -0.0013  0.0001 -0.0037  0.0010 -0.0136
                                     0.0126  0.0014
32. (1.95740) LP ( 2) O  6           s(  0.05%)p99.99( 99.90%)d 1.06(  0.05%)
                                     0.0000  0.0218 -0.0013  0.0046  0.0002
                                     0.5246  0.0126  0.0028 -0.0002  0.4027
                                     0.0085  0.0031 -0.0009 -0.7490 -0.0169
                                     0.0037  0.0022 -0.0117 -0.0043  0.0108
                                     0.0074  0.0142
33. (1.97531) LP ( 1) O  7           s( 44.64%)p 1.24( 55.33%)d 0.00(  0.03%)
                                     0.0000  0.6681  0.0076  0.0006  0.0001
                                     0.3080 -0.0001 -0.0065  0.0015 -0.6754
                                    -0.0089  0.0057  0.0006  0.0463  0.0029
                                     0.0003  0.0003  0.0125  0.0013  0.0022
                                     0.0075  0.0099
34. (1.95773) LP ( 2) O  7           s(  3.36%)p28.73( 96.60%)d 0.01(  0.04%)
                                     0.0000  0.1832  0.0068 -0.0013 -0.0003
                                     0.7547  0.0201  0.0006 -0.0002  0.4990
                                     0.0063  0.0027 -0.0023 -0.3834 -0.0023
                                     0.0035 -0.0003  0.0039  0.0050 -0.0062
                                    -0.0177  0.0021
82. (0.00718) BD*( 1) O  3- H 28
              ( 25.35%)   0.5035* O  3 s( 21.00%)p 3.76( 78.87%)d 0.01(  0.13%)
                                     0.0000 -0.4582  0.0085 -0.0007  0.0001
                                     0.4043  0.0071 -0.0026  0.0001  0.7790
                                    -0.0312  0.0053  0.0024 -0.1311 -0.0037
                                     0.0000  0.0002 -0.0290  0.0104  0.0104
                                     0.0030  0.0163
              ( 74.65%)  -0.8640* H 28 s( 99.88%)p 0.00(  0.12%)
                                    -0.9994  0.0034 -0.0006  0.0000 -0.0124
                                    -0.0330  0.0016
83. (0.01943) BD*( 1) O  4- C  9
              ( 33.27%)   0.5768* O  4 s( 31.41%)p 2.18( 68.51%)d 0.00(  0.08%)
                                     0.0000 -0.5604  0.0080  0.0056  0.0001
                                     0.7095 -0.0095 -0.0054  0.0021  0.0815
                                     0.0014 -0.0069 -0.0005  0.4181 -0.0065
                                    -0.0044 -0.0006 -0.0098 -0.0212 -0.0095
                                    -0.0109  0.0037
              ( 66.73%)  -0.8169* C  9 s( 20.96%)p 3.76( 78.82%)d 0.01(  0.22%)
                                     0.0000 -0.4556  0.0451  0.0010  0.0004
                                    -0.7778  0.0422  0.0020 -0.0049 -0.0652
                                     0.0156 -0.0003 -0.0020 -0.4204  0.0079
                                    -0.0089  0.0073 -0.0031 -0.0361 -0.0011
                                    -0.0283  0.0073
84. (0.00867) BD*( 1) O  4- H 29
              ( 25.07%)   0.5007* O  4 s( 21.28%)p 3.69( 78.59%)d 0.01(  0.13%)
                                     0.0000 -0.4612  0.0078 -0.0015 -0.0001
                                    -0.4807  0.0286 -0.0076 -0.0008  0.7422
                                    -0.0059  0.0019  0.0012  0.0543  0.0111
                                    -0.0019  0.0001  0.0194  0.0031 -0.0126
                                     0.0223  0.0165
              ( 74.93%)  -0.8656* H 29 s( 99.88%)p 0.00(  0.12%)
                                    -0.9994  0.0038  0.0009 -0.0001  0.0214
                                    -0.0277  0.0021
85. (0.01895) BD*( 1) O  5- C 10
              ( 34.07%)   0.5837* O  5 s( 31.03%)p 2.22( 68.89%)d 0.00(  0.08%)
                                     0.0000 -0.5569 -0.0088  0.0049 -0.0005
                                    -0.3855  0.0117  0.0005 -0.0020 -0.6708
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                                     0.0085  0.0043  0.0005  0.3002 -0.0033
                                    -0.0023 -0.0005 -0.0115  0.0044  0.0198
                                     0.0142  0.0059
              ( 65.93%)  -0.8120* C 10 s( 21.77%)p 3.58( 78.02%)d 0.01(  0.21%)
                                     0.0000 -0.4647  0.0422 -0.0018 -0.0004
                                     0.4424  0.0081  0.0022  0.0023  0.7122
                                     0.0402  0.0005 -0.0061 -0.2746  0.0029
                                     0.0068 -0.0061 -0.0307  0.0145  0.0225
                                     0.0136  0.0163
  86. (0.02025) BD*( 1) O  5- H 30
              ( 23.51%)   0.4849* O  5 s( 23.71%)p 3.21( 76.16%)d 0.01(  0.12%)
                                     0.0000 -0.4869 -0.0086  0.0000  0.0004
                                     0.7965 -0.0237  0.0010  0.0027  0.0981
                                    -0.0229  0.0054  0.0002  0.3413  0.0028
                                    -0.0014 -0.0008  0.0054 -0.0269  0.0048
                                    -0.0213  0.0040
              ( 76.49%)  -0.8746* H 30 s( 99.83%)p 0.00(  0.17%)
                                    -0.9991  0.0056  0.0002  0.0002 -0.0385
                                    -0.0095 -0.0099
  87. (0.00600) BD*( 1) O  6- C 13
              ( 34.06%)   0.5836* O  6 s( 29.99%)p 2.33( 69.92%)d 0.00(  0.09%)
                                     0.0000 -0.5474  0.0148  0.0038 -0.0002
                                     0.6061 -0.0121 -0.0026  0.0019  0.2252
                                     0.0086  0.0095  0.0002  0.5298 -0.0080
                                     0.0049 -0.0005 -0.0132 -0.0217 -0.0170
                                    -0.0030 -0.0014
              ( 65.94%)  -0.8121* C 13 s( 22.28%)p 3.48( 77.49%)d 0.01(  0.23%)
                                     0.0000 -0.4694  0.0496 -0.0007  0.0002
                                    -0.6639 -0.0373  0.0013  0.0048 -0.2221
                                    -0.0461  0.0011  0.0009 -0.5296 -0.0280
                                    -0.0037  0.0079 -0.0113 -0.0409 -0.0066
                                    -0.0209 -0.0039
  88. (0.01209) BD*( 1) O  6- H 31
              ( 25.09%)   0.5009* O  6 s( 22.32%)p 3.47( 77.53%)d 0.01(  0.14%)
                                     0.0000 -0.4724  0.0071 -0.0026  0.0002
                                    -0.5929  0.0303 -0.0025 -0.0011  0.6448
                                    -0.0108  0.0033 -0.0003 -0.0823  0.0166
                                     0.0023  0.0001  0.0284  0.0007 -0.0050
                                     0.0157  0.0189
              ( 74.91%)  -0.8655* H 31 s( 99.85%)p 0.00(  0.15%)
                                    -0.9992  0.0032  0.0004  0.0005  0.0273
                                    -0.0260  0.0095
 107. (0.35937) BD*( 2) C 15- C 17
              ( 48.31%)   0.6950* C 15 s(  0.01%)p 1.00( 99.96%)d 0.00(  0.04%)
                                     0.0000  0.0047  0.0076 -0.0023 -0.0005
                                    -0.4940  0.0066 -0.0085  0.0025 -0.3007
                                    -0.0056 -0.0120 -0.0020 -0.8152 -0.0123
                                    -0.0072 -0.0093 -0.0071  0.0093 -0.0118
                                     0.0089 -0.0019
              ( 51.69%)  -0.7190* C 17 s(  0.00%)p 1.00( 99.95%)d 0.00(  0.05%)
                                     0.0000  0.0011 -0.0004  0.0002 -0.4977
                                    -0.0033 -0.0048  0.0017 -0.2870 -0.0021
                                    -0.0052  0.0010 -0.8181 -0.0096 -0.0092
                                     0.0057 -0.0042 -0.0097  0.0037 -0.0086
                                     0.0166

SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

     Threshold for printing:   0.10 kcal/mol
                                                                 E(2) E(NL)-E(L) F(L,NL)
      Donor (L) NBO              Acceptor (NL) NBO            kcal/mol   a.u.    a.u.
 ===========================================================================================

