Supporting Information for

Why O_x Appears and Disappears in the S_3 State of Photosystem II: Insights from the Low Oxidation State Model

Alireza Ariafard,[a] *Matthew Longhurst,*[b] *Gerhard F. Swiegers,*[b] *Robert Stranger*[a]

[a] Research School of Chemistry, Australian National University, Canberra, Australia

[b] Intelligent Polymer Research Institute, University of Wollongong, Wollongong, Australia

Table of contents:

Fig. S1 Optimised structures and relative free energies (kcal mol^{-1}) for the unrestrained O$_x$-formation pathway during the S$_2$ → S$_3$ transition in the LOS model. Values outside parentheses correspond to the IEFPCM/B3LYP-D3/6-311+G(2d,p),SDD//IEFPCM/B3LYP-D3/6-31G(d),SDD level, and those in parentheses to the IEFPCM/B3LYP*-D3/6-311+G(2d,p),SDD//IEFPCM/B3LYP-D3/6-31G(d),SDD level.

Fig. S2 Optimised structures and relative free energies (kcal mol⁻¹) for the Mn₁–ligand-restrained O_x-formation pathway during the $S_2 \rightarrow S_3$ transition in the LOS model. Values outside parentheses correspond to the IEFPCM/B3LYP-D3/6-311+G(2d,p),SDD//IEFPCM/B3LYP-D3/6-31G(d),SDD level, and those in parentheses to the IEFPCM/B3LYP*-D3/6-311+G(2d,p),SDD//IEFPCM/B3LYP-D3/6-31G(d),SDD level.
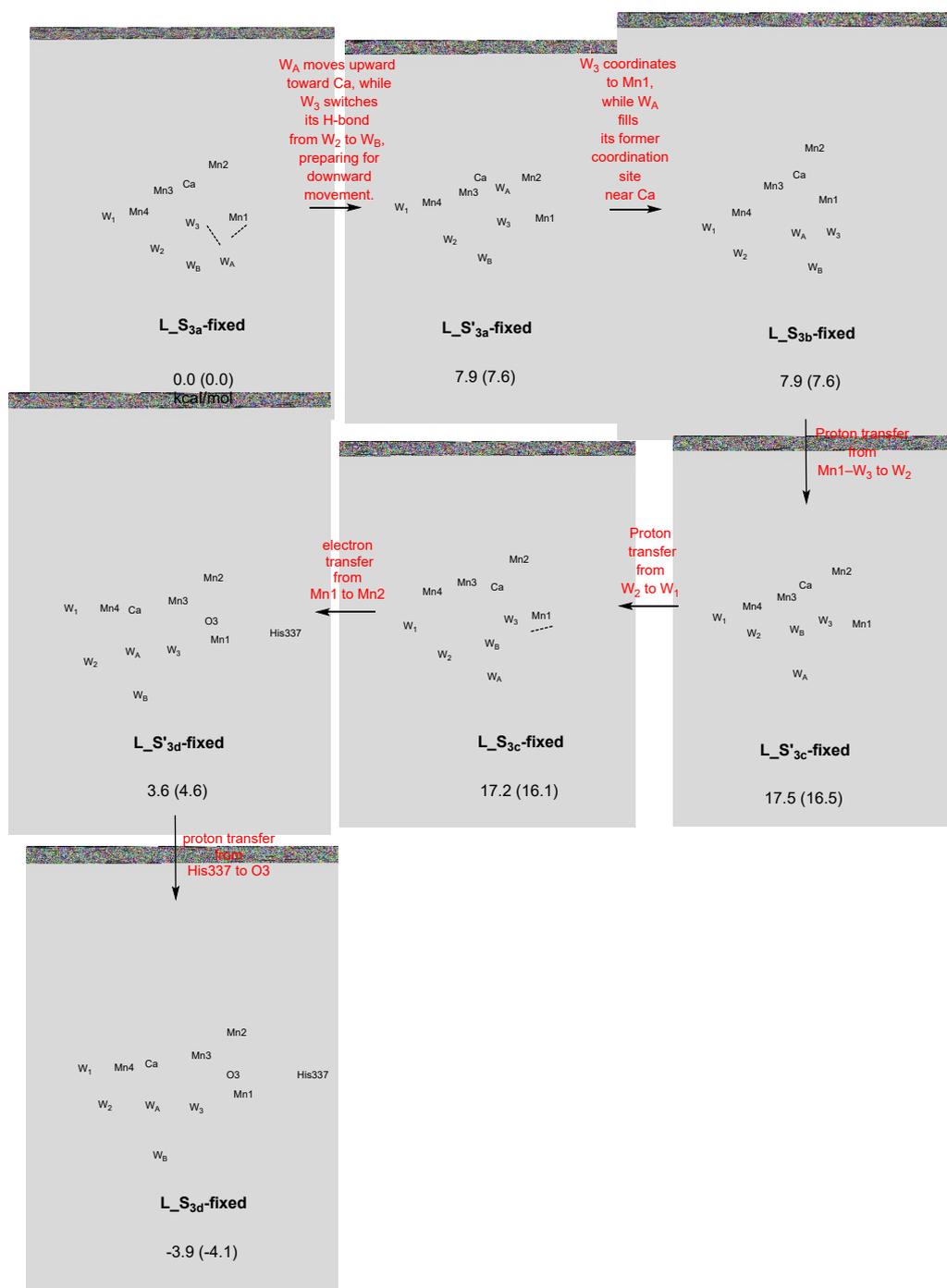
Comparison of the L_S$_{3a}$ and L_S$_{3aa}$ structures. In high-resolution XFEL structures of the OEC, a water molecule is typically observed between W$_3$ and Glu189 and another between W$_3$ and W2. In our LOS model, we simply label these two experimentally observed waters as W$_A$ (between W$_3$ and Glu189) and W$_B$ (between W$_3$ and W$_2$). Whereas in Siegbahn's original HOS model, W$_A$ and W$_B$ were introduced as additional waters migrating toward the OEC, in our model they correspond directly to crystallographically observed water sites in the XFEL structures.

As discussed in the manuscript, our calculations start from the intermediate **L_S$_{3a}$** (Fig. 3 and Figs S1 and S2). Our initial exploration of **L_S$_{3a}$** considered a conformer consistent with experimentally reported XFEL models, containing a water molecule between W$_3$ and Glu189 and another between W$_3$ and W$_2$. However, this intermediate (denoted **L_S$_{3aa}$**, Fig. S3) was found to be less stable than **L_S$_{3a}$** at both the B3LYP and B3LYP* levels of theory, in terms of both electronic energy and free energy. Accordingly, the **L_S$_{3a}$** structure shown in Fig. S1 and S2 was adopted as the reference point for the mechanistic calculations presented in this study.

The higher stability of **L_S$_{3a}$** relative to **L_S$_{3aa}$** can be attributed to differences in the hydrogen-bonding environment around W$_2$. In **L_S$_{3a}$**, W$_2$ is an OH ligand with high electron density localized on the oxygen atom, enabling simultaneous hydrogen-bond interactions with both W$_3$ and W$_B$. These simultaneous interactions provide additional stabilization. In contrast, in **L_S$_{3aa}$**, W$_2$ forms a hydrogen bond only with W$_B$, while the interaction with W$_3$ is absent, leading to reduced stabilization.

A similar hydrogen-bond-based rationale was employed by us under the subtitle *"Effect of the W3' Water Molecule on Proton Transfer and O–O Coupling"* in the Supporting Information of our recent publication (ref 17).
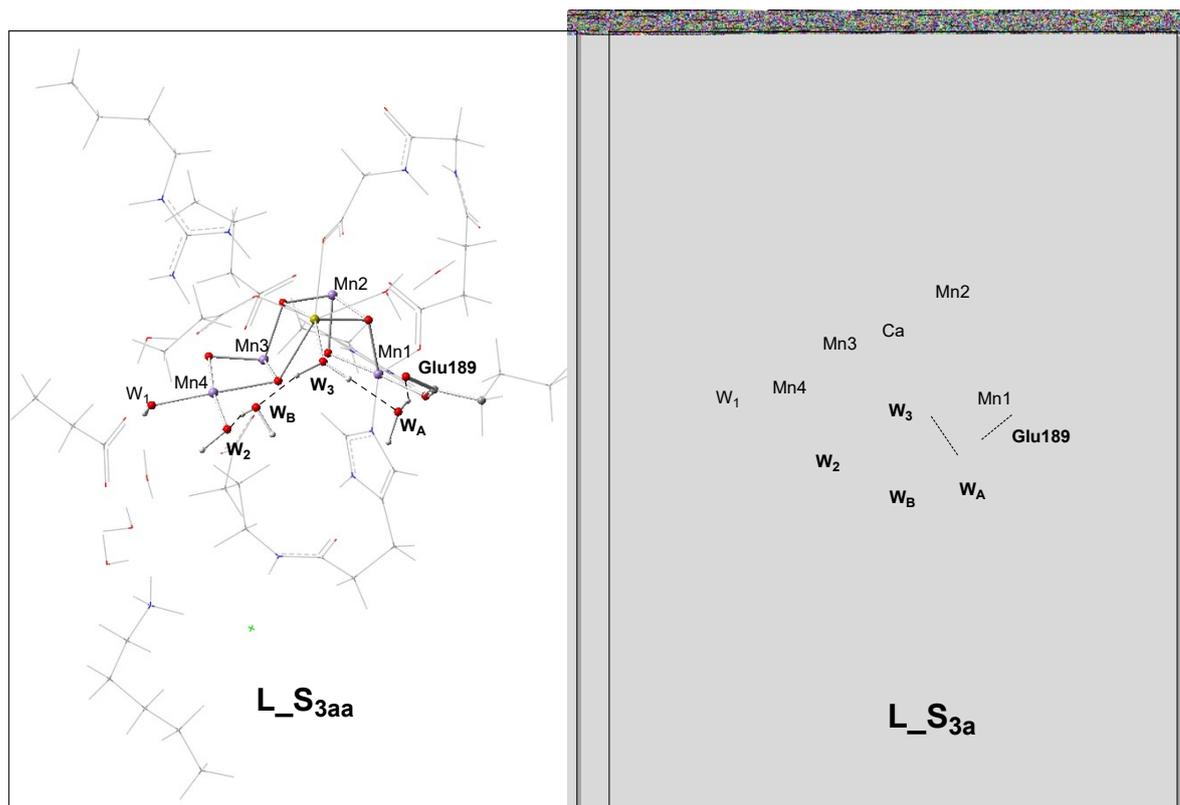
Fig. S3 3D structures for **L_S$_{3a}$** and **L_S$_{3aa}$**.