 within unit  1
   21. LP ( 1) O  1           79. BD*( 1) O  2- C 12      5.38    0.97   0.064
   21. LP ( 1) O  1           85. BD*( 1) O  5- C 10      0.11    0.97   0.009
   21. LP ( 1) O  1           87. BD*( 1) O  6- C 13      0.50    0.99   0.020
   21. LP ( 1) O  1           94. BD*( 1) C  9- C 11      0.63    1.02   0.023
   21. LP ( 1) O  1           95. BD*( 1) C  9- H 22      0.16    1.04   0.011
   21. LP ( 1) O  1           96. BD*( 1) C 10- C 12      0.74    1.02   0.025
   21. LP ( 1) O  1           97. BD*( 1) C 10- H 23      0.13    1.04   0.011
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21. LP (1) O 1	98. BD*(1) C 11- C 13	1.90	1.03	0.040
21. LP (1) O 1	99. BD*(1) C 11- H 24	1.45	1.04	0.035
21. LP (1) O 1	100. BD*(1) C 12- H 25	1.19	1.02	0.031
21. LP (1) O 1	124. RY (6) O 1	0.16	2.11	0.016
21. LP (1) O 1	289. RY (1) C 11	0.93	1.60	0.034
21. LP (1) O 1	290. RY (2) C 11	1.35	2.23	0.049
21. LP (1) O 1	291. RY (3) C 11	0.10	2.24	0.014
21. LP (1) O 1	306. RY (1) C 12	2.28	1.75	0.056
21. LP (1) O 1	307. RY (2) C 12	0.26	2.75	0.024
21. LP (1) O 1	308. RY (3) C 12	0.18	2.47	0.019
21. LP (1) O 1	310. RY (5) C 12	0.26	2.54	0.023
21. LP (1) O 1	312. RY (7) C 12	0.10	2.36	0.014
21. LP (1) O 1	315. RY (10) C 12	0.32	2.93	0.027
21. LP (1) O 1	322. RY (17) C 12	0.12	3.16	0.017
21. LP (1) O 1	323. RY (1) C 13	0.25	1.54	0.018
22. LP (2) O 1	83. BD*(1) O 4- C 9	1.33	0.75	0.028
22. LP (2) O 1	85. BD*(1) O 5- C 10	1.05	0.77	0.025
22. LP (2) O 1	94. BD*(1) C 9- C 11	6.53	0.82	0.065
22. LP (2) O 1	96. BD*(1) C 10- C 12	6.98	0.82	0.067
22. LP (2) O 1	99. BD*(1) C 11- H 24	6.65	0.84	0.067
22. LP (2) O 1	100. BD*(1) C 12- H 25	7.49	0.81	0.070
22. LP (2) O 1	101. BD*(1) C 13- H 26	0.12	0.86	0.009
22. LP (2) O 1	122. RY (4) O 1	0.12	1.93	0.013
22. LP (2) O 1	272. RY (1) C 10	0.16	1.46	0.014
22. LP (2) O 1	289. RY (1) C 11	0.21	1.40	0.015
22. LP (2) O 1	292. RY (4) C 11	0.95	2.10	0.040
22. LP (2) O 1	294. RY (6) C 11	0.11	2.30	0.014
22. LP (2) O 1	296. RY (8) C 11	0.10	2.41	0.014
22. LP (2) O 1	299. RY (11) C 11	0.10	1.48	0.011
22. LP (2) O 1	306. RY (1) C 12	0.19	1.55	0.015
22. LP (2) O 1	308. RY (3) C 12	0.21	2.27	0.020
22. LP (2) O 1	309. RY (4) C 12	0.99	1.87	0.038
22. LP (2) O 1	311. RY (6) C 12	0.41	1.97	0.025
22. LP (2) O 1	313. RY (8) C 12	0.11	2.17	0.014
22. LP (2) O 1	475. RY (1) H 24	0.21	1.16	0.014
22. LP (2) O 1	481. RY (1) H 25	0.17	1.31	0.013
23. LP (1) O 2	79. BD*(1) O 2- C 12	0.17	0.96	0.011
23. LP (1) O 2	92. BD*(1) C 8- C 10	0.44	1.02	0.019
23. LP (1) O 2	96. BD*(1) C 10- C 12	1.69	1.01	0.037
23. LP (1) O 2	100. BD*(1) C 12- H 25	3.45	1.00	0.053
23. LP (1) O 2	103. BD*(1) C 14- C 15	0.30	1.20	0.017
23. LP (1) O 2	104. BD*(1) C 14- C 16	0.75	1.20	0.027
23. LP (1) O 2	105. BD*(2) C 14- C 16	9.60	0.64	0.070
23. LP (1) O 2	108. BD*(1) C 15- C 18	0.10	1.04	0.009
23. LP (1) O 2	110. BD*(1) C 16- H 32	0.13	1.09	0.011
23. LP (1) O 2	273. RY (2) C 10	0.15	1.77	0.015
23. LP (1) O 2	307. RY (2) C 12	1.94	2.74	0.065
23. LP (1) O 2	308. RY (3) C 12	0.10	2.46	0.014
23. LP (1) O 2	309. RY (4) C 12	0.14	2.06	0.015
23. LP (1) O 2	311. RY (6) C 12	0.17	2.16	0.017
23. LP (1) O 2	312. RY (7) C 12	0.30	2.35	0.023
23. LP (1) O 2	320. RY (15) C 12	0.14	2.93	0.018
23. LP (1) O 2	340. RY (1) C 14	1.82	2.11	0.055
23. LP (1) O 2	341. RY (2) C 14	0.14	1.68	0.014
23. LP (1) O 2	344. RY (5) C 14	0.53	2.22	0.031
23. LP (1) O 2	348. RY (9) C 14	0.17	1.87	0.016
24. LP (2) O 2	77. BD*(1) O 1- C 11	0.62	0.77	0.020
24. LP (2) O 2	78. BD*(1) O 1- C 12	16.45	0.77	0.100
24. LP (2) O 2	86. BD*(1) O 5- H 30	0.22	0.92	0.013
24. LP (2) O 2	89. BD*(1) O 7- C 18	0.13	0.75	0.009
24. LP (2) O 2	92. BD*(1) C 8- C 10	0.26	0.84	0.013
24. LP (2) O 2	96. BD*(1) C 10- C 12	1.01	0.83	0.026
24. LP (2) O 2	97. BD*(1) C 10- H 23	0.18	0.85	0.011
24. LP (2) O 2	100. BD*(1) C 12- H 25	3.25	0.82	0.046
24. LP (2) O 2	103. BD*(1) C 14- C 15	7.73	1.02	0.079
24. LP (2) O 2	104. BD*(1) C 14- C 16	7.44	1.02	0.078
24. LP (2) O 2	106. BD*(1) C 15- C 17	0.47	1.02	0.019
24. LP (2) O 2	109. BD*(1) C 16- C 19	0.40	1.03	0.018
24. LP (2) O 2	114. BD*(1) C 18- H 35	0.27	0.85	0.014
24. LP (2) O 2	306. RY (1) C 12	0.80	1.56	0.032
24. LP (2) O 2	308. RY (3) C 12	0.28	2.28	0.022

24. LP (2) O 2	310. RY (5) C 12	0.49	2.35	0.030
24. LP (2) O 2	311. RY (6) C 12	0.21	1.98	0.018
24. LP (2) O 2	315. RY (10) C 12	0.20	2.74	0.021
24. LP (2) O 2	342. RY (3) C 14	1.30	2.50	0.051
24. LP (2) O 2	343. RY (4) C 14	0.10	1.48	0.011
24. LP (2) O 2	374. RY (2) C 16	0.17	1.49	0.014
24. LP (2) O 2	481. RY (1) H 25	0.11	1.32	0.011
25. LP (1) O 3	84. BD*(1) O 4- H 29	0.24	1.13	0.015
25. LP (1) O 3	91. BD*(1) C 8- C 9	1.76	1.07	0.039
25. LP (1) O 3	92. BD*(1) C 8- C 10	1.25	1.07	0.033
25. LP (1) O 3	93. BD*(1) C 8- H 21	0.95	1.07	0.028
25. LP (1) O 3	94. BD*(1) C 9- C 11	0.37	1.06	0.018
25. LP (1) O 3	96. BD*(1) C 10- C 12	0.14	1.05	0.011
25. LP (1) O 3	97. BD*(1) C 10- H 23	0.20	1.07	0.013
25. LP (1) O 3	238. RY (1) C 8	1.77	1.61	0.048
25. LP (1) O 3	240. RY (3) C 8	0.85	1.57	0.033
25. LP (1) O 3	241. RY (4) C 8	0.15	2.20	0.016
25. LP (1) O 3	242. RY (5) C 8	0.35	2.26	0.025
25. LP (1) O 3	245. RY (8) C 8	0.12	3.28	0.018
25. LP (1) O 3	257. RY (3) C 9	0.19	1.42	0.015
25. LP (1) O 3	499. RY (1) H 28	0.11	2.28	0.014
25. LP (1) O 3	500. RY (2) H 28	1.05	2.57	0.046
26. LP (2) O 3	84. BD*(1) O 4- H 29	0.20	0.90	0.012
26. LP (2) O 3	85. BD*(1) O 5- C 10	0.17	0.77	0.010
26. LP (2) O 3	92. BD*(1) C 8- C 10	6.07	0.83	0.064
26. LP (2) O 3	93. BD*(1) C 8- H 21	8.69	0.83	0.076
26. LP (2) O 3	96. BD*(1) C 10- C 12	0.71	0.82	0.022
26. LP (2) O 3	238. RY (1) C 8	0.16	1.37	0.013
26. LP (2) O 3	239. RY (2) C 8	0.40	1.53	0.022
26. LP (2) O 3	241. RY (4) C 8	1.07	1.97	0.041
26. LP (2) O 3	242. RY (5) C 8	0.12	2.03	0.014
26. LP (2) O 3	248. RY (11) C 8	0.17	1.44	0.014
26. LP (2) O 3	272. RY (1) C 10	0.14	1.47	0.013
26. LP (2) O 3	457. RY (1) H 21	0.18	1.18	0.013
26. LP (2) O 3	499. RY (1) H 28	1.65	2.05	0.052
27. LP (1) O 4	77. BD*(1) O 1- C 11	0.47	0.99	0.019
27. LP (1) O 4	88. BD*(1) O 6- H 31	2.58	1.17	0.049
27. LP (1) O 4	91. BD*(1) C 8- C 9	1.09	1.07	0.031
27. LP (1) O 4	92. BD*(1) C 8- C 10	0.12	1.07	0.010
27. LP (1) O 4	93. BD*(1) C 8- H 21	0.18	1.07	0.012
27. LP (1) O 4	94. BD*(1) C 9- C 11	1.76	1.06	0.039
27. LP (1) O 4	95. BD*(1) C 9- H 22	1.05	1.07	0.030
27. LP (1) O 4	255. RY (1) C 9	1.84	1.60	0.048
27. LP (1) O 4	257. RY (3) C 9	0.47	1.42	0.023
27. LP (1) O 4	258. RY (4) C 9	0.22	2.26	0.020
27. LP (1) O 4	259. RY (5) C 9	0.41	2.33	0.028
27. LP (1) O 4	269. RY (15) C 9	0.12	3.67	0.019
27. LP (1) O 4	289. RY (1) C 11	0.14	1.64	0.014
27. LP (1) O 4	505. RY (1) H 29	0.32	2.31	0.024
27. LP (1) O 4	506. RY (2) H 29	0.89	2.57	0.043
28. LP (2) O 4	81. BD*(1) O 3- C 8	0.21	0.77	0.011
28. LP (2) O 4	88. BD*(1) O 6- H 31	0.75	0.94	0.024
28. LP (2) O 4	91. BD*(1) C 8- C 9	5.51	0.84	0.061
28. LP (2) O 4	92. BD*(1) C 8- C 10	0.72	0.84	0.022
28. LP (2) O 4	94. BD*(1) C 9- C 11	0.12	0.83	0.009
28. LP (2) O 4	95. BD*(1) C 9- H 22	8.66	0.85	0.076
28. LP (2) O 4	238. RY (1) C 8	0.17	1.38	0.013
28. LP (2) O 4	255. RY (1) C 9	0.17	1.37	0.014
28. LP (2) O 4	256. RY (2) C 9	0.46	1.57	0.024
28. LP (2) O 4	258. RY (4) C 9	0.90	2.03	0.038
28. LP (2) O 4	259. RY (5) C 9	0.16	2.10	0.016
28. LP (2) O 4	463. RY (1) H 22	0.23	1.27	0.015
28. LP (2) O 4	505. RY (1) H 29	1.35	2.08	0.047
28. LP (2) O 4	506. RY (2) H 29	0.25	2.35	0.022
29. LP (1) O 5	78. BD*(1) O 1- C 12	0.13	0.97	0.010
29. LP (1) O 5	82. BD*(1) O 3- H 28	0.13	1.11	0.011
29. LP (1) O 5	91. BD*(1) C 8- C 9	0.42	1.04	0.019
29. LP (1) O 5	92. BD*(1) C 8- C 10	2.01	1.05	0.041
29. LP (1) O 5	96. BD*(1) C 10- C 12	1.05	1.03	0.029
29. LP (1) O 5	97. BD*(1) C 10- H 23	1.58	1.05	0.036
29. LP (1) O 5	100. BD*(1) C 12- H 25	0.25	1.03	0.014