Why oxidation occurs at Mn3 during the S$_2$ → S$_3$ transition. Our assignment of the oxidation sequence in the LOS model follows the literature, in which the order of Mn oxidation states has been discussed in detail. We previously reviewed and summarised these studies in 2021 (see ref2).

Nevertheless, this assignment is further supported by our calculations (Fig. S4). As shown in Fig. 3, in the S$_3$ state of the LOS model only Mn2 is in the +IV oxidation state, while the remaining Mn centres are +III. Consequently, oxidation during the S$_2$ → S$_3$ transition must occur at Mn1, Mn3, or Mn4. Computational attempts to localise oxidation at Mn1 consistently collapsed to oxidation at Mn3 or Mn4. This behaviour arises because Mn1 is intrinsically five-coordinate in the S$_2$ state, making its oxidation unfavourable, whereas Mn3 and Mn4 are six-coordinate and therefore more readily oxidised. Although we were able to locate an S$_3$ state in which Mn4 is oxidised instead of Mn3, at the B3LYP (B3LYP*) level, this state is approximately 16.5 (16.0) kcal/mol higher in free energy than the case in which Mn3 is oxidised (Fig. S4), demonstrating that oxidation at Mn3 during the S$_2$ → S$_3$ transition is energetically preferred, in agreement with previous studies (ref 2).

The lower propensity of Mn4 to undergo oxidation relative to Mn3 is likely associated with its ligand environment, which includes the bridging carboxylate ligands Asp170 and Glu333. These weak σ-donor ligands stabilise the Mn4 d$_z^2$ orbital along the Asp170–Mn4–Glu333 axis, lowering its energy and reducing its tendency to undergo oxidation.
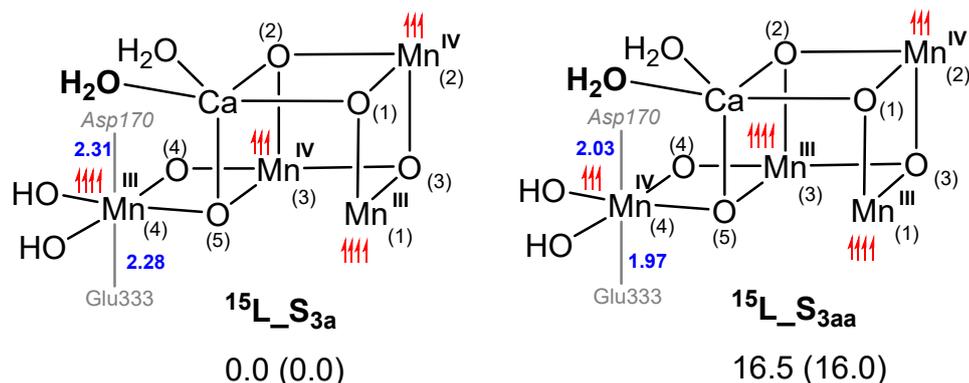
Fig. S4 Calculated structures of **L_S3a** and **L_S3aa** and their relative free energies in the LOS model. The relative free energies outside parentheses correspond to the IEFPCM/B3LYP-D3/6-311+G(2d,p),SDD//IEFPCM/B3LYP-D3/6-31G(d),SDD level, and those in parentheses to the IEFPCM/B3LYP*-D3/6-311+G(2d,p),SDD//IEFPCM/B3LYP-D3/6-31G(d),SDD level.

Justification of the structural model used in this study. We note that the structural model adopted from Siegbahn remains appropriate and consistent with current crystallographic understanding of the OEC. In this model, all first- and second-coordination-sphere ligands are explicitly included and correctly positioned, indicating that the essential structural features of the active site are fully retained. Importantly, the structures employed in this work were not treated as rigid single-point models; rather, they were fully geometry-optimised prior to subsequent single-point energy calculations. As a result, any potential inaccuracies in structural parameters present in the initial coordinates are eliminated during optimisation.

Moreover, this structural model continues to be used by Siegbahn himself in his more recent studies (J. Phys. Chem. B 2023, 127, 6643–6647), supporting its ongoing validity. In addition, in our own recent work (ref. 14), we explicitly demonstrated that the Siegbahn model is fully appropriate for describing the OEC. In that study, we investigated the mechanistic details of O–O bond formation and O_2 release within the LOS framework and showed that calculations performed using the Siegbahn model yield results very similar to those obtained using a model constructed from more recent crystallographic data reported by Bhowmick et al. (ref. 16).
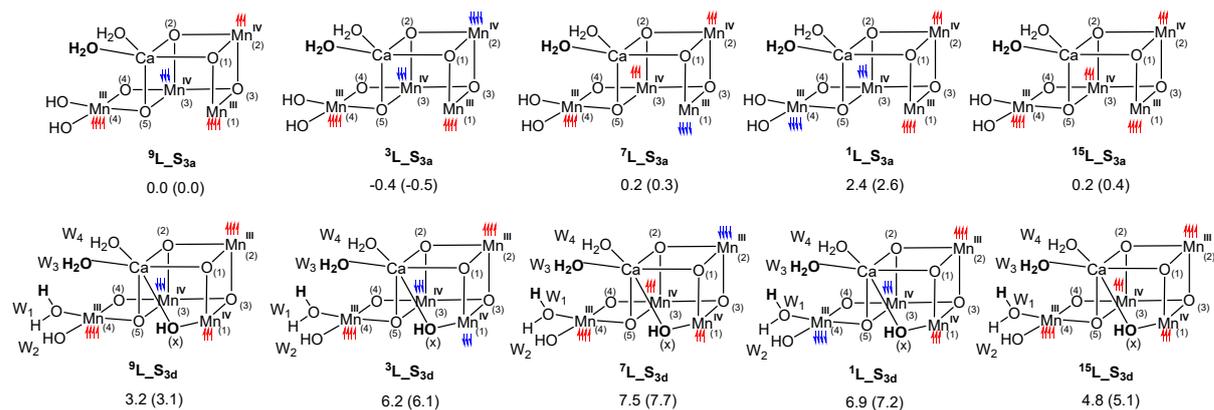
Fig. S5 Optimised free-OEC structures of **L_S₃ₐ** and **L_S₃d** computed for multiple spin states (antiferromagnetic singlet, triplet, septet, and nonet, and ferromagnetic 15-et), with relative free energies given in kcal/mol, where ¹⁵**L_S₃ₐ** is considered as the reference energy point. The relative free energies outside parentheses refer to calculations performed at the IEFPCM/B3LYP-D3/6-311+G(2d,p),SDD//IEFPCM/B3LYP-D3/6-31G(d),SDD level, whereas those in parentheses refer to calculations performed at the IEFPCM/B3LYP-D3/6-311+G(2d,p),SDD//IEFPCM/B3LYP-D3/6-31G(d),SDD level.
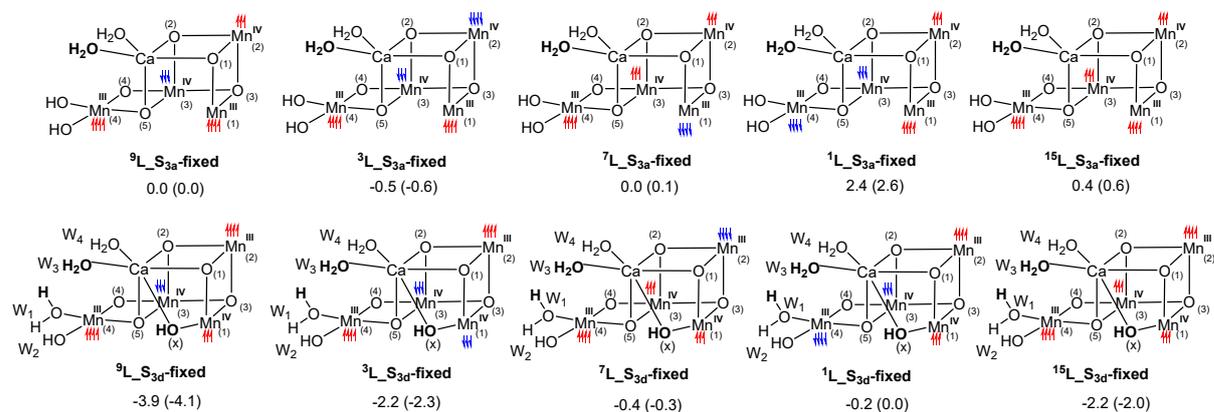
Fig. S6 Optimised fixed-OEC structures of **L_S₃ₐ-fixed** and **L_S₃d-fixed** computed for multiple spin states (antiferromagnetic singlet, triplet, septet, and nonet, and ferromagnetic 15-et), with relative free energies given in kcal/mol, where ¹⁵**L_S₃ₐ-fixed** is considered as the reference energy point. The relative free energies outside parentheses refer to calculations performed at the IEFPCM/B3LYP-D3/6-311+G(2d,p),SDD//IEFPCM/B3LYP-D3/6-31G(d),SDD level, whereas those in parentheses refer to calculations performed at the IEFPCM/B3LYP-D3/6-311+G(2d,p),SDD//IEFPCM/B3LYP-D3/6-31G(d),SDD level.

Contribution of His337 to Mn1 → Mn2 electron transfer in the constrained model.
When electron transfer occurs from Mn1 to Mn2 in **L_S$_{3c}$-fixed**, the oxidation state of Mn2 is reduced from +IV to +III, stabilising the system by approximately 13.6 kcal/mol and leading to formation of **L_S′$_{3d}$-fixed** (Fig. S7). This stabilisation arises from the Mn1–ligand restraints, which enforce a Mn(IV)-type coordination geometry at Mn1. Upon reduction of Mn2, a Jahn–Teller distortion is induced at this centre, resulting in increased basicity of O3. This effect is clearly reflected in the shortening of the O3–H(His337) distance from 1.72 Å in **L_S$_{3c}$-fixed** to 1.60 Å in **L_S′$_{3d}$-fixed** (Fig. S7). The increased basicity of O3 favours full proton transfer from His337, leading to formation of **L_S$_{3d}$-fixed**, which is approximately 7 kcal/mol more stable than **L_S′$_{3d}$-fixed**.

L_S₃c-fixed

17.2 (16.1)

L_S'₃d-fixed

3.6 (4.6)

L_S₃d-fixed

-3.9 (-4.1)
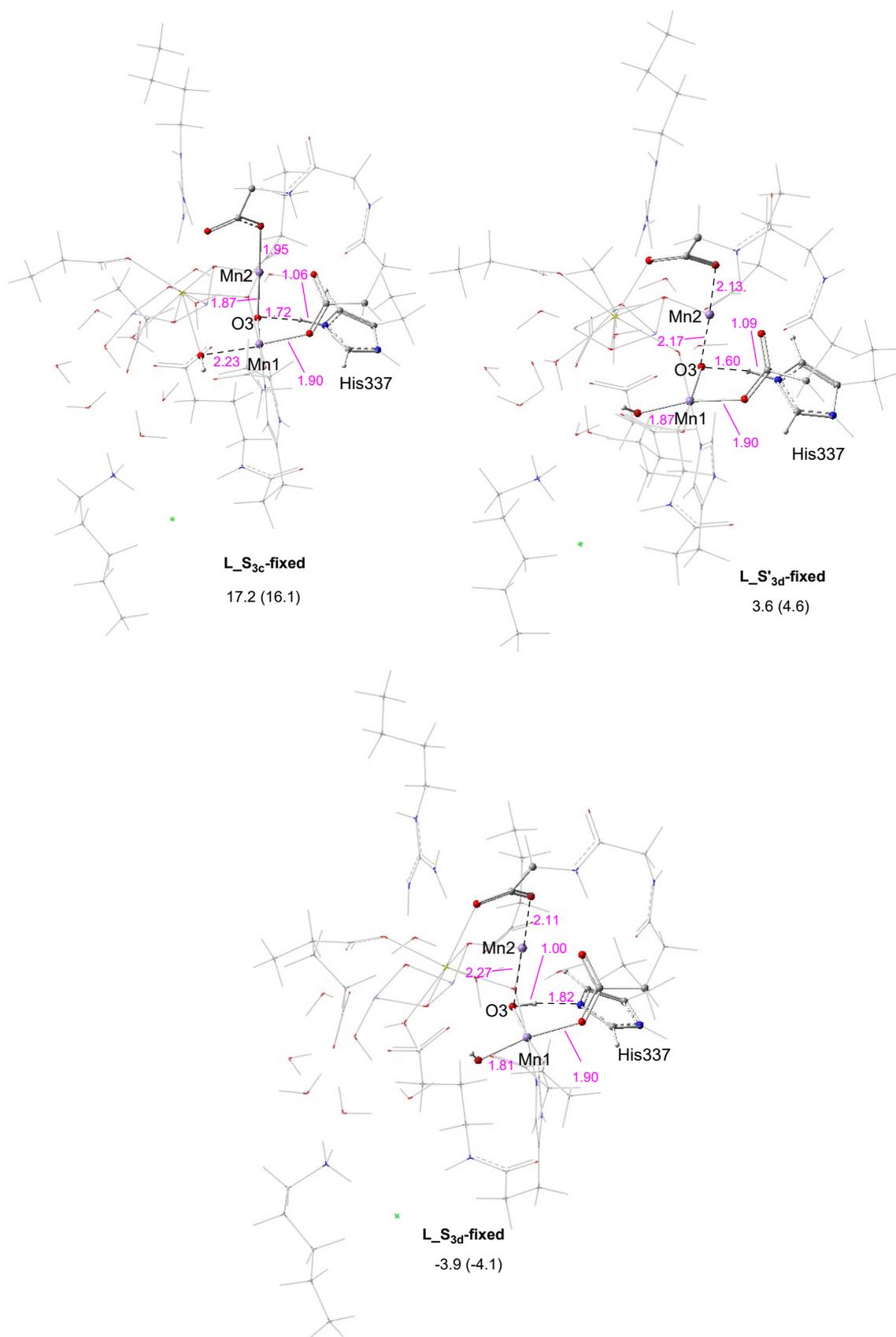
Fig. S7 Structural changes and relative free energies associated with Mn1 → Mn2 electron transfer under geometric constraints in the fixed-OEC model. Selected bond distances are given in Å.

Table S1. Mulliken spin densities on Mn atoms for all calculated intermediates along the O_x-formation pathway under unrestrained and Mn_1–ligand-restrained conditions, obtained at the IEFPCM/B3LYP-D3/6-311+G(2d,p),SDD//IEFPCM/B3LYP-D3/6-31G(d),SDD level in a solvent with $\varepsilon = 6.0$.

Species	Mn1	Mn2	Mn3	Mn4
L_S$_{3b}$	3.99	3.08	-2.91	3.99
L_S$_{3b}$-fixed	4.05	3.05	-2.91	3.99
L_S$'_{3a}$-fixed	4.14	3.07	-2.98	4.02
L_S$'_{3a}$	4.18	3.08	-2.96	4.01
L_S$'_{3c}$-fixed	4.04	3.06	-2.88	3.99
L_S$'_{3c}$	4.04	3.11	-2.91	3.98
L_S$'_{3d}$-fixed	3.08	3.96	-2.99	4.02
L_S$'_{3d}$	3.03	4.01	-3.00	4.03
L_S$_{3a}$-fixed	4.07	3.1	-2.94	4.00
L_S$_{3b}$	4.08	3.08	-2.91	3.99
L_S$_{3c}$-fixed	4.04	3.08	-2.91	4.02
L_S$_{3c}$	4.02	3.08	-2.96	4.01
L_S$_{3d}$-fixed	3.07	3.97	-2.97	4.02
L_S$_{3d}$	3.03	4.01	-3.00	4.03

Computational Details. Gaussian 16[1] was used to fully optimize all the structures reported in this study at the B3LYP level of theory.[2] For all calculations, solvent effects were incorporated

using the IEFPCM solvation model[3] with a dielectric constant (ε) of 6.0. The Grimme empirical dispersion was added with the GD3 term for all the calculations.[4] For geometry optimizations, the SDD basis set with effective core potential (ECP) was chosen to describe the Ca and Mn ions and the 6-31G(d) basis set was employed for all other atoms.[5] This basis set combination will be referred to as BS1. Transition structures were located using the Berny algorithm. Frequency calculations were performed at the same level of theory as the structural optimisations to confirm that each transition structure exhibits a single imaginary frequency corresponding to the intended reaction coordinate, and to obtain the enthalpy and entropy corrections required for calculating Gibbs free energies. Intrinsic reaction coordinate (IRC) calculations were used to confirm the connectivity between transition structures and minima.[6] To enhance the precision of the energies derived from the IEFPCM/B3LYP-D3/SDD, 6-31G(d) calculations, single-point energy calculations were carried out on all structures using both the B3LYP*-D3 and B3LYP-D3 functionals with a larger basis set (BS2), while still applying the IEFPCM solvation model. This larger basis set employs the SDD effective core potential (ECP) for Mn and Ca and the 6-311+G(2d,p) basis set for all other atoms, which includes diffuse functions as recommended for this type of system.[7]