29. LP (1) O 5	272. RY (1) C 10	1.89	1.68	0.050
29. LP (1) O 5	274. RY (3) C 10	0.85	1.89	0.036
29. LP (1) O 5	276. RY (5) C 10	0.35	2.35	0.026
29. LP (1) O 5	285. RY (14) C 10	0.23	3.34	0.025
29. LP (1) O 5	511. RY (1) H 30	1.03	2.65	0.047
29. LP (1) O 5	513. RY (3) H 30	0.13	2.23	0.015
30. LP (2) O 5	78. BD*(1) O 1- C 12	1.26	0.75	0.028
30. LP (2) O 5	79. BD*(1) O 2- C 12	0.18	0.76	0.010
30. LP (2) O 5	82. BD*(1) O 3- H 28	0.17	0.89	0.011
30. LP (2) O 5	93. BD*(1) C 8- H 21	0.13	0.83	0.009
30. LP (2) O 5	96. BD*(1) C 10- C 12	7.74	0.81	0.071
30. LP (2) O 5	97. BD*(1) C 10- H 23	8.05	0.83	0.073
30. LP (2) O 5	113. BD*(1) C 18- H 34	0.24	0.84	0.013
30. LP (2) O 5	272. RY (1) C 10	0.25	1.46	0.017
30. LP (2) O 5	274. RY (3) C 10	0.45	1.67	0.025
30. LP (2) O 5	275. RY (4) C 10	0.97	1.74	0.037
30. LP (2) O 5	276. RY (5) C 10	0.14	2.13	0.016
30. LP (2) O 5	277. RY (6) C 10	0.16	2.23	0.017
30. LP (2) O 5	306. RY (1) C 12	0.23	1.54	0.017
30. LP (2) O 5	406. RY (1) C 18	0.11	1.30	0.011
30. LP (2) O 5	469. RY (1) H 23	0.16	1.24	0.013
30. LP (2) O 5	512. RY (2) H 30	1.37	2.10	0.048
31. LP (1) O 6	77. BD*(1) O 1- C 11	0.14	0.96	0.010
31. LP (1) O 6	98. BD*(1) C 11- C 13	1.27	1.03	0.032
31. LP (1) O 6	99. BD*(1) C 11- H 24	0.25	1.04	0.014
31. LP (1) O 6	101. BD*(1) C 13- H 26	3.32	1.06	0.053
31. LP (1) O 6	102. BD*(1) C 13- H 27	0.83	1.05	0.026
31. LP (1) O 6	323. RY (1) C 13	1.95	1.54	0.049
31. LP (1) O 6	325. RY (3) C 13	0.47	2.15	0.028
31. LP (1) O 6	326. RY (4) C 13	0.38	2.40	0.027
31. LP (1) O 6	335. RY (13) C 13	0.17	1.73	0.015
31. LP (1) O 6	518. RY (2) H 31	1.15	2.50	0.048
31. LP (1) O 6	520. RY (4) H 31	0.10	1.66	0.012
32. LP (2) O 6	77. BD*(1) O 1- C 11	1.18	0.73	0.026
32. LP (2) O 6	98. BD*(1) C 11- C 13	6.03	0.81	0.062
32. LP (2) O 6	101. BD*(1) C 13- H 26	0.15	0.84	0.010
32. LP (2) O 6	102. BD*(1) C 13- H 27	8.96	0.82	0.076
32. LP (2) O 6	323. RY (1) C 13	0.35	1.31	0.019
32. LP (2) O 6	324. RY (2) C 13	0.76	1.37	0.029
32. LP (2) O 6	325. RY (3) C 13	0.92	1.92	0.037
32. LP (2) O 6	493. RY (1) H 27	0.15	1.01	0.011
32. LP (2) O 6	517. RY (1) H 31	1.84	1.98	0.054
33. LP (1) O 7	86. BD*(1) O 5- H 30	2.97	1.14	0.052
33. LP (1) O 7	107. BD*(2) C 15- C 17	0.36	0.67	0.014
33. LP (1) O 7	108. BD*(1) C 15- C 18	3.50	1.08	0.055
33. LP (1) O 7	113. BD*(1) C 18- H 34	2.04	1.07	0.042
33. LP (1) O 7	114. BD*(1) C 18- H 35	0.12	1.07	0.010
33. LP (1) O 7	406. RY (1) C 18	1.31	1.53	0.040
33. LP (1) O 7	408. RY (3) C 18	0.65	1.89	0.031
33. LP (1) O 7	409. RY (4) C 18	0.29	2.74	0.025
33. LP (1) O 7	413. RY (8) C 18	0.10	3.94	0.018
33. LP (1) O 7	559. RY (1) H 38	0.29	2.34	0.023
33. LP (1) O 7	560. RY (2) H 38	1.07	2.53	0.046
34. LP (2) O 7	86. BD*(1) O 5- H 30	4.75	0.94	0.060
34. LP (2) O 7	107. BD*(2) C 15- C 17	0.37	0.47	0.012
34. LP (2) O 7	108. BD*(1) C 15- C 18	2.16	0.88	0.039
34. LP (2) O 7	113. BD*(1) C 18- H 34	1.77	0.87	0.035
34. LP (2) O 7	114. BD*(1) C 18- H 35	8.52	0.87	0.077
34. LP (2) O 7	407. RY (2) C 18	1.53	1.52	0.043
34. LP (2) O 7	408. RY (3) C 18	0.29	1.69	0.020
34. LP (2) O 7	409. RY (4) C 18	0.31	2.54	0.025
34. LP (2) O 7	511. RY (1) H 30	0.11	2.46	0.014
34. LP (2) O 7	541. RY (1) H 35	0.11	0.99	0.009
34. LP (2) O 7	559. RY (1) H 38	1.51	2.14	0.051
34. LP (2) O 7	560. RY (2) H 38	0.22	2.33	0.020

Salicin (Conformer XI)

Summary of Natural Population Analysis:

Atom No	Natural Charge	Natural Population			
		Core	Valence	Rydberg	Total
O 1	-0.65171	2.00000	6.62705	0.02467	8.65171
O 2	-0.58745	2.00000	6.56488	0.02257	8.58745
O 3	-0.76253	2.00000	6.74885	0.01367	8.76253
O 4	-0.74843	2.00000	6.73504	0.01340	8.74843
O 5	-0.79052	2.00000	6.77492	0.01561	8.79052
O 6	-0.73699	2.00000	6.72351	0.01348	8.73699
O 7	-0.76701	2.00000	6.75332	0.01369	8.76701
C 8	0.09856	1.99999	3.87518	0.02627	5.90144
C 9	0.09483	1.99999	3.87931	0.02586	5.90517
C 10	0.05583	1.99999	3.91893	0.02524	5.94417
C 11	0.09589	1.99999	3.88002	0.02409	5.90411
C 12	0.45694	1.99999	3.51014	0.03292	5.54306
C 13	-0.03204	1.99999	4.00854	0.02351	6.03204
C 14	0.32802	1.99999	3.64751	0.02448	5.67198
C 15	-0.11942	1.99999	4.10118	0.01824	6.11942
C 16	-0.26848	1.99999	4.25130	0.01718	6.26848
C 17	-0.16624	1.99999	4.14989	0.01636	6.16624
C 18	-0.03073	1.99999	4.01043	0.02031	6.03073
C 19	-0.18619	1.99999	4.16975	0.01645	6.18619
C 20	-0.22763	1.99999	4.21011	0.01752	6.22763
H 21	0.17660	0.00000	0.82045	0.00295	0.82340

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   H 22    0.17464      0.00000     0.82225    0.00311     0.82536
   H 23    0.19063      0.00000     0.80655    0.00282     0.80937
   H 24    0.18616      0.00000     0.81122    0.00263     0.81384
   H 25    0.17442      0.00000     0.82313    0.00245     0.82558
   H 26    0.15974      0.00000     0.83785    0.00241     0.84026
   H 27    0.20426      0.00000     0.79392    0.00181     0.79574
   H 28    0.48663      0.00000     0.50931    0.00406     0.51337
   H 29    0.48275      0.00000     0.51315    0.00410     0.51725
   H 30    0.51521      0.00000     0.48052    0.00427     0.48479
   H 31    0.46815      0.00000     0.52725    0.00460     0.53185
   H 32    0.24468      0.00000     0.75307    0.00225     0.75532
   H 33    0.21297      0.00000     0.78503    0.00200     0.78703
   H 34    0.18898      0.00000     0.80896    0.00206     0.81102
   H 35    0.17194      0.00000     0.82583    0.00223     0.82806
   H 36    0.21489      0.00000     0.78353    0.00158     0.78511
   H 37    0.21624      0.00000     0.78205    0.00171     0.78376
   H 38    0.47641      0.00000     0.51988    0.00372     0.52359
 ===============================================================
 * Total *  0.00000     39.99990   111.54382    0.45628   152.00000

    (Occupancy)   Bond orbital / Coefficients / Hybrids
 ------------------ Lewis ---------------------------------------------------------