The choice of B3LYP*, a modified hybrid functional with 15% exact Hartree–Fock exchange, is based on its reliable performance in describing spin-state energetics in transition metal (TM) systems[8] and its good agreement with experimental redox behaviour in the OEC system.[9]

The antiferromagnetic electronic configurations were obtained through the application of the broken symmetry (BS) approach.[10]

In the OEC model (Figure 9), all amino acid residues directly bound to Mn and Ca are included, namely His332, Glu189, Asp342, Ala344, Glu354, Asp170, and Glu333. Additionally, the model incorporates His337 and Arg357, and the backbones of Leu343 and Ser169, as well as

a portion of Gly171. Seven water molecules, positioned at crystallographic locations, are also included. The cluster in the LOS model formally has a -1 net charge. We have adopted this structural model from a recent computational study by Siegbahn et al.,[11] who interpreted the 1.9 Å crystallographic data of PSII [12] as representative of the S_3 state and used it to build their computational model. In this setup, the α-carbons and peptide chains were fixed, to account for the constraints imposed by the enzyme surroundings on the active site.
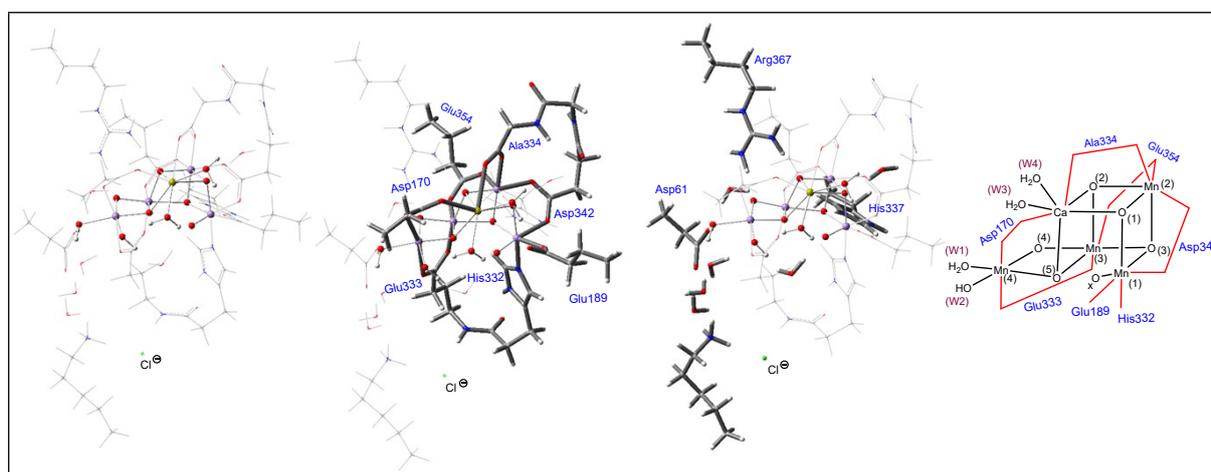
Fig. S8 Model complex used in this study for S_3 state. The first structure from the left represents the active site of PSII. The second structure includes the first coordination sphere ligands along with the active site. The third structure encompasses the second coordination sphere ligands and the active site.

Table S2. Cartesian coordinates for all optimised structures, together with total potential energies, enthalpies, and Gibbs free energies calculated at the IEFPCM/B3LYP-D3/SDD,6-31G(d) level, and single-point energies obtained at the IEFPCM/B3LYP-D3/SDD,6-

311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)   and   IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d) levels in a solvent with $\varepsilon = 6.0$.

In the Cartesian coordinates, a '-1' sign following an atom indicates it was fixed, while a '0' signifies it remained fully unconstrained during the optimization process.

L-S$_{3b}$-fixed
E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.92397 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.359758 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.599082 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.759802 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.686268 au

Mn	0	1.2383339931	2.5084942895	-1.6380279340
Mn	0	-1.0145508553	-2.4958009278	-0.6217060387
Mn	0	-0.0646239796	0.8998360928	0.2135867607
Mn	0	-2.6350378351	-0.4563649680	0.3570810508
O	0	0.3333742274	0.8244998044	-1.4903451799
O	0	-1.8816637638	1.0362497362	-0.2632716605
O	0	-2.4708345523	-1.4070866246	-1.1730143806
O	0	-0.9154927660	-1.1163489926	0.6810987157
Ca	0	-1.6943708582	0.4372922866	-2.6850369436
C	-1	0.5592308420	4.7792480410	-5.3708585874
H	-1	0.6334039215	5.6907385829	-4.7962188267
H	-1	0.7468677331	4.8954757818	-6.4278203588
H	0	1.3609606312	4.1350592309	-4.9878036142
C	0	-0.7797402297	4.0596397263	-5.1103743267
H	0	-0.8888858017	3.2063978421	-5.7898467275
H	0	-1.6322097232	4.7211850573	-5.3235735579
C	0	-0.9777434304	3.4936542870	-3.6849199471
O	0	-1.8770550855	2.6000400557	-3.5521295060
O	0	-0.2574943867	3.9215399943	-2.7420450626
C	-1	-3.0037496340	-6.4493825185	-5.5450793098
H	-1	-2.0477974075	-6.9141074566	-5.7363661176
H	-1	-3.7386472224	-6.5541053738	-6.3295231003
H	0	-3.4337937260	-7.0587246674	-4.7311368149
C	0	-2.7704925175	-5.0538729435	-4.9966485158
H	0	-3.7113825571	-4.5128872199	-4.8356697852
H	0	-2.1622847381	-4.4542105793	-5.6798800739
C	0	-2.0393349936	-5.2216255622	-3.6616196953
H	0	-1.2665582162	-5.9996139299	-3.7628089168
H	0	-2.7178841209	-5.5622630631	-2.8733325390
C	0	-1.3125212888	-3.9891261949	-3.2026560418
O	0	-0.8449219491	-3.2091914200	-4.0667590742
O	0	-1.1933858831	-3.8623712230	-1.9295674131
C	-1	5.0196256773	-4.7185871238	0.8372928093
H	0	5.7481004173	-5.5150331705	1.0262538172
H	0	5.3674433130	-4.1440088062	-0.0249532319
C	0	4.9097142779	-3.8327680645	2.0740289162
O	0	4.3181681849	-4.2420014022	3.0958562267
C	0	3.6407460726	-5.3936989914	0.5450730143
H	0	3.4397398283	-6.1012305266	1.3584279795
H	0	3.7147674738	-5.9727636101	-0.3795021338
C	0	2.4753034665	-4.4448018923	0.4340044806
N	0	2.2616267351	-3.4880253056	1.4148207835
H	0	2.7852358160	-3.4504596849	2.2870943006
C	0	1.4558533035	-4.2450090146	-0.4694129905
H	0	1.2272246013	-4.7657737357	-1.3855476943
C	0	1.2136160006	-2.7319976744	1.0847930752
H	0	0.9231632930	-1.8401848245	1.6048501917

N	0	0.6619915620	-3.1771306405	-0.0429196851
N	0	5.3231550395	-2.5639205409	1.9336794067
H	0	5.8887424827	-2.3275000216	1.1112314554
C	-1	5.0243228601	-1.5220196920	2.9101905152
H	0	5.9270675071	-0.9089677899	3.0274448163
H	0	4.8249622915	-2.0072908806	3.8680080406
C	0	3.8422041483	-0.6274173612	2.5017342012
H	0	3.6896284799	0.1252987573	3.2855518586
H	0	2.9278245432	-1.2208138522	2.4764683638
C	0	4.0539656690	0.0563936490	1.1502997002
H	0	4.5228233678	-0.6352421539	0.4384460531
H	0	4.7388296846	0.9077397345	1.2400421403
C	0	2.8136824750	0.5765941812	0.4304836198
O	0	2.9956630021	1.1732696997	-0.6440975128
O	0	1.6616970011	0.3073844813	0.9551217232
C	-1	-5.4759574907	-4.0370836111	2.1272933470
H	0	-5.3643843037	-3.3305117973	2.9562311538
H	0	-5.9540910307	-4.9393799547	2.5283915704
C	0	-4.1038214246	-4.4140661117	1.5496890626
H	0	-4.2237291357	-5.1005445081	0.7057714575
H	0	-3.5204658678	-4.9547777523	2.3053615974
C	0	-3.2354832245	-3.2592011761	1.0550545467
O	0	-3.6193687447	-2.0727147625	1.2537326763
O	0	-2.1349733360	-3.5596223200	0.4841580032
C	0	-6.3989231612	-3.4554213635	1.0618672868
O	0	-6.2490102792	-3.6880597175	-0.1463096952
N	0	-7.4361015951	-2.7221337914	1.5301525064
H	0	-7.4446154687	-2.4621153612	2.5070254502
C	-1	-8.4394195755	-2.1178760328	0.6602203237
H	0	-9.3508730189	-1.9516161697	1.2344546036
H	0	-8.6439836967	-2.8139993329	-0.1583385368
C	0	-7.9853734109	-0.7480870321	0.1000503410
O	0	-8.5185671937	0.2962885665	0.4782675372
N	0	-6.9851894480	-0.8058466134	-0.8140592309
H	0	-6.5628094711	-1.7019437588	-1.0353825065
C	0	-6.3825534388	0.3718244719	-1.4107616375
H	0	-6.5779072653	0.4060119836	-2.4864799250
H	0	-6.8452171679	1.2481336732	-0.9462963916
C	0	-4.8597403906	0.4450847021	-1.2152683478
O	0	-4.1469365757	0.8150561114	-2.1616543855
O	0	-4.4532935649	0.1218313573	-0.0309368465
C	-1	-3.3821743588	3.4531607476	5.1921402038
H	-1	-3.4114417042	3.1163730636	6.2178685665
H	-1	-4.1944375015	4.1154992887	4.9315448238
H	0	-2.4752851958	4.0709666846	5.1104946913
C	0	-3.3330318879	2.3711044480	4.1165644316
H	0	-3.4782884160	2.8577835343	3.1442114504
H	0	-4.1538975704	1.6533972711	4.2233225716
C	0	-1.9896859494	1.6394859579	4.0903909306
H	0	-1.9673785531	0.8892733973	4.8900856055
H	0	-1.1643638567	2.3325070648	4.2749416912
C	0	-1.7406185888	0.9834757626	2.7461523648
O	0	-0.5982850720	1.1447507215	2.2321892569
O	0	-2.7023501069	0.3221144191	2.2328021425
C	-1	-5.4264639332	8.9982416046	2.4370920317
H	-1	-5.2895529622	8.5477230174	3.4090442416
H	-1	-6.4604882469	9.2517746269	2.2557944679
H	0	-4.8685119934	9.9431320911	2.4375655019
C	0	-4.8715352328	8.0592531116	1.3600957593
H	0	-3.7828846726	7.9937882370	1.4975049607

H	0	-5.0224403249	8.4850346842	0.3593812197
C	0	-5.5030990127	6.6609186681	1.4193558719
H	0	-6.5651786034	6.7285541566	1.1533330993
H	0	-5.4573244947	6.2736182180	2.4465669024
C	0	-4.8421136453	5.6409768698	0.4885534317
H	0	-4.8608302998	6.0053724404	-0.5489888171
H	0	-5.3900906927	4.6936471260	0.5220734043
N	0	-3.4685652195	5.3796389171	0.9175841508
H	0	-2.9575281078	6.1427886347	1.3384214221
C	0	-2.7449280900	4.2938930126	0.5791153522
N	0	-3.2368737795	3.3889284793	-0.2734758086
H	0	-2.7395258056	2.4875099660	-0.3821832375
H	0	-3.9102824621	3.6506443750	-0.9777551697
N	0	-1.5609988087	4.0737974046	1.1505738922
H	0	-1.2132235885	4.6406678867	1.9121723277
H	0	-0.8438935878	3.4817523466	0.6766175401
C	-1	-0.9664442738	-1.6288481342	7.5194669553
H	-1	0.0245840315	-1.2330372607	7.3532976494
H	-1	-1.1424827945	-1.8760671804	8.5559316170
H	0	-1.7098453838	-0.8911781659	7.1996420772
C	0	-1.1327671065	-2.9676886661	6.7727594456
H	0	-2.1063275100	-3.4081997929	7.0286448932
H	0	-0.3764911511	-3.6754859633	7.1368183500
C	0	-1.0389203012	-2.8872832907	5.2846882438
N	0	-0.9947173471	-4.0210187136	4.4817416724
C	0	-1.0432519104	-1.8333188916	4.4134577914
H	0	-1.0430354773	-0.7784786714	4.6083634776
C	0	-0.9819287576	-3.6693361761	3.1889056212
H	0	-0.9546830288	-4.3340562457	2.3412247481
N	0	-1.0242595143	-2.3407897595	3.1299805520
H	0	-1.0353263298	-1.7875389134	2.2271312990
C	-1	3.8190585520	6.0725486238	2.6326123397
H	-1	4.6895105957	6.5758783397	2.2384199635
H	-1	3.3597853872	6.5606426272	3.4795082672
H	0	3.0595497021	6.0338275799	1.8439891293
C	0	4.2203923542	4.6210193323	3.0080015879
H	0	5.1777387279	4.6027644955	3.5399975587
H	0	3.4494593454	4.1877864420	3.6552045913
C	0	4.2734290736	3.7636504871	1.7421389208
O	0	3.1729420498	3.5728490053	1.1714643506
O	0	5.3972725127	3.3355960449	1.3075708431
C	-1	12.0869694440	-2.4779816574	-0.7431934922
H	-1	13.1351204712	-2.2217057459	-0.7890121660
H	-1	11.8537399039	-3.3423967046	-1.3471682440
H	0	11.8795402465	-2.7803374089	0.2932320561
C	0	11.1951675494	-1.2708763705	-1.1123506766
H	0	11.6397756777	-0.7296619901	-1.9602304539
H	0	10.2126980609	-1.6263929523	-1.4439513043
C	0	10.9914770736	-0.3102757552	0.0744345924
H	0	10.2723721291	-0.7646472081	0.7701777013
H	0	11.9347114670	-0.2140903604	0.6306711521
C	0	10.5441119182	1.1136107998	-0.2990985310
H	0	10.4697944223	1.7260319448	0.6100627376
H	0	11.3256096337	1.5755698526	-0.9175419873
C	0	9.2394126200	1.2555085824	-1.0851549392
H	0	9.1125878544	2.2946213802	-1.4017336406
H	0	9.2350808069	0.6283667438	-1.9803627876
N	0	8.0160458264	0.8980542487	-0.2993009494
H	0	7.1782930567	1.3370029818	-0.7467676736
H	0	7.8703171773	-0.1391829501	-0.2625578677

H	0	8.0182640622	1.2859653342	0.6742146308
O	0	1.8474179565	1.9724472761	-3.3954744631
H	0	2.6289306310	2.5081207627	-3.6516677697
O	0	0.4035043517	2.5817214251	0.1116651766
O	0	0.8965894494	3.6010154820	2.8380895322
H	0	0.4621940657	2.7691244181	2.5774255558
H	0	1.6133649415	3.6719351607	2.1653427836
O	0	-2.8349214969	-1.1839154244	-4.1852871738
H	0	-3.5592182126	-1.6212461707	-3.6932929517
H	0	-2.1860595215	-1.8995544040	-4.3496992523
O	0	-4.6432585142	-2.4598143546	-2.2339414663
H	0	-3.8681214236	-2.1008251261	-1.7221724303
H	0	-5.0120398091	-3.1567837658	-1.6623507095
O	0	2.3403661192	4.0089665398	-1.4250436511
H	0	2.7368159037	3.8620016501	-0.5354265141
O	0	5.9552038465	2.5600717779	-1.2092822016
H	0	5.5297737355	2.7747863520	-0.3271702932
H	0	6.4244859185	3.3817765800	-1.4298074566
O	0	4.1875678717	3.5703644480	-3.2853919372
H	0	4.7251554440	2.9493952047	-2.7557498486
O	0	7.5887668852	2.0923298184	2.2054325197
H	0	6.7884069697	2.6415535997	1.9761565174
H	0	7.2522983166	1.4253167323	2.8236147640
O	0	2.5962243915	-0.5327212108	-2.8695615921
H	0	2.9105964984	-0.3002206210	-1.9765542175
H	0	-0.9701852381	-4.9772980568	4.8143976944
H	0	3.5315843482	3.8765750606	-2.5912268325
Cl	0	7.5043251062	-2.1883784749	-0.4245031057
H	0	2.3375600426	0.3918223369	-3.1653446985
O	0	0.0577359779	-1.4399300100	-2.4601049447
H	0	0.4083941184	-0.2737527143	-4.5779869121
O	0	-0.0662692917	0.5714134419	-4.6171203120
H	0	0.9818928888	-1.0705036396	-2.4593273707
H	0	0.6180428561	1.2235448191	-4.2811010412
H	0	-0.0164381076	-2.1324742435	-3.1608563942

L_S'$_{3a}$-fixed
E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.923834 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.358957 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.599076 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.760882 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.686904 au