21. (1.95891) LP ( 1) O  1           s( 42.08%)p 1.38( 57.89%)d 0.00(  0.03%)
                                      0.0000  0.6484  0.0167  0.0020  0.0000
                                     -0.2631  0.0041  0.0016 -0.0017 -0.7086
                                     -0.0065  0.0004 -0.0004  0.0867 -0.0042
                                      0.0021 -0.0005 -0.0101  0.0016  0.0020
                                      0.0123  0.0061
  22. (1.92944) LP ( 2) O  1           s(  0.00%)p 1.00( 99.96%)d 0.00(  0.03%)
                                      0.0000 -0.0031  0.0044 -0.0041 -0.0001
                                     -0.1573  0.0021  0.0035 -0.0002  0.1745
                                      0.0065 -0.0022 -0.0011  0.9717  0.0133
                                     -0.0046 -0.0048 -0.0017  0.0058  0.0170
                                     -0.0040 -0.0026
  23. (1.95044) LP ( 1) O  2           s( 34.01%)p 1.94( 65.96%)d 0.00(  0.04%)
                                      0.0000  0.5830  0.0126  0.0031  0.0001
                                     -0.3351 -0.0031  0.0017 -0.0010  0.2289
                                     -0.0003  0.0013 -0.0007 -0.7034 -0.0106
                                      0.0051 -0.0003  0.0028 -0.0109  0.0040
                                     -0.0011 -0.0148
  24. (1.88251) LP ( 2) O  2           s(  2.43%)p40.20( 97.53%)d 0.02(  0.04%)
                                      0.0000  0.1557  0.0009 -0.0022  0.0003
                                      0.3009 -0.0023 -0.0041  0.0014 -0.8901
                                     -0.0094  0.0011  0.0041 -0.3038 -0.0040
                                      0.0038  0.0010 -0.0044  0.0044 -0.0178
                                      0.0037 -0.0082
  25. (1.98003) LP ( 1) O  3           s( 47.74%)p 1.09( 52.22%)d 0.00(  0.03%)
                                      0.0000  0.6909  0.0084  0.0022  0.0001
                                      0.3931  0.0055  0.0002  0.0011 -0.0764
                                     -0.0059  0.0010 -0.0012  0.6015  0.0009
                                      0.0015  0.0006 -0.0006 -0.0135  0.0044
                                     -0.0056 -0.0095
  26. (1.95992) LP ( 2) O  3           s(  0.05%)p99.99( 99.90%)d 0.91(  0.05%)
                                      0.0000  0.0223 -0.0018  0.0032  0.0001
                                      0.7317  0.0141 -0.0008 -0.0020  0.5213
                                      0.0103  0.0021 -0.0002 -0.4375 -0.0072
                                     -0.0031  0.0018 -0.0052 -0.0067 -0.0103
                                     -0.0109  0.0129
  27. (1.98043) LP ( 1) O  4           s( 47.96%)p 1.08( 52.01%)d 0.00(  0.04%)
                                      0.0000  0.6925  0.0077  0.0027  0.0001
                                      0.5863  0.0000  0.0012  0.0013 -0.3146
                                     -0.0044  0.0011 -0.0013 -0.2780 -0.0027
                                      0.0005 -0.0010  0.0124  0.0114 -0.0029
                                     -0.0070  0.0035
  28. (1.95839) LP ( 2) O  4           s(  0.12%)p99.99( 99.83%)d 0.40(  0.05%)
                                      0.0000  0.0349  0.0038 -0.0021  0.0000
                                     -0.0801 -0.0030  0.0019  0.0001  0.6176
                                      0.0108  0.0001 -0.0019 -0.7811 -0.0158
                                     -0.0027  0.0019 -0.0114  0.0127 -0.0017
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                                    -0.0047 -0.0134
29. (1.97774) LP ( 1) O  5          s( 44.29%)p 1.26( 55.68%)d 0.00(  0.03%)
                                     0.0000  0.6654  0.0103  0.0023  0.0002
                                     0.3164  0.0057 -0.0034  0.0013  0.6581
                                     0.0051  0.0033  0.0013 -0.1532 -0.0005
                                    -0.0024  0.0004 -0.0120  0.0030  0.0038
                                     0.0104  0.0064
30. (1.95384) LP ( 2) O  5          s(  0.27%)p99.99( 99.69%)d 0.16(  0.04%)
                                     0.0000  0.0517 -0.0007  0.0034  0.0002
                                    -0.1549 -0.0045 -0.0056 -0.0007  0.2446
                                     0.0057 -0.0018 -0.0003  0.9553  0.0187
                                     0.0023 -0.0039  0.0011 -0.0075 -0.0177
                                     0.0063  0.0042
31. (1.98123) LP ( 1) O  6          s( 48.85%)p 1.05( 51.11%)d 0.00(  0.04%)
                                     0.0000  0.6989  0.0114  0.0004  0.0000
                                     0.4971  0.0045  0.0021  0.0022 -0.3155
                                    -0.0022  0.0018 -0.0004 -0.4055 -0.0017
                                     0.0013 -0.0005  0.0110  0.0138 -0.0054
                                    -0.0035  0.0013
32. (1.95752) LP ( 2) O  6          s(  0.02%)p99.99( 99.93%)d 3.04(  0.05%)
                                     0.0000  0.0120 -0.0002  0.0055  0.0001
                                    -0.0341 -0.0023 -0.0030 -0.0001 -0.7983
                                    -0.0182  0.0008  0.0021  0.6002  0.0136
                                    -0.0034 -0.0015  0.0138 -0.0106 -0.0029
                                     0.0093  0.0117
33. (1.97988) LP ( 1) O  7          s( 37.48%)p 1.67( 62.49%)d 0.00(  0.03%)
                                     0.0000  0.6122  0.0054 -0.0023  0.0000
                                    -0.1390 -0.0077 -0.0079  0.0012  0.2845
                                    -0.0013  0.0021  0.0000  0.7242  0.0054
                                     0.0018 -0.0002 -0.0013 -0.0009 -0.0092
                                     0.0002 -0.0156
34. (1.95526) LP ( 2) O  7          s( 11.85%)p 7.43( 88.11%)d 0.00(  0.03%)
                                     0.0000  0.3441  0.0115  0.0025  0.0000
                                     0.9282  0.0212 -0.0046 -0.0010 -0.1215
                                    -0.0048 -0.0047  0.0006 -0.0648  0.0020
                                    -0.0012  0.0022 -0.0011 -0.0154  0.0011
                                    -0.0075  0.0052
82. (0.00777) BD*( 1) O  3- H 28
              ( 25.35%)   0.5035* O  3 s( 21.00%)p 3.76( 78.86%)d 0.01(  0.14%)
                                     0.0000 -0.4582  0.0082 -0.0008  0.0001
                                     0.5523 -0.0073  0.0001 -0.0004 -0.6903
                                     0.0258 -0.0042 -0.0016  0.0777  0.0165
                                    -0.0033  0.0002  0.0289 -0.0148  0.0124
                                    -0.0006  0.0122
              ( 74.65%)  -0.8640* H 28 s( 99.87%)p 0.00(  0.13%)
                                    -0.9994  0.0038 -0.0004  0.0001 -0.0220
                                     0.0282  0.0018
83. (0.01803) BD*( 1) O  4- C  9
              ( 33.90%)   0.5822* O  4 s( 31.11%)p 2.21( 68.81%)d 0.00(  0.08%)
                                     0.0000 -0.5576  0.0085  0.0059  0.0001
                                     0.7998 -0.0077 -0.0081  0.0015  0.2113
                                    -0.0062  0.0032  0.0008  0.0601 -0.0005
                                     0.0017  0.0006 -0.0032  0.0037 -0.0032
                                    -0.0241  0.0144
              ( 66.10%)  -0.8130* C  9 s( 21.45%)p 3.65( 78.33%)d 0.01(  0.21%)
                                     0.0000 -0.4611  0.0443 -0.0008  0.0002
                                    -0.8450 -0.0433  0.0022  0.0065 -0.2347
                                     0.0073 -0.0030 -0.0005 -0.1095 -0.0134
                                     0.0035  0.0011 -0.0222 -0.0073 -0.0039
                                    -0.0308  0.0247
84. (0.00765) BD*( 1) O  4- H 29
              ( 25.56%)   0.5056* O  4 s( 20.79%)p 3.80( 79.07%)d 0.01(  0.14%)
                                     0.0000 -0.4559  0.0074 -0.0014  0.0000
                                    -0.0938  0.0229 -0.0056 -0.0003 -0.6879
                                     0.0183 -0.0014 -0.0007 -0.5547  0.0114
                                    -0.0014  0.0001  0.0078  0.0070 -0.0318
                                     0.0164 -0.0031
              ( 74.44%)  -0.8628* H 29 s( 99.87%)p 0.00(  0.13%)
                                    -0.9993  0.0034 -0.0007 -0.0001  0.0093
                                     0.0285  0.0210
85. (0.01922) BD*( 1) O  5- C 10
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              ( 34.18%)   0.5847* O  5 s( 30.93%)p 2.23( 68.99%)d 0.00(  0.08%)
                                        0.0000 -0.5561  0.0100  0.0046 -0.0002
                                       -0.3918  0.0116  0.0020 -0.0025  0.7006
                                       -0.0086 -0.0043 -0.0002 -0.2128  0.0046
                                        0.0000  0.0005  0.0118 -0.0038  0.0103
                                        0.0185  0.0137
              ( 65.82%)  -0.8113* C 10 s( 21.76%)p 3.59( 78.03%)d 0.01(  0.21%)
                                        0.0000 -0.4646  0.0421 -0.0044  0.0000
                                        0.4667 -0.0204  0.0078  0.0018 -0.7166
                                        0.0393  0.0010  0.0060  0.2166  0.0034
                                       -0.0046 -0.0035  0.0322 -0.0131  0.0170
                                        0.0159  0.0179
 86. (0.02718) BD*( 1) O  5- H 30
              ( 23.15%)   0.4811* O  5 s( 24.50%)p 3.08( 75.38%)d 0.01(  0.12%)
                                        0.0000 -0.4949  0.0085 -0.0004  0.0006
                                        0.8484 -0.0268 -0.0014  0.0032  0.1231
                                        0.0199 -0.0059 -0.0002  0.1328 -0.0084
                                       -0.0009 -0.0005 -0.0215 -0.0054 -0.0017
                                       -0.0200  0.0182
              ( 76.85%)  -0.8767* H 30 s( 99.84%)p 0.00(  0.16%)
                                       -0.9992  0.0067  0.0001  0.0001 -0.0385
                                        0.0015 -0.0093
 87. (0.00792) BD*( 1) O  6- C 13
              ( 33.79%)   0.5813* O  6 s( 30.28%)p 2.30( 69.63%)d 0.00(  0.09%)
                                        0.0000 -0.5501  0.0138  0.0030 -0.0001
                                       -0.0852  0.0120 -0.0063 -0.0005 -0.5016
                                        0.0019 -0.0057 -0.0003 -0.6612  0.0091
                                       -0.0056 -0.0004  0.0045  0.0052 -0.0265
                                        0.0067 -0.0107
              ( 66.21%)  -0.8137* C 13 s( 22.06%)p 3.52( 77.71%)d 0.01(  0.24%)
                                        0.0000 -0.4669  0.0508 -0.0013  0.0008
                                        0.1139 -0.0221  0.0008  0.0004  0.5464
                                        0.0459  0.0014 -0.0016  0.6795  0.0331
                                       -0.0030 -0.0083 -0.0075 -0.0149 -0.0379
                                        0.0138 -0.0215
 88. (0.00966) BD*( 1) O  6- H 31
              ( 26.18%)   0.5117* O  6 s( 20.85%)p 3.79( 79.01%)d 0.01(  0.14%)
                                        0.0000 -0.4565  0.0088 -0.0022  0.0001
                                        0.8614 -0.0255 -0.0024  0.0013  0.1003
                                       -0.0149 -0.0038  0.0000  0.1916 -0.0219
                                       -0.0031  0.0001  0.0036 -0.0006 -0.0019
                                       -0.0329  0.0185
              ( 73.82%)  -0.8592* H 31 s( 99.86%)p 0.00(  0.14%)
                                       -0.9993  0.0045 -0.0002 -0.0002 -0.0337
                                       -0.0065 -0.0138

107. (0.35451) BD*( 2) C 15- C 17
              ( 47.71%)   0.6908* C 15 s(  0.00%)p 1.00( 99.97%)d 0.00(  0.03%)
                                        0.0000  0.0040  0.0016 -0.0022 -0.0002
                                        0.2591 -0.0087  0.0053 -0.0008  0.7563
                                       -0.0092  0.0152 -0.0062  0.6000  0.0073
                                        0.0047  0.0029 -0.0062  0.0020  0.0028
                                        0.0070  0.0144
              ( 52.29%)  -0.7231* C 17 s(  0.00%)p 1.00( 99.95%)d 0.00(  0.05%)
                                        0.0000  0.0013 -0.0022  0.0000  0.2662
                                        0.0027  0.0035 -0.0001  0.7598  0.0088
                                        0.0108 -0.0028  0.5925  0.0048  0.0091
                                       -0.0021  0.0156  0.0094 -0.0075  0.0055
                                       -0.0090