Mn	0	1.2276938926	2.2009512433	-1.8674230717
Mn	0	-1.0515136183	-2.5041100009	-0.5137569779
Mn	0	-0.0747091025	0.7764670950	0.1534267391
Mn	0	-2.6601225562	-0.4531029208	0.4586379612
O	0	0.2107055676	0.4638406887	-1.5629991966
O	0	-1.9164654588	1.0120938673	-0.2105765974
O	0	-2.4902133639	-1.4071409499	-1.0941050168
O	0	-0.9562611188	-1.1247251508	0.7894025440
Ca	0	-2.0398491636	0.5154400956	-2.6130504465
C	-1	0.5409880620	4.6158132693	-5.4978300476
H	-1	0.6203369418	5.5451288549	-4.9532166012
H	-1	0.7211059720	4.6978961868	-6.5592934761
H	0	1.3218487121	3.9599642335	-5.0909940745
C	0	-0.8213008831	3.9335924609	-5.2784455227
H	0	-0.9633813245	3.1332961250	-6.0144823659
H	0	-1.6495165392	4.6368870048	-5.4483039713
C	0	-1.0427594374	3.2854255166	-3.9033950756
O	0	-2.0023069532	2.4446927465	-3.8319836622

O	0	-0.3017128917	3.5969919850	-2.9366318337
C	-1	-3.0357448567	-6.6078128683	-5.2868207417
H	-1	-2.0817226534	-7.0797144615	-5.4700012324
H	-1	-3.7764134870	-6.7365970428	-6.0622032401
H	0	-3.4558975040	-7.1490171277	-4.4234158248
C	0	-2.7977066926	-5.1607401866	-4.8724036253
H	0	-3.7426210089	-4.6355049333	-4.6898877529
H	0	-2.2782830765	-4.6116267812	-5.6666770571
C	0	-1.9559724005	-5.1446231578	-3.5972784228
H	0	-1.0072998021	-5.6801247414	-3.7460554319
H	0	-2.4689954597	-5.6727246335	-2.7828757005
C	0	-1.6173408586	-3.7613687903	-3.1021746434
O	0	-1.9180826919	-2.7663074116	-3.7786589725
O	0	-0.9952165690	-3.7264281744	-1.9672928803
C	-1	5.0355150413	-4.6844650920	0.9789892571
H	0	5.7295307626	-5.4989424270	1.2147168489
H	0	5.4375235039	-4.1411603178	0.1201550753
C	0	4.9089925143	-3.7631968060	2.1899825041
O	0	4.2679044235	-4.1254026738	3.2015557582
C	0	3.6503710275	-5.3294552604	0.6400148778
H	0	3.4173374288	-6.0468595517	1.4362911364
H	0	3.7438994064	-5.8978089151	-0.2893402838
C	0	2.4867550005	-4.3775340294	0.5128315827
N	0	2.2286362025	-3.4609858358	1.5216766807
H	0	2.7528202682	-3.4311911650	2.3972263896
C	0	1.4848924093	-4.1683415099	-0.4078152677
H	0	1.2854781622	-4.6605841598	-1.3459680429
C	0	1.1735789484	-2.7176445133	1.1959006818
H	0	0.8512474583	-1.8562896530	1.7448860195
N	0	0.6554682237	-3.1310691458	0.0368186383
N	0	5.3787389826	-2.5175770861	2.0367888189
H	0	5.9798049474	-2.3227004569	1.2278103619
C	-1	5.0587874039	-1.4231950488	2.9483918092
H	0	5.9515929679	-0.7913587623	3.0292687135
H	0	4.8548197381	-1.8469529746	3.9342219642
C	0	3.8613606388	-0.5807672652	2.4645940871
H	0	3.7061037870	0.2417172876	3.1743657016
H	0	2.9562050274	-1.1876587417	2.5065333244
C	0	4.0463388071	-0.0264197203	1.0483612899
H	0	4.4964173160	-0.7847845622	0.3958828458
H	0	4.7356554633	0.8260180357	1.0506159713
C	0	2.7934284760	0.4363182461	0.3047330098
O	0	2.9475809094	0.9780971382	-0.7966369460
O	0	1.6472156233	0.1884577419	0.8673130407
C	-1	-5.4496933810	-3.9478307051	2.3219667638
H	0	-5.3006447254	-3.2039053147	3.1112811477
H	0	-5.9470473432	-4.8129133407	2.7776422164
C	0	-4.1037582674	-4.3912282188	1.7367105041
H	0	-4.2532849525	-5.1169752385	0.9319867118
H	0	-3.5123010075	-4.9002891309	2.5081926610
C	0	-3.2375909321	-3.2719069096	1.1738972393
O	0	-3.5824965353	-2.0762671350	1.3816521963
O	0	-2.1728901932	-3.6089921954	0.5500793207
C	0	-6.3749833547	-3.3850289571	1.2460993826
O	0	-6.2071089958	-3.6134185118	0.0403677868
N	0	-7.4328463210	-2.6751428223	1.7030683565
H	0	-7.4651123339	-2.4238056270	2.6819452293
C	-1	-8.4215348684	-2.0725600763	0.8155515637
H	0	-9.3734292004	-2.0012208842	1.3432543442
H	0	-8.5340213170	-2.7231009568	-0.0552684222

```
C    0   -8.0082827312   -0.6487538781    0.3970633341
O    0   -8.4963802004    0.3409840640    0.9448346213
N    0   -7.0791475505   -0.5935286419   -0.5880397626
H    0   -6.6470286310   -1.4481826759   -0.9238222274
C    0   -6.4836105354    0.6485564316   -1.0352984811
H    0   -6.7198178438    0.8421709276   -2.0854515286
H    0   -6.9077668808    1.4559596156   -0.4304456723
C    0   -4.9577864443    0.6615924444   -0.8974536764
O    0   -4.2845258219    1.2044935259   -1.7864442571
O    0   -4.5006329645    0.0987346556    0.1715172728
C   -1   -3.3254035313    3.6338383685    5.1302867786
H   -1   -3.3476292847    3.3300948809    6.1664562170
H   -1   -4.1387871070    4.2885939102    4.8544679115
H    0   -2.4235974092    4.2557342816    5.0261671169
C    0   -3.2625107045    2.5041030849    4.1000165225
H    0   -3.5128836674    2.9221491824    3.1165857888
H    0   -4.0108115483    1.7288602491    4.2983993341
C    0   -1.8656454379    1.8861203049    4.0095611912
H    0   -1.6786408288    1.2428664818    4.8798129394
H    0   -1.0965928420    2.6636298210    4.0321351791
C    0   -1.6599167198    1.0998080407    2.7277747165
O    0   -0.5364643523    1.2153386986    2.1645477214
O    0   -2.6338539561    0.3821285219    2.3140045688
C   -1   -5.3833473503    9.0906525517    2.2138886209
H   -1   -5.2399156604    8.6712905868    3.1987569383
H   -1   -6.4183709443    9.3396504228    2.0320087119
H    0   -4.8288672211   10.0371616871    2.1817994470
C    0   -4.8218145164    8.1147410699    1.1740646665
H    0   -3.7269789446    8.1118252457    1.2716465676
H    0   -5.0339689377    8.4635984018    0.1549161963
C    0   -5.3723119033    6.6946130467    1.3575414605
H    0   -6.4517968661    6.6927792233    1.1611943506
H    0   -5.2390971450    6.3764977863    2.4007279281
C    0   -4.7251902734    5.6503260327    0.4473194124
H    0   -4.8432119369    5.9397144012   -0.6074209021
H    0   -5.2222603987    4.6851987314    0.5884796857
N    0   -3.3099166816    5.4746430541    0.7779974891
H    0   -2.7853802119    6.2965787016    1.0440584907
C    0   -2.5804063372    4.3999275684    0.4078665471
N    0   -3.1341089606    3.4301801609   -0.3219617254
H    0   -2.6793530288    2.5054310744   -0.3626116144
H    0   -3.9498494051    3.5775591428   -0.8952494370
N    0   -1.3137972865    4.2754713893    0.7991977767
H    0   -0.9219668219    4.7713048313    1.5897408095
H    0   -0.6943636809    3.5487550593    0.3839819581
C   -1   -0.8986034279   -1.3743343334    7.6016959663
H   -1    0.0916402751   -0.9853852920    7.4158152527
H   -1   -1.0674183668   -1.5880130745    8.6467838690
H    0   -1.6457308641   -0.6478649818    7.2658836838
C    0   -1.0820502725   -2.7445918219    6.9161862176
H    0   -2.0432079951   -3.1774674707    7.2261665747
H    0   -0.3092666652   -3.4321362151    7.2835352436
C    0   -1.0398250318   -2.7273093518    5.4247915547
N    0   -0.9189366058   -3.8857365928    4.6661771784
C    0   -1.1564852549   -1.7137086206    4.5147879912
H    0   -1.2670147780   -0.6574949880    4.6672157905
C    0   -0.9607304375   -3.5868007283    3.3604574178
H    0   -0.8908728438   -4.2806109754    2.5385383680
N    0   -1.1123798878   -2.2695074648    3.2537578133
H    0   -1.1336531062   -1.7476023872    2.3372198332
```