SECOND ORDER PERTURBATION THEORY ANALYSIS OF FOCK MATRIX IN NBO BASIS

     Threshold for printing:   0.10 kcal/mol
                                                          E(2) E(NL)-E(L) F(L,NL)
     Donor (L) NBO              Acceptor (NL) NBO      kcal/mol   a.u.    a.u.
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 within unit  1
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21. LP (1) O 1	79. BD*(1) O 2- C 12	5.13	0.97	0.063
21. LP (1) O 1	85. BD*(1) O 5- C 10	0.11	0.98	0.009
21. LP (1) O 1	88. BD*(1) O 6- H 31	0.36	1.12	0.018
21. LP (1) O 1	94. BD*(1) C 9- C 11	0.67	1.04	0.024
21. LP (1) O 1	95. BD*(1) C 9- H 22	0.13	1.04	0.011
21. LP (1) O 1	96. BD*(1) C 10- C 12	0.69	1.02	0.024
21. LP (1) O 1	97. BD*(1) C 10- H 23	0.13	1.04	0.010
21. LP (1) O 1	98. BD*(1) C 11- C 13	1.72	1.05	0.038
21. LP (1) O 1	99. BD*(1) C 11- H 24	1.27	1.05	0.033
21. LP (1) O 1	100. BD*(1) C 12- H 25	0.95	1.05	0.028
21. LP (1) O 1	102. BD*(1) C 13- H 27	0.48	1.08	0.020
21. LP (1) O 1	109. BD*(1) C 16- C 19	0.21	1.24	0.014
21. LP (1) O 1	110. BD*(1) C 16- H 32	0.72	1.12	0.025
21. LP (1) O 1	120. RY (2) O 1	0.12	1.51	0.012
21. LP (1) O 1	122. RY (4) O 1	0.12	1.68	0.013
21. LP (1) O 1	125. RY (7) O 1	0.10	1.90	0.013
21. LP (1) O 1	289. RY (1) C 11	1.45	1.51	0.042
21. LP (1) O 1	290. RY (2) C 11	0.78	2.16	0.037
21. LP (1) O 1	291. RY (3) C 11	0.12	2.20	0.014
21. LP (1) O 1	292. RY (4) C 11	0.15	2.33	0.017
21. LP (1) O 1	293. RY (5) C 11	0.11	2.12	0.013
21. LP (1) O 1	295. RY (7) C 11	0.12	3.85	0.019
21. LP (1) O 1	299. RY (11) C 11	0.10	3.23	0.016
21. LP (1) O 1	306. RY (1) C 12	2.25	1.74	0.056
21. LP (1) O 1	308. RY (3) C 12	0.52	2.35	0.031
21. LP (1) O 1	309. RY (4) C 12	0.15	2.35	0.017
21. LP (1) O 1	310. RY (5) C 12	0.17	2.57	0.018
21. LP (1) O 1	312. RY (7) C 12	0.13	4.48	0.021
21. LP (1) O 1	316. RY (11) C 12	0.12	4.11	0.020
22. LP (2) O 1	83. BD*(1) O 4- C 9	1.17	0.78	0.027
22. LP (2) O 1	85. BD*(1) O 5- C 10	1.09	0.78	0.026
22. LP (2) O 1	88. BD*(1) O 6- H 31	0.35	0.92	0.016
22. LP (2) O 1	94. BD*(1) C 9- C 11	6.25	0.84	0.065
22. LP (2) O 1	96. BD*(1) C 10- C 12	6.51	0.81	0.065
22. LP (2) O 1	99. BD*(1) C 11- H 24	6.58	0.85	0.067
22. LP (2) O 1	100. BD*(1) C 12- H 25	7.12	0.85	0.069
22. LP (2) O 1	110. BD*(1) C 16- H 32	0.28	0.92	0.014
22. LP (2) O 1	122. RY (4) O 1	0.12	1.48	0.012
22. LP (2) O 1	272. RY (1) C 10	0.15	1.38	0.013
22. LP (2) O 1	292. RY (4) C 11	0.81	2.13	0.037
22. LP (2) O 1	294. RY (6) C 11	0.11	2.20	0.014
22. LP (2) O 1	308. RY (3) C 12	0.17	2.15	0.017
22. LP (2) O 1	309. RY (4) C 12	0.97	2.15	0.041
22. LP (2) O 1	313. RY (8) C 12	0.17	3.06	0.020
22. LP (2) O 1	463. RY (1) H 22	0.11	1.22	0.010
22. LP (2) O 1	475. RY (1) H 24	0.18	1.35	0.014
22. LP (2) O 1	481. RY (1) H 25	0.13	1.35	0.012
23. LP (1) O 2	77. BD*(1) O 1- C 11	0.28	0.92	0.014
23. LP (1) O 2	78. BD*(1) O 1- C 12	2.74	0.92	0.045
23. LP (1) O 2	96. BD*(1) C 10- C 12	0.86	0.98	0.026
23. LP (1) O 2	100. BD*(1) C 12- H 25	3.68	1.01	0.054
23. LP (1) O 2	103. BD*(1) C 14- C 15	1.03	1.18	0.031
23. LP (1) O 2	104. BD*(1) C 14- C 16	5.93	1.18	0.075
23. LP (1) O 2	105. BD*(2) C 14- C 16	2.56	0.62	0.035
23. LP (1) O 2	106. BD*(1) C 15- C 17	0.19	1.19	0.014
23. LP (1) O 2	108. BD*(1) C 15- C 18	0.13	1.04	0.010
23. LP (1) O 2	109. BD*(1) C 16- C 19	0.19	1.20	0.013
23. LP (1) O 2	110. BD*(1) C 16- H 32	0.20	1.08	0.013
23. LP (1) O 2	114. BD*(1) C 18- H 35	0.33	1.01	0.016
23. LP (1) O 2	307. RY (2) C 12	2.89	1.87	0.066
23. LP (1) O 2	309. RY (4) C 12	0.12	2.32	0.015
23. LP (1) O 2	315. RY (10) C 12	0.20	3.77	0.025
23. LP (1) O 2	319. RY (14) C 12	0.13	3.42	0.019
23. LP (1) O 2	340. RY (1) C 14	1.90	2.04	0.056
23. LP (1) O 2	343. RY (4) C 14	0.24	2.06	0.020
23. LP (1) O 2	344. RY (5) C 14	0.46	2.13	0.028
23. LP (1) O 2	481. RY (1) H 25	0.12	1.52	0.012
24. LP (2) O 2	77. BD*(1) O 1- C 11	0.35	0.77	0.015
24. LP (2) O 2	78. BD*(1) O 1- C 12	12.63	0.77	0.088
24. LP (2) O 2	79. BD*(1) O 2- C 12	0.16	0.78	0.010
24. LP (2) O 2	92. BD*(1) C 8- C 10	0.44	0.85	0.017

24. LP (2) O 2	96. BD*(1) C 10- C 12	6.07	0.83	0.063
24. LP (2) O 2	97. BD*(1) C 10- H 23	0.22	0.86	0.012
24. LP (2) O 2	103. BD*(1) C 14- C 15	3.06	1.02	0.050
24. LP (2) O 2	104. BD*(1) C 14- C 16	2.18	1.03	0.042
24. LP (2) O 2	105. BD*(2) C 14- C 16	19.52	0.46	0.085
24. LP (2) O 2	106. BD*(1) C 15- C 17	0.20	1.04	0.013
24. LP (2) O 2	107. BD*(2) C 15- C 17	0.14	0.47	0.007
24. LP (2) O 2	114. BD*(1) C 18- H 35	0.15	0.86	0.010
24. LP (2) O 2	306. RY (1) C 12	0.51	1.55	0.025
24. LP (2) O 2	308. RY (3) C 12	0.13	2.16	0.015
24. LP (2) O 2	310. RY (5) C 12	0.84	2.38	0.040
24. LP (2) O 2	342. RY (3) C 14	0.93	1.79	0.036
24. LP (2) O 2	343. RY (4) C 14	1.13	1.91	0.041
24. LP (2) O 2	344. RY (5) C 14	0.14	1.98	0.015
25. LP (1) O 3	84. BD*(1) O 4- H 29	0.22	1.14	0.014
25. LP (1) O 3	91. BD*(1) C 8- C 9	1.78	1.07	0.039
25. LP (1) O 3	92. BD*(1) C 8- C 10	1.25	1.06	0.033
25. LP (1) O 3	93. BD*(1) C 8- H 21	0.93	1.06	0.028
25. LP (1) O 3	94. BD*(1) C 9- C 11	0.36	1.06	0.018
25. LP (1) O 3	96. BD*(1) C 10- C 12	0.14	1.04	0.011
25. LP (1) O 3	97. BD*(1) C 10- H 23	0.22	1.07	0.014
25. LP (1) O 3	238. RY (1) C 8	1.92	1.62	0.050
25. LP (1) O 3	240. RY (3) C 8	0.66	1.55	0.028
25. LP (1) O 3	241. RY (4) C 8	0.22	2.15	0.019
25. LP (1) O 3	242. RY (5) C 8	0.36	2.27	0.026
25. LP (1) O 3	245. RY (8) C 8	0.15	2.56	0.017
25. LP (1) O 3	249. RY (12) C 8	0.12	3.17	0.017
25. LP (1) O 3	257. RY (3) C 9	0.13	1.46	0.013
25. LP (1) O 3	500. RY (2) H 28	1.08	2.60	0.047
26. LP (2) O 3	84. BD*(1) O 4- H 29	0.21	0.90	0.012
26. LP (2) O 3	85. BD*(1) O 5- C 10	0.19	0.77	0.011
26. LP (2) O 3	92. BD*(1) C 8- C 10	6.07	0.83	0.063
26. LP (2) O 3	93. BD*(1) C 8- H 21	8.78	0.83	0.076
26. LP (2) O 3	95. BD*(1) C 9- H 22	0.10	0.83	0.008
26. LP (2) O 3	96. BD*(1) C 10- C 12	0.76	0.80	0.022
26. LP (2) O 3	238. RY (1) C 8	0.13	1.39	0.012
26. LP (2) O 3	239. RY (2) C 8	0.42	1.49	0.022
26. LP (2) O 3	241. RY (4) C 8	1.11	1.92	0.041
26. LP (2) O 3	242. RY (5) C 8	0.17	2.04	0.016
26. LP (2) O 3	272. RY (1) C 10	0.12	1.37	0.012
26. LP (2) O 3	457. RY (1) H 21	0.22	1.16	0.014
26. LP (2) O 3	499. RY (1) H 28	1.69	2.05	0.053
27. LP (1) O 4	77. BD*(1) O 1- C 11	0.54	0.97	0.021
27. LP (1) O 4	91. BD*(1) C 8- C 9	1.87	1.06	0.040
27. LP (1) O 4	92. BD*(1) C 8- C 10	0.22	1.06	0.014
27. LP (1) O 4	93. BD*(1) C 8- H 21	0.19	1.06	0.013
27. LP (1) O 4	94. BD*(1) C 9- C 11	1.61	1.05	0.037
27. LP (1) O 4	95. BD*(1) C 9- H 22	0.43	1.06	0.019
27. LP (1) O 4	102. BD*(1) C 13- H 27	0.12	1.09	0.010
27. LP (1) O 4	255. RY (1) C 9	2.04	1.64	0.052
27. LP (1) O 4	257. RY (3) C 9	0.49	1.45	0.024
27. LP (1) O 4	258. RY (4) C 9	0.17	2.21	0.017
27. LP (1) O 4	259. RY (5) C 9	0.50	2.39	0.031
27. LP (1) O 4	268. RY (14) C 9	0.12	1.90	0.013
27. LP (1) O 4	289. RY (1) C 11	0.23	1.53	0.017
27. LP (1) O 4	506. RY (2) H 29	1.15	2.57	0.049
28. LP (2) O 4	77. BD*(1) O 1- C 11	0.13	0.74	0.009
28. LP (2) O 4	81. BD*(1) O 3- C 8	0.18	0.76	0.010
28. LP (2) O 4	91. BD*(1) C 8- C 9	4.71	0.83	0.056
28. LP (2) O 4	92. BD*(1) C 8- C 10	0.64	0.83	0.021
28. LP (2) O 4	94. BD*(1) C 9- C 11	0.41	0.82	0.016
28. LP (2) O 4	95. BD*(1) C 9- H 22	10.23	0.82	0.082
28. LP (2) O 4	238. RY (1) C 8	0.19	1.39	0.014
28. LP (2) O 4	256. RY (2) C 9	0.44	1.52	0.023
28. LP (2) O 4	258. RY (4) C 9	1.25	1.98	0.044
28. LP (2) O 4	463. RY (1) H 22	0.22	1.21	0.015
28. LP (2) O 4	505. RY (1) H 29	1.76	2.05	0.054
29. LP (1) O 5	82. BD*(1) O 3- H 28	0.17	1.11	0.012
29. LP (1) O 5	91. BD*(1) C 8- C 9	0.47	1.04	0.020
29. LP (1) O 5	92. BD*(1) C 8- C 10	2.08	1.04	0.041
29. LP (1) O 5	96. BD*(1) C 10- C 12	0.75	1.01	0.025