C	-1	3.8600617365	6.1602196402	2.4364757748
H	-1	4.7282038123	6.6494967379	2.0201196164
H	-1	3.4074730454	6.6757916799	3.2705916280
H	0	3.0951992831	6.1244135914	1.6524252947
C	0	4.2330582685	4.7030264549	2.8117855175
H	0	5.1886640410	4.6605321097	3.3451762908
H	0	3.4525970085	4.2856377910	3.4587320138
C	0	4.2714450886	3.8322168002	1.5499870799
O	0	3.1828618743	3.7150286307	0.9359988283
O	0	5.3748048876	3.3091515818	1.1732522954
C	-1	12.0937508283	-2.5051533902	-0.7232169006
H	-1	13.1418297084	-2.2518927056	-0.7847551524
H	-1	11.8551903625	-3.3881415618	-1.2975127181
H	0	11.8883477348	-2.7687077888	0.3238528621
C	0	11.2130148711	-1.3042311436	-1.1326713640
H	0	11.6544797479	-0.8042187102	-2.0072055866
H	0	10.2221181863	-1.6602838089	-1.4362996076
C	0	11.0407213656	-0.2966252986	0.0183258802
H	0	10.3305541563	-0.7199724271	0.7414927303
H	0	11.9950311696	-0.1870599438	0.5528086520
C	0	10.5937028792	1.1136959081	-0.4011126631
H	0	10.5376727954	1.7610560427	0.4849287022
H	0	11.3631021790	1.5494808239	-1.0527952003
C	0	9.2732852544	1.2226908816	-1.1639034846
H	0	9.1261671459	2.2515192500	-1.5045335236
H	0	9.2578488466	0.5723208175	-2.0422299079
N	0	8.0726466255	0.8711944287	-0.3424521252
H	0	7.2202428854	1.2692460069	-0.7996750056
H	0	7.9553447465	-0.1654504914	-0.2457521844
H	0	8.0767352397	1.3108895191	0.6083185903
O	0	1.8885494081	1.6515656381	-3.5519973938
H	0	2.7315998522	2.1303870713	-3.7083862007
O	0	0.4267224526	2.4155104566	-0.1146145922
O	0	0.9355995766	3.7082611288	2.5957575474
H	0	0.5366412662	2.8507133947	2.3610064933
H	0	1.6628219286	3.7891703682	1.9339588515
O	0	-3.7645289944	-0.4616482450	-4.0644333979
H	0	-4.2041969230	-1.2053851211	-3.6085010247
H	0	-3.3803930808	-0.8363883870	-4.8950647163
O	0	-4.8199672356	-2.3196856186	-2.0699484800
H	0	-3.9675317358	-2.0332361144	-1.6518542815
H	0	-5.2058885173	-2.9458153385	-1.4290497199
O	0	2.3136312489	3.7197304898	-1.7014537398
H	0	2.6937994068	3.6495289214	-0.7961949514
O	0	6.0067056043	2.4696130207	-1.2966654653
H	0	5.5752712166	2.7253750467	-0.4283169544
H	0	6.4504846211	3.2879979194	-1.5740703084
O	0	4.2489047734	3.2541847018	-3.4478707486
H	0	4.7923749749	2.6963478516	-2.8575837602
O	0	7.6240247499	2.1840242001	2.1036573330
H	0	6.8037756089	2.6952301033	1.8602227390
H	0	7.3133932358	1.5270534206	2.7457045390
O	0	1.8736118233	-0.9419962596	-3.1486797454
H	0	1.4254428472	-0.7459837297	-2.2959072596
H	0	-0.8098504233	-4.8222182088	5.0363361529
H	0	3.5535807694	3.5787457499	-2.8013280875
Cl	0	7.6534539058	-2.2375617469	-0.2119466445
H	0	2.1171564342	0.0052992481	-3.3848052181
O	0	-0.5745291646	-0.5480508516	-4.2378318033
H	0	-2.2550567335	-2.2780813123	-5.6379699368

```
O    0   -2.3462291643   -1.4815648330   -6.1970373374
H    0    0.3801134479   -0.5771111373   -3.9464380576
H    0   -1.5887464289   -0.9415426779   -5.8869979568
H    0   -0.9029900124   -1.4476427322   -3.9996604624
```

L_S'₃ₐ
E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.948304 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.382585 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.62515 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.785426 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.710891 au

```
Mn   0    1.1895234586    2.1383802805   -1.8726801409
Mn   0   -0.9644695573   -2.3531490173   -0.7189831381
Mn   0   -0.1238992331    0.7601466913    0.1735073343
Mn   0   -2.6876879632   -0.5104830459    0.4384901924
O    0    0.1528932744    0.4034447473   -1.5386287261
O    0   -1.9645309512    0.9899028206   -0.1850342403
O    0   -2.4895330016   -1.3826766300   -1.1771125931
O    0   -0.9511471339   -1.1419894282    0.7311759379
Ca   0   -2.0940664057    0.5937882281   -2.6229621866
C   -1    0.5472649505    4.5368639876   -5.5813020197
H   -1    0.6276269520    5.4713769874   -5.0458070197
H   -1    0.7249039506    4.6088109873   -6.6439180197
H    0    1.3241567299    3.8811178643   -5.1669465428
C    0   -0.8212228041    3.8714789846   -5.3533137273
H    0   -0.9548418601    3.0395351915   -6.0556205453
H    0   -1.6425778035    4.5692898976   -5.5712538845
C    0   -1.0803077478    3.2807399392   -3.9585083202
O    0   -2.0917222154    2.5021248604   -3.8698718167
O    0   -0.3235747945    3.5643106416   -2.9954992262
C   -1   -3.0259830672   -6.6850960068   -5.2544260197
H   -1   -2.0722610680   -7.1584990083   -5.4352840197
H   -1   -3.7684090674   -6.8214880056   -6.0268210197
H    0   -3.4410584321   -7.2013865031   -4.3741606787
C    0   -2.7982246960   -5.2209319123   -4.8958659927
H    0   -3.7479897942   -4.7089796001   -4.7016778770
H    0   -2.3200827244   -4.6895659551   -5.7277118961
C    0   -1.9152171104   -5.1254522952   -3.6534839945
H    0   -0.9566835774   -5.6412629682   -3.8054769375
H    0   -2.3862897882   -5.6222822129   -2.7946576102
C    0   -1.6070705663   -3.7079935017   -3.2440443167
O    0   -2.0174895505   -2.7568008310   -3.9247987634
O    0   -0.8857846295   -3.5894220316   -2.1713363267
C   -1    5.0592439359   -4.6998000196    0.9739439803
H    0    5.7939310301   -5.4798998902    1.2064034772
H    0    5.4255751637   -4.1531348601    0.1011721388
C    0    4.9316634852   -3.7669582848    2.1765486597
O    0    4.3138097507   -4.1264400775    3.2030035202
C    0    3.7024108823   -5.3980576316    0.6629133885
H    0    3.4796296063   -6.0892002884    1.4846641190
H    0    3.8094562867   -5.9950670365   -0.2467001625
C    0    2.5497265189   -4.4492120830    0.4994264091
N    0    2.2445731362   -3.5649795764    1.5241386408
H    0    2.7332022540   -3.5593400876    2.4205283503
C    0    1.6457797303   -4.1581094670   -0.4958541245
H    0    1.5076972309   -4.6050154720   -1.4676391686
C    0    1.2564999174   -2.7591327207    1.1342775118
H    0    0.9195202624   -1.9035691019    1.6822952159
N    0    0.8392244537   -3.1023165271   -0.0799157391
N    0    5.3928746450   -2.5203422699    2.0043555389
```