29. LP (1) O 5	97. BD*(1) C 10- H 23	2.15	1.04	0.042
29. LP (1) O 5	100. BD*(1) C 12- H 25	0.20	1.04	0.013
29. LP (1) O 5	239. RY (2) C 8	0.13	1.69	0.013
29. LP (1) O 5	272. RY (1) C 10	1.79	1.58	0.047
29. LP (1) O 5	273. RY (2) C 10	0.43	2.06	0.027
29. LP (1) O 5	274. RY (3) C 10	0.30	2.13	0.022
29. LP (1) O 5	275. RY (4) C 10	0.20	1.65	0.016
29. LP (1) O 5	276. RY (5) C 10	0.25	2.14	0.021
29. LP (1) O 5	280. RY (9) C 10	0.12	2.64	0.016
29. LP (1) O 5	286. RY (15) C 10	0.20	3.62	0.024
29. LP (1) O 5	511. RY (1) H 30	1.19	2.56	0.049
29. LP (1) O 5	513. RY (3) H 30	0.15	2.03	0.015
30. LP (2) O 5	78. BD*(1) O 1- C 12	1.38	0.74	0.029
30. LP (2) O 5	79. BD*(1) O 2- C 12	0.19	0.75	0.011
30. LP (2) O 5	82. BD*(1) O 3- H 28	0.30	0.89	0.015
30. LP (2) O 5	93. BD*(1) C 8- H 21	0.14	0.82	0.010
30. LP (2) O 5	96. BD*(1) C 10- C 12	8.72	0.80	0.074
30. LP (2) O 5	97. BD*(1) C 10- H 23	7.13	0.83	0.069
30. LP (2) O 5	272. RY (1) C 10	0.43	1.36	0.022
30. LP (2) O 5	273. RY (2) C 10	0.16	1.84	0.015
30. LP (2) O 5	274. RY (3) C 10	1.06	1.92	0.040
30. LP (2) O 5	277. RY (6) C 10	0.28	1.99	0.021
30. LP (2) O 5	306. RY (1) C 12	0.24	1.52	0.017
30. LP (2) O 5	469. RY (1) H 23	0.18	1.26	0.013
30. LP (2) O 5	512. RY (2) H 30	1.43	2.05	0.048
31. LP (1) O 6	78. BD*(1) O 1- C 12	0.10	0.97	0.009
31. LP (1) O 6	98. BD*(1) C 11- C 13	1.33	1.06	0.033
31. LP (1) O 6	99. BD*(1) C 11- H 24	0.17	1.06	0.012
31. LP (1) O 6	101. BD*(1) C 13- H 26	0.70	1.05	0.024
31. LP (1) O 6	102. BD*(1) C 13- H 27	3.01	1.08	0.051
31. LP (1) O 6	323. RY (1) C 13	1.80	1.59	0.048
31. LP (1) O 6	325. RY (3) C 13	0.56	2.12	0.031
31. LP (1) O 6	326. RY (4) C 13	0.29	2.15	0.022
31. LP (1) O 6	327. RY (5) C 13	0.12	1.79	0.013
31. LP (1) O 6	338. RY (16) C 13	0.23	3.25	0.024
31. LP (1) O 6	496. RY (4) H 27	0.10	2.75	0.015
31. LP (1) O 6	518. RY (2) H 31	1.12	2.36	0.046
31. LP (1) O 6	520. RY (4) H 31	0.19	2.39	0.019
32. LP (2) O 6	77. BD*(1) O 1- C 11	0.30	0.73	0.013
32. LP (2) O 6	94. BD*(1) C 9- C 11	0.86	0.81	0.024
32. LP (2) O 6	98. BD*(1) C 11- C 13	5.62	0.82	0.061
32. LP (2) O 6	101. BD*(1) C 13- H 26	8.89	0.82	0.076
32. LP (2) O 6	102. BD*(1) C 13- H 27	0.17	0.85	0.011
32. LP (2) O 6	289. RY (1) C 11	0.22	1.28	0.015
32. LP (2) O 6	323. RY (1) C 13	0.26	1.35	0.017
32. LP (2) O 6	324. RY (2) C 13	0.80	1.44	0.030
32. LP (2) O 6	325. RY (3) C 13	0.93	1.88	0.037
32. LP (2) O 6	487. RY (1) H 26	0.14	1.03	0.011
32. LP (2) O 6	517. RY (1) H 31	1.89	1.98	0.055
33. LP (1) O 7	86. BD*(1) O 5- H 30	2.65	1.12	0.049
33. LP (1) O 7	107. BD*(2) C 15- C 17	0.17	0.65	0.009
33. LP (1) O 7	108. BD*(1) C 15- C 18	0.71	1.07	0.025
33. LP (1) O 7	113. BD*(1) C 18- H 34	3.45	1.04	0.054
33. LP (1) O 7	114. BD*(1) C 18- H 35	0.49	1.04	0.020
33. LP (1) O 7	407. RY (2) C 18	1.01	1.81	0.038
33. LP (1) O 7	408. RY (3) C 18	0.27	1.72	0.019
33. LP (1) O 7	409. RY (4) C 18	0.60	2.29	0.033
33. LP (1) O 7	559. RY (1) H 38	1.09	2.27	0.045
33. LP (1) O 7	560. RY (2) H 38	0.51	2.51	0.032
34. LP (2) O 7	86. BD*(1) O 5- H 30	10.38	1.00	0.091
34. LP (2) O 7	107. BD*(2) C 15- C 17	0.38	0.53	0.013
34. LP (2) O 7	108. BD*(1) C 15- C 18	0.85	0.94	0.025
34. LP (2) O 7	113. BD*(1) C 18- H 34	2.04	0.92	0.039
34. LP (2) O 7	114. BD*(1) C 18- H 35	6.84	0.92	0.071
34. LP (2) O 7	190. RY (4) O 5	0.18	2.01	0.017
34. LP (2) O 7	407. RY (2) C 18	1.08	1.69	0.038
34. LP (2) O 7	409. RY (4) C 18	0.39	2.17	0.026
34. LP (2) O 7	410. RY (5) C 18	0.18	1.73	0.016
34. LP (2) O 7	511. RY (1) H 30	0.17	2.43	0.018
34. LP (2) O 7	513. RY (3) H 30	0.12	1.90	0.014
34. LP (2) O 7	535. RY (1) H 34	0.13	1.09	0.010

34. LP (2) O 7	559. RY (1) H 38	0.85	2.15	0.038
34. LP (2) O 7	560. RY (2) H 38	0.76	2.39	0.038

11. Cartesian co-ordinates of the 14 low energy S_0 structures of salicin optimized at the M06-2X/6-311++G(d,p) level of theory

Conformer I				
Center Number	**Atomic Number**	**X**	**Y**	**Z**
1	8	0.993282	-1.04209	0.303348
2	8	-0.927931	0.131864	0.644755
3	8	3.125365	2.449846	-0.261215
4	8	4.286547	-0.061054	-0.865868
5	8	0.288257	2.47842	-0.357496
6	8	3.006519	-2.341189	1.627843
7	8	-2.531618	2.539864	0.252264
8	6	2.331618	1.318171	-0.550688
9	6	3.102311	0.086942	-0.112792
10	6	0.990648	1.373582	0.152365
11	6	2.257695	-1.163803	-0.350053
12	6	0.243757	0.073984	-0.111335
13	6	2.899167	-2.415907	0.22398
14	6	-2.053384	-0.473877	0.15474
15	6	-3.253831	0.212848	0.366422
16	6	-2.025512	-1.701153	-0.493774
17	6	-4.435539	-0.366756	-0.082165
18	6	-3.219991	1.562589	1.034804
19	6	-3.221563	-2.254259	-0.945474
20	6	-4.426922	-1.595704	-0.738152
21	1	2.153668	1.254427	-1.635265
22	1	3.328438	0.164544	0.958279
23	1	1.145604	1.457341	1.236872
24	1	2.11363	-1.289287	-1.433481
25	1	-0.004887	-0.012796	-1.180901
26	1	3.908219	-2.513726	-0.176345
27	1	2.307324	-3.287496	-0.079856
28	1	2.596608	3.232593	-0.450328
29	1	4.767576	0.77127	-0.808756
30	1	-0.606735	2.504721	0.021256
31	1	2.123991	-2.167719	1.971731
32	1	-1.081777	-2.218597	-0.617726
33	1	-5.373248	0.155102	0.079931
34	1	-4.239796	1.898812	1.244704
35	1	-2.673366	1.513581	1.97637
36	1	-3.206542	-3.212344	-1.451063
37	1	-5.354751	-2.033864	-1.083706
38	1	-2.958054	2.5982	-0.608029

Conformer II				
Center Number	**Atomic Number**	**X**	**Y**	**Z**
1	8	-1.040763	0.91671	0.549479
2	8	0.907407	-0.257591	0.690531
3	8	-3.185121	-2.506676	-0.237253
4	8	-4.365054	0.03448	-0.608877
5	8	-0.341592	-2.52179	-0.445813
6	8	-2.091622	3.448207	0.402194
7	8	2.509671	-2.603742	0.06668
8	6	-2.394625	-1.359985	-0.47296
9	6	-3.148831	-0.161681	0.076523
10	6	-1.028922	-1.467147	0.177948
11	6	-2.301575	1.095792	-0.09596
12	6	-0.298063	-0.143768	-0.000072
13	6	-2.930132	2.321792	0.537159
14	6	2.003857	0.397864	0.199362
15	6	3.219413	-0.284391	0.319457
16	6	1.935686	1.662363	-0.370213
17	6	4.376324	0.340107	-0.132915
18	6	3.222364	-1.678575	0.890586
19	6	3.107478	2.261066	-0.827864
20	6	4.32806	1.609406	-0.705561
21	1	-2.253942	-1.218676	-1.555287
22	1	-3.328659	-0.325106	1.149033
23	1	-1.146702	-1.642192	1.256161
24	1	-2.1415	1.283004	-1.168025
25	1	-0.102911	0.043207	-1.067942
26	1	-3.138264	2.107524	1.5933
27	1	-3.86978	2.545467	0.033627
28	1	-2.673455	-3.275754	-0.510586
29	1	-4.818115	-0.815349	-0.636839
30	1	0.567164	-2.569587	-0.103296
31	1	-1.258229	3.229975	0.830929
32	1	0.98152	2.171896	-0.43896
33	1	5.325473	-0.178251	-0.041248
34	1	4.252058	-2.019087	1.035087
35	1	2.713241	-1.702902	1.853853
36	1	3.060552	3.247749	-1.272798
37	1	5.236786	2.082876	-1.055271
38	1	2.905154	-2.598634	-0.810214

Conformer III				
Center Number	**Atomic Number**	**X**	**Y**	**Z**
1	8	0.951014	-0.905824	0.609035
2	8	-1.03626	0.208337	0.704724
3	8	2.971444	2.59019	-0.22842
4	8	4.280718	0.11383	-0.416344
5	8	0.131718	2.467227	-0.535793
6	8	4.033013	-2.66638	-0.111438
7	8	-2.718527	2.453453	-0.100613
8	6	2.234899	1.405173	-0.450583
9	6	3.004183	0.260816	0.177778
10	6	0.846366	1.474146	0.153903
11	6	2.227242	-1.04309	-0.005306
12	6	0.175988	0.11174	0.021939
13	6	2.923302	-2.235583	0.640324
14	6	-2.10336	-0.516978	0.247053
15	6	-3.343043	0.129538	0.299581
16	6	-1.983642	-1.817932	-0.222425
17	6	-4.470378	-0.565314	-0.124607
18	6	-3.406716	1.557475	0.775059
19	6	-3.126313	-2.487624	-0.654394
20	6	-4.369515	-1.869911	-0.602825
21	1	2.139831	1.219841	-1.530902
22	1	3.107614	0.454307	1.254698
23	1	0.925412	1.703325	1.225517
24	1	2.113899	-1.247296	-1.080768
25	1	-0.008928	-0.119515	-1.039358
26	1	2.217363	-3.066169	0.682392
27	1	3.203348	-1.974887	1.669513
28	1	2.440116	3.329184	-0.543982
29	1	4.694332	0.98411	-0.439123
30	1	-0.787955	2.491136	-0.220293
31	1	4.601188	-1.901902	-0.262284
32	1	-1.012752	-2.298619	-0.223806
33	1	-5.437914	-0.075147	-0.084569
34	1	-4.450512	1.866732	0.884322
35	1	-2.912468	1.665641	1.740335
36	1	-3.039663	-3.503482	-1.020925
37	1	-5.255548	-2.398243	-0.931669
38	1	-3.0964	2.369585	-0.981297

Conformer IV				
Center Number	**Atomic Number**	**X**	**Y**	**Z**
1	8	-0.52322	0.595879	0.13201
2	8	0.791459	-1.144566	0.741382
3	8	-3.968418	-1.558285	0.420155
4	8	-3.972605	0.938191	-0.894279
5	8	-1.464567	-2.905769	0.406242
6	8	-0.373328	3.172213	-0.945199
7	8	1.399474	1.987265	1.490003
8	6	-2.788439	-1.030632	-0.147751
9	6	-2.904968	0.487237	-0.095243
10	6	-1.545812	-1.508776	0.586191
11	6	-1.618913	1.121914	-0.615563
12	6	-0.339478	-0.792514	0.003768
13	6	-1.565615	2.628773	-0.43407
14	6	2.006885	-0.858562	0.123818
15	6	2.801296	0.172859	0.626476
16	6	2.411576	-1.634212	-0.954588
17	6	4.021625	0.41184	-0.004829
18	6	2.367251	1.003599	1.81434
19	6	3.6301	-1.372241	-1.569718
20	6	4.436643	-0.343858	-1.095313
21	1	-2.708584	-1.336312	-1.201821
22	1	-3.049201	0.784834	0.953942
23	1	-1.620516	-1.246457	1.649349
24	1	-1.485933	0.87827	-1.678269
25	1	-0.206597	-1.052317	-1.05691
26	1	-1.6885	2.858897	0.633155
27	1	-2.395615	3.076689	-0.980762
28	1	-3.898217	-2.518598	0.417923
29	1	-4.755525	0.437506	-0.640367
30	1	-0.720131	-3.235484	0.919347
31	1	0.365052	2.905641	-0.383138
32	1	1.773686	-2.442314	-1.29587
33	1	4.652267	1.211158	0.369503
34	1	1.988934	0.345385	2.603349
35	1	3.23254	1.538991	2.206045
36	1	3.949032	-1.975334	-2.411071
37	1	5.387821	-0.134984	-1.56919
38	1	0.596234	1.512439	1.237155

Conformer V				
Center Number	**Atomic Number**	**X**	**Y**	**Z**
1	8	-1.055756	0.911228	0.567597
2	8	0.908852	-0.238927	0.679891
3	8	-3.148921	-2.526932	-0.302284
4	8	-4.369678	0.002853	-0.602229
5	8	-0.297673	-2.485705	-0.513766
6	8	-2.148801	3.428563	0.476176
7	8	2.537855	-2.551897	0.12597
8	6	-2.376115	-1.361813	-0.508612
9	6	-3.147685	-0.190334	0.073713
10	6	-1.007952	-1.463224	0.137394
11	6	-2.320958	1.084393	-0.070857
12	6	-0.298848	-0.124944	-0.007424
13	6	-2.967042	2.285379	0.591602
14	6	2.004014	0.413056	0.178405
15	6	3.221657	-0.260277	0.307272
16	6	1.927634	1.667773	-0.41196
17	6	4.371714	0.357498	-0.169595
18	6	3.249389	-1.619026	0.949123
19	6	3.092799	2.262281	-0.889124
20	6	4.315422	1.614424	-0.766492
21	1	-2.239603	-1.190058	-1.586827
22	1	-3.320748	-0.382756	1.142543
23	1	-1.120711	-1.668803	1.210949
24	1	-2.166672	1.298826	-1.138633
25	1	-0.107302	0.088488	-1.070577
26	1	-3.1651	2.044847	1.644109
27	1	-3.913395	2.503495	0.098264
28	1	-2.634934	-3.278314	-0.61664
29	1	-4.806979	-0.854136	-0.652761
30	1	0.633519	-2.459381	-0.234088
31	1	-1.305306	3.211847	0.885691
32	1	0.97129	2.173146	-0.482285
33	1	5.322228	-0.157727	-0.080471
34	1	4.288827	-1.939271	1.061405
35	1	2.783064	-1.575929	1.938383
36	1	3.039312	3.24085	-1.350881
37	1	5.219942	2.081033	-1.135687
38	1	2.731372	-3.440746	0.435986

Conformer VI				
Center Number	**Atomic Number**	**X**	**Y**	**Z**
1	8	-1.005373	0.877254	0.578804
2	8	0.928534	-0.318025	0.715833
3	8	-3.200341	-2.510091	-0.173406
4	8	-4.351634	0.031895	-0.541456
5	8	-0.360478	-2.565959	-0.438827
6	8	-2.103888	3.427837	0.063518
7	8	2.521925	-2.594384	-0.12479
8	6	-2.395026	-1.375337	-0.421504
9	6	-3.126449	-0.163347	0.130108
10	6	-1.020317	-1.504938	0.205142
11	6	-2.25417	1.076013	-0.071313
12	6	-0.277524	-0.188617	0.027688
13	6	-2.876358	2.324591	0.504422
14	6	2.00814	0.386778	0.253779
15	6	3.230348	-0.293244	0.278867
16	6	1.912359	1.697159	-0.196831
17	6	4.369611	0.377158	-0.153421
18	6	3.262145	-1.727781	0.737773
19	6	3.067029	2.340701	-0.636818
20	6	4.294767	1.690282	-0.61239
21	1	-2.268948	-1.238389	-1.506255
22	1	-3.293048	-0.311462	1.206869
23	1	-1.122115	-1.687144	1.283795
24	1	-2.096801	1.231904	-1.149193
25	1	-0.079297	-0.001475	-1.040265
26	1	-2.868322	2.244035	1.598063
27	1	-3.909849	2.389246	0.150836
28	1	-2.702773	-3.286688	-0.451481
29	1	-4.796738	-0.822129	-0.573892
30	1	0.567788	-2.599649	-0.151365
31	1	-2.450159	4.22868	0.461667
32	1	0.953246	2.202913	-0.178001
33	1	5.324465	-0.138583	-0.135186
34	1	4.298661	-2.070099	0.814585
35	1	2.792381	-1.830406	1.715972
36	1	3.00162	3.3631	-0.989415
37	1	5.189175	2.2	-0.948236
38	1	2.863433	-2.498577	-1.018921

Conformer VII				
Center Number	**Atomic Number**	**X**	**Y**	**Z**
1	8	-0.912155	0.999791	0.443674
2	8	0.892228	-0.303837	0.92365
3	8	-3.356777	-2.291956	0.110863
4	8	-4.259904	0.245461	-0.737706
5	8	-0.528975	-2.60906	0.056695
6	8	-1.702217	3.555633	-0.26393
7	8	2.291985	-2.747654	0.381421
8	6	-2.446416	-1.279205	-0.264271
9	6	-3.096656	0.059546	0.036574
10	6	-1.1254	-1.404372	0.470035
11	6	-2.117853	1.180056	-0.300672
12	6	-0.253036	-0.20362	0.132016
13	6	-2.639238	2.554494	0.066365
14	6	2.035137	0.282902	0.423234
15	6	2.898312	-0.482314	-0.368658
16	6	2.329324	1.597388	0.755992
17	6	4.072644	0.117222	-0.821355
18	6	2.56622	-1.909545	-0.736422
19	6	3.503473	2.177045	0.28643
20	6	4.37575	1.437626	-0.504046
21	1	-2.249812	-1.335177	-1.345778
22	1	-3.332037	0.101878	1.109875
23	1	-1.302369	-1.391899	1.554062
24	1	-1.8932	1.155202	-1.377024
25	1	0.017515	-0.212375	-0.936609
26	1	-2.872786	2.567497	1.139081
27	1	-3.551465	2.75594	-0.49404
28	1	-2.915442	-3.140148	-0.006575
29	1	-4.793685	-0.5516	-0.648119
30	1	0.342396	-2.708148	0.475035
31	1	-0.866275	3.302084	0.140149
32	1	1.632533	2.139256	1.383737
33	1	4.757192	-0.462161	-1.432158
34	1	1.662	-1.953602	-1.348886
35	1	3.387865	-2.326273	-1.327153
36	1	3.737007	3.203344	0.542615
37	1	5.293112	1.88394	-0.867512
38	1	2.940413	-2.578111	1.070627

Conformer VIII				
Center Number	**Atomic Number**	**X**	**Y**	**Z**
1	8	0.96633	-0.900205	0.633034
2	8	-1.035475	0.19052	0.69555
3	8	2.938916	2.599935	-0.308803
4	8	4.28224	0.138583	-0.419716
5	8	0.09251	2.422519	-0.605888
6	8	4.075097	-2.634595	-0.033736
7	8	-2.743175	2.4084	-0.033348
8	6	2.217815	1.398436	-0.49412
9	6	3.002916	0.284454	0.168629
10	6	0.829304	1.464564	0.109912
11	6	2.245027	-1.035772	0.023739
12	6	0.179093	0.090103	0.017043
13	6	2.958283	-2.198241	0.704365
14	6	-2.102438	-0.530409	0.227898
15	6	-3.343394	0.10853	0.293326
16	6	-1.97583	-1.821457	-0.267355
17	6	-4.464835	-0.579458	-0.15548
18	6	-3.428893	1.50466	0.842855
19	6	-3.112769	-2.486425	-0.71835
20	6	-4.357564	-1.872035	-0.661788
21	1	2.124767	1.17911	-1.568014
22	1	3.102234	0.511102	1.239498
23	1	0.905622	1.725739	1.174627
24	1	2.135996	-1.273051	-1.04536
25	1	-0.001178	-0.171246	-1.03767
26	1	2.264514	-3.037403	0.770532
27	1	3.233594	-1.90328	1.725587
28	1	2.405599	3.319781	-0.662361
29	1	4.681992	1.014136	-0.47019
30	1	-0.842936	2.372636	-0.343339
31	1	4.631866	-1.866513	-0.20702
32	1	-1.002867	-2.298097	-0.275124
33	1	-5.433185	-0.092042	-0.115154
34	1	-4.480712	1.792063	0.924024
35	1	-2.972938	1.544682	1.837
36	1	-3.020985	-3.494196	-1.105324
37	1	-5.240126	-2.393659	-1.010007
38	1	-2.9831	3.307273	0.207499

Conformer IX				
Center Number	**Atomic Number**	**X**	**Y**	**Z**
1	8	-0.48846	0.552845	0.203526
2	8	0.743691	-1.288421	0.743809
3	8	-4.005536	-1.549358	0.348238
4	8	-3.934444	1.012657	-0.828046
5	8	-1.524388	-2.941214	0.310735
6	8	-0.323279	3.073631	-0.883508
7	8	1.771483	2.404632	1.010838
8	6	-2.80593	-1.021731	-0.178468
9	6	-2.882915	0.490559	-0.048428
10	6	-1.582784	-1.5512	0.544983
11	6	-1.572246	1.10986	-0.530688
12	6	-0.351209	-0.835715	0.011457
13	6	-1.533819	2.603678	-0.312893
14	6	1.981511	-0.968261	0.194381
15	6	2.652262	0.182074	0.601359
16	6	2.523918	-1.839624	-0.744964
17	6	3.896083	0.443037	0.021005
18	6	2.072661	1.157487	1.602307
19	6	3.762428	-1.560451	-1.30534
20	6	4.45016	-0.411061	-0.921947
21	1	-2.71941	-1.277057	-1.245249
22	1	-3.024924	0.739411	1.013336
23	1	-1.662625	-1.331634	1.617519
24	1	-1.444028	0.902043	-1.602757
25	1	-0.207897	-1.051219	-1.059871
26	1	-1.560924	2.802356	0.765462
27	1	-2.408817	3.051943	-0.791389
28	1	-3.944608	-2.510051	0.322358
29	1	-4.723944	0.498299	-0.626572
30	1	-0.763008	-3.291762	0.784241
31	1	-0.226245	4.011545	-0.700979
32	1	1.965907	-2.727719	-1.020721
33	1	4.420965	1.345082	0.317459
34	1	1.194134	0.721906	2.082113
35	1	2.820505	1.362572	2.371661
36	1	4.190259	-2.237484	-2.034822
37	1	5.416924	-0.186322	-1.355904
38	1	1.104481	2.268	0.322783

Conformer X				
Center Number	**Atomic Number**	**X**	**Y**	**Z**
1	8	-0.85177	0.967697	0.52829
2	8	1.039855	-0.240726	0.911618
3	8	-3.092565	-2.463322	0.114595
4	8	-4.188736	0.034471	-0.549441
5	8	-0.241399	-2.593155	-0.029237
6	8	-3.742698	2.804969	-0.652524
7	8	2.58128	-2.571165	0.308849
8	6	-2.25343	-1.384454	-0.243032
9	6	-2.96272	-0.102186	0.145074
10	6	-0.907489	-1.452342	0.451736
11	6	-2.075009	1.098519	-0.185303
12	6	-0.12786	-0.178712	0.150914
13	6	-2.706331	2.424621	0.221452
14	6	2.133215	0.438431	0.41686
15	6	3.048397	-0.252286	-0.384799
16	6	2.32753	1.767956	0.762427
17	6	4.178516	0.434575	-0.82598
18	6	2.811525	-1.689381	-0.785594
19	6	3.458285	2.435111	0.302679
20	6	4.385589	1.768869	-0.49051
21	1	-2.08776	-1.383177	-1.33087
22	1	-3.140819	-0.112761	1.229591
23	1	-1.057108	-1.500558	1.538906
24	1	-1.885802	1.121556	-1.268934
25	1	0.117618	-0.124567	-0.922806
26	1	-1.939847	3.199206	0.17298
27	1	-3.054437	2.353171	1.260566
28	1	-2.606349	-3.279121	-0.046877
29	1	-4.669475	-0.796128	-0.46032
30	1	0.640453	-2.655302	0.37495
31	1	-4.358778	2.065977	-0.718469
32	1	1.585859	2.253639	1.384365
33	1	4.903289	-0.086258	-1.443069
34	1	1.916944	-1.774323	-1.408231
35	1	3.662745	-2.039972	-1.377351
36	1	3.615227	3.473415	0.568763
37	1	5.270179	2.283951	-0.844293
38	1	3.195008	-2.361217	1.018368

Conformer XI				
Center Number	**Atomic Number**	**X**	**Y**	**Z**
1	8	1.193017	-0.904921	-0.651435
2	8	-0.924606	-0.266924	-1.257848
3	8	1.943285	2.497508	1.525279
4	8	4.05576	0.770094	0.818298
5	8	-0.294631	2.402533	-0.191443
6	8	3.158822	-2.718418	-1.364809
7	8	-2.967868	2.029001	-0.952557
8	6	1.83628	1.633684	0.413174
9	6	2.697888	0.416538	0.688551
10	6	0.394851	1.229111	0.157007
11	6	2.565625	-0.552871	-0.479915
12	6	0.366235	0.193695	-0.970083
13	6	3.309562	-1.85463	-0.261359
14	6	-1.741026	-0.714194	-0.240829
15	6	-3.059227	-0.246191	-0.2601
16	6	-1.325065	-1.62989	0.722036
17	6	-3.947592	-0.702411	0.709358
18	6	-3.488915	0.741843	-1.305362
19	6	-2.229083	-2.06173	1.687302
20	6	-3.541253	-1.603856	1.686207
21	1	2.220263	2.135775	-0.487768
22	1	2.333335	-0.073877	1.603586
23	1	-0.014681	0.778605	1.071149
24	1	2.937972	-0.072774	-1.396575
25	1	0.706219	0.660028	-1.902928
26	1	2.939383	-2.320683	0.662129
27	1	4.372626	-1.646661	-0.144761
28	1	1.325548	3.22405	1.387194
29	1	4.099879	1.516996	1.425426
30	1	-1.238075	2.213239	-0.333065
31	1	2.214988	-2.796486	-1.537469
32	1	-0.308276	-1.995877	0.704183
33	1	-4.969109	-0.33762	0.696482
34	1	-3.106792	0.442945	-2.284653
35	1	-4.581076	0.784379	-1.340856
36	1	-1.902028	-2.770872	2.438456
37	1	-4.242255	-1.947489	2.436482
38	1	-3.127826	2.640749	-1.676821

Conformer XII				
Center Number	**Atomic Number**	**X**	**Y**	**Z**
1	8	-0.999116	0.880353	0.567156
2	8	0.933246	-0.316535	0.715611
3	8	-3.190075	-2.520644	-0.161159
4	8	-4.345658	0.023352	-0.540081
5	8	-0.354951	-2.56858	-0.436236
6	8	-2.190936	3.493611	0.147286
7	8	2.521399	-2.588691	-0.153648
8	6	-2.39008	-1.383366	-0.412728
9	6	-3.123285	-0.172888	0.137867
10	6	-1.012691	-1.506905	0.208444
11	6	-2.256987	1.070358	-0.064499
12	6	-0.271187	-0.190434	0.024053
13	6	-2.881386	2.318802	0.528393
14	6	2.013638	0.391339	0.259158
15	6	3.234382	-0.291761	0.269386
16	6	1.920538	1.709777	-0.167365
17	6	4.373429	0.3825	-0.157519
18	6	3.267192	-1.731123	0.712917
19	6	3.074834	2.357754	-0.601844
20	6	4.30034	1.70293	-0.595259
21	1	-2.267624	-1.247466	-1.498224
22	1	-3.294059	-0.319411	1.214021
23	1	-1.108742	-1.685971	1.288137
24	1	-2.114233	1.216503	-1.148077
25	1	-0.070442	-0.010077	-1.044874
26	1	-2.812174	2.255933	1.616183
27	1	-3.936413	2.355804	0.242396
28	1	-2.68883	-3.296079	-0.436132
29	1	-4.796807	-0.827703	-0.565769
30	1	0.575939	-2.599808	-0.156827
31	1	-2.434897	3.713234	-0.754807
32	1	0.964	2.218678	-0.128993
33	1	5.327209	-0.135459	-0.150388
34	1	4.303748	-2.07506	0.780665
35	1	2.802999	-1.842879	1.692794
36	1	3.011677	3.387357	-0.933247
37	1	5.194888	2.215689	-0.926018
38	1	2.860071	-2.488104	-1.048297

Conformer XIII				
Center Number	**Atomic Number**	**X**	**Y**	**Z**
1	8	-0.544906	0.592891	0.215787
2	8	0.738516	-1.199799	0.776352
3	8	-4.004326	-1.597684	0.366896
4	8	-3.990476	0.948122	-0.859229
5	8	-1.483537	-2.923751	0.350901
6	8	-0.422217	3.187917	-0.795829
7	8	1.820804	2.460769	0.830846
8	6	-2.818001	-1.044062	-0.164874
9	6	-2.933396	0.468473	-0.060059
10	6	-1.584472	-1.532649	0.570605
11	6	-1.637791	1.120423	-0.536758
12	6	-0.37351	-0.785145	0.03453
13	6	-1.618361	2.623257	-0.329625
14	6	1.968604	-0.936861	0.197113
15	6	2.689187	0.200464	0.558678
16	6	2.480896	-1.861089	-0.70757
17	6	3.957717	0.370253	-0.001069
18	6	2.139734	1.243636	1.501187
19	6	3.734435	-1.659123	-1.26867
20	6	4.479644	-0.53918	-0.910832
21	1	-2.721029	-1.313292	-1.227281
22	1	-3.094337	0.730073	0.996092
23	1	-1.677917	-1.30495	1.64024
24	1	-1.487519	0.902023	-1.603699
25	1	-0.219018	-1.013609	-1.032481
26	1	-1.771906	2.827715	0.739313
27	1	-2.444836	3.064451	-0.887714
28	1	-3.923305	-2.556656	0.340044
29	1	-4.773847	0.432623	-0.639128
30	1	-0.736089	-3.25338	0.859506
31	1	0.300684	2.845239	-0.248236
32	1	1.886625	-2.734017	-0.954348
33	1	4.550817	1.232742	0.291337
34	1	1.21324	0.900851	1.952988
35	1	2.869731	1.442854	2.293358
36	1	4.133475	-2.379659	-1.972146
37	1	5.465234	-0.382409	-1.331435
38	1	2.611012	2.801293	0.401857

Conformer XIV				
Center Number	**Atomic Number**	**X**	**Y**	**Z**
1	8	-0.465334	0.524546	0.175796
2	8	0.693872	-1.349515	0.738961
3	8	-4.073939	-1.385872	0.381399
4	8	-3.877164	1.133566	-0.88034
5	8	-1.668411	-2.908043	0.355668
6	8	-0.139413	3.087465	-0.899423
7	8	1.862545	2.332038	1.035311
8	6	-2.8532	-0.933637	-0.168293
9	6	-2.851931	0.585421	-0.084222
10	6	-1.654351	-1.51174	0.561695
11	6	-1.51361	1.126835	-0.580619
12	6	-0.395911	-0.865031	0.006845
13	6	-1.364912	2.62498	-0.396625
14	6	1.926238	-1.027874	0.186553
15	6	2.604561	0.117582	0.596502
16	6	2.461873	-1.883667	-0.77026
17	6	3.839587	0.392805	0.006422
18	6	2.05545	1.051933	1.640451
19	6	3.691904	-1.592688	-1.343299
20	6	4.38166	-0.44624	-0.956681
21	1	-2.788236	-1.222876	-1.227801
22	1	-2.981922	0.872788	0.969662
23	1	-1.719045	-1.266889	1.629869
24	1	-1.389035	0.881361	-1.644896
25	1	-0.269759	-1.110785	-1.060177
26	1	-1.476165	2.852195	0.673833
27	1	-2.165517	3.128023	-0.939883
28	1	-4.0701	-2.348502	0.363022
29	1	-4.694411	0.678553	-0.650163
30	1	-0.926889	-3.289767	0.835917
31	1	0.572609	2.684127	-0.379441
32	1	1.901878	-2.768283	-1.052027
33	1	4.367567	1.29101	0.307977
34	1	1.116132	0.668222	2.037536
35	1	2.783622	1.140957	2.454586
36	1	4.110997	-2.258293	-2.088144
37	1	5.339905	-0.211059	-1.403258
38	1	1.666986	2.973667	1.7236