H	0	5.9828313422	-2.3315610352	1.1862548784
C	-1	5.0862059411	-1.4197940196	2.9119339803
H	0	5.9693606253	-0.7708173573	2.9529876440
H	0	4.9229361354	-1.8331205059	3.9098670558
C	0	3.8566037457	-0.6074357980	2.4579344585
H	0	3.6924621285	0.2086194919	3.1730681594
H	0	2.9710827825	-1.2423908996	2.5146307217
C	0	4.0075016111	-0.0456253362	1.0413471442
H	0	4.4562106624	-0.7962408196	0.3790261922
H	0	4.6880708696	0.8142960115	1.0353343403
C	0	2.7432321827	0.4087203233	0.3146625730
O	0	2.8840523553	0.9178675718	-0.8049548429
O	0	1.6039874879	0.1935309400	0.9031142112
C	-1	-5.4230240629	-3.9528820030	2.3340849803
H	0	-5.2382883117	-3.1840920337	3.0915899846
H	0	-5.9402049225	-4.7832606144	2.8310426025
C	0	-4.1069646783	-4.4521050367	1.7401622119
H	0	-4.2927059515	-5.2016354949	0.9656830135
H	0	-3.5158018509	-4.9501123439	2.5184971009
C	0	-3.2211302054	-3.3758574748	1.1158378266
O	0	-3.5527800840	-2.1613241457	1.2979572398
O	0	-2.1893919135	-3.7693930716	0.4992470084
C	0	-6.3509044821	-3.3977314257	1.2555120399
O	0	-6.1896145851	-3.6364271564	0.0508300023
N	0	-7.4071277900	-2.6822953174	1.7088228209
H	0	-7.4396877730	-2.4241475440	2.6859030275
C	-1	-8.3988430600	-2.0928639983	0.8166509803
H	0	-9.3533090016	-2.0302216090	1.3414065407
H	0	-8.5025036552	-2.7481104044	-0.0515227374
C	0	-7.9980382314	-0.6689600980	0.3976391486
O	0	-8.4641682362	0.3183327948	0.9682080818
N	0	-7.1016173341	-0.6100789178	-0.6172399118
H	0	-6.6708490792	-1.4639025346	-0.9568916332
C	0	-6.5008912335	0.6316568054	-1.0528340706
H	0	-6.7273866237	0.8323139006	-2.1036916002
H	0	-6.9273731975	1.4374531392	-0.4473741693
C	0	-4.9777844583	0.6416493824	-0.9030822921
O	0	-4.3044287725	1.2287519153	-1.7632076464
O	0	-4.5246367943	0.0274965820	0.1397368628
C	-1	-3.2942590509	3.6558789937	5.0646689803
H	-1	-3.3140060513	3.3620769937	6.1037509803
H	-1	-4.1084530498	4.3077619949	4.7844709803
H	0	-2.3823084158	4.2590188782	4.9437906682
C	0	-3.2731166401	2.5279778826	4.0308324092
H	0	-3.3576459389	2.9889688741	3.0378066625
H	0	-4.1431440951	1.8700304679	4.1334480127
C	0	-1.9849679336	1.6957840751	4.0748617931
H	0	-2.0591361791	0.9585000700	4.8830106535
H	0	-1.1171677409	2.3299859271	4.2766828301
C	0	-1.7407710488	0.9921389738	2.7522087843
O	0	-0.6240445239	1.1773041242	2.1934760659
O	0	-2.6919128126	0.2642507848	2.3010775135
C	-1	-5.3603990423	9.0839809969	2.1008699803
H	-1	-5.2145770429	8.6741149967	3.0893789803
H	-1	-6.3959070419	9.3309719986	1.9190099803
H	0	-4.8051908772	10.0296350369	2.0571796697
C	0	-4.8126292869	8.0981865044	1.0677819340
H	0	-3.7180144882	8.0825195965	1.1643661385
H	0	-5.0213084060	8.4422795040	0.0463732044
C	0	-5.3856256677	6.6901481538	1.2660174740

H	0	-6.4615112794	6.6981419434	1.0515889068
H	0	-5.2728479555	6.3883004654	2.3163797714
C	0	-4.7313764159	5.6274734183	0.3866282507
H	0	-4.8404302314	5.8902743661	-0.6759781171
H	0	-5.2249990254	4.6638019741	0.5475252410
N	0	-3.3191364447	5.4703275521	0.7362343708
H	0	-2.8009460866	6.3025054101	0.9813789106
C	0	-2.5838410514	4.3914725637	0.3963369739
N	0	-3.1336189394	3.4045167300	-0.3106524991
H	0	-2.6888053497	2.4732454113	-0.3151695942
H	0	-3.9483951096	3.5357839301	-0.8890723352
N	0	-1.3177550543	4.2804086921	0.7938972205
H	0	-0.9345467067	4.7891002691	1.5798786672
H	0	-0.6987516207	3.5474547589	0.3890189061
C	-1	-0.8604130587	-1.3277790102	7.5783439803
H	-1	0.1292939419	-0.9403880118	7.3864499803
H	-1	-1.0267520591	-1.5314700099	8.6258209803
H	0	-1.6076707578	-0.6057432710	7.2327621984
C	0	-1.0332053712	-2.7011097175	6.8948176673
H	0	-1.9996762368	-3.1322951392	7.1898546963
H	0	-0.2676750588	-3.3885731219	7.2783972994
C	0	-0.9726723187	-2.6996234475	5.4017621057
N	0	-1.0336663444	-3.8741021871	4.6587842621
C	0	-0.9238517659	-1.6943717306	4.4760543877
H	0	-0.8299887730	-0.6339716381	4.6133053560
C	0	-1.0331618899	-3.5920508670	3.3487264193
H	0	-1.0747132964	-4.2963712824	2.5332806886
N	0	-0.9809590320	-2.2696366525	3.2218984407
H	0	-1.0087057149	-1.7694204848	2.2956713654
C	-1	3.8842799531	6.1580719823	2.3301239803
H	-1	4.7513259539	6.6435469809	1.9070869803
H	-1	3.4334859539	6.6815059830	3.1603059803
H	0	3.1166393213	6.1132551514	1.5486577298
C	0	4.2540470584	4.7053383120	2.7298564892
H	0	5.2169067537	4.6700913796	3.2506351712
H	0	3.4812257833	4.3082772416	3.3984101478
C	0	4.2698570354	3.8012438204	1.4915075159
O	0	3.1667666175	3.6462990609	0.9123780147
O	0	5.3720685131	3.2877551423	1.0978373483
C	-1	12.1129409393	-2.5351850307	-0.7654220197
H	-1	13.1608069397	-2.2822700324	-0.8318130197
H	-1	11.8732869379	-3.4236960303	-1.3306730197
H	0	11.9099762472	-2.7885905811	0.2846383941
C	0	11.2292504855	-1.3395459641	-1.1852716194
H	0	11.6687377469	-0.8470602440	-2.0650534653
H	0	10.2388543249	-1.7007819266	-1.4845744895
C	0	11.0550857293	-0.3208062657	-0.0442946629
H	0	10.3475530143	-0.7390904429	0.6843731076
H	0	12.0099029531	-0.2025813703	0.4874516421
C	0	10.6031203629	1.0841285857	-0.4770405668
H	0	10.5518005303	1.7412900059	0.4020546027
H	0	11.3682714076	1.5134975274	-1.1379180217
C	0	9.2779168922	1.1843918227	-1.2331711196
H	0	9.1303580879	2.2086323682	-1.5872193909
H	0	9.2559562087	0.5216510501	-2.1020965862
N	0	8.0818323066	0.8461444829	-0.3994585047
H	0	7.2255701610	1.2363043697	-0.8562566566
H	0	7.9649451484	-0.1894431875	-0.2890310928
H	0	8.0917099243	1.2993573081	0.5447471077
O	0	1.8376094907	1.5720864583	-3.5522140868

H	0	2.6815621421	2.0456335196	-3.7223125874
O	0	0.3776551438	2.3919066990	-0.1283110741
O	0	0.9279670878	3.6542939154	2.6030612645
H	0	0.4903119936	2.8122879661	2.3850095368
H	0	1.6471131262	3.7047903733	1.9303034720
O	0	-3.8126018855	-0.4189247260	-4.0544498529
H	0	-4.2219246498	-1.1901494507	-3.6177432092
H	0	-3.4398207386	-0.7532817181	-4.9072535700
O	0	-4.8233475301	-2.3724238730	-2.0902401947
H	0	-3.9661527867	-2.0767462963	-1.6955992486
H	0	-5.2067225047	-2.9639425934	-1.4149394367
O	0	2.2827219266	3.6517223216	-1.7277418383
H	0	2.6674064378	3.5856860295	-0.8235350422
O	0	5.9886809983	2.4121803789	-1.3582389060
H	0	5.5628694822	2.6816752215	-0.4908653112
H	0	6.4175925436	3.2301798926	-1.6592667497
O	0	4.1969780863	3.1590945024	-3.4925209262
H	0	4.7485062841	2.6059718641	-2.9051498857
O	0	7.6421960046	2.1984825627	2.0276825886
H	0	6.8170336472	2.6993081437	1.7799220261
H	0	7.3396419110	1.5515363895	2.6836809546
O	0	1.7795389890	-1.0173981862	-3.2019139633
H	0	1.3740141359	-0.8469255503	-2.3254783219
H	0	-1.0686174768	-4.8103766216	5.0433957695
H	0	3.5142840075	3.4960745732	-2.8395217153
Cl	0	7.6619775285	-2.2585565283	-0.2551794080
H	0	2.0304076083	-0.0656245416	-3.4191477412
O	0	-0.6739099532	-0.5110496615	-4.2386263021
H	0	-2.3400287338	-2.1647829636	-5.7959782676
O	0	-2.4282355482	-1.3147032036	-6.2681451352
H	0	0.2789024330	-0.5981207050	-3.9528833405
H	0	-1.6621149796	-0.8141297179	-5.9156154562
H	0	-1.0477508379	-1.4065207611	-4.0477026087

L_S'₃c-fixed

E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.912665 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.347974 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.58755 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.744786 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.672319 au

Mn	0	1.1897694878	2.4493035269	-1.6042638214
Mn	0	-1.0797709892	-2.4782111693	-0.6462118333
Mn	0	-0.1555281169	0.8795177781	0.2084478806
Mn	0	-2.7210507624	-0.4515792473	0.3375106583
O	0	0.2899527285	0.8056007169	-1.4919106365
O	0	-1.9469178333	1.0340061548	-0.3015129259
O	0	-2.5785682561	-1.4306242673	-1.1621273527
O	0	-0.9842842852	-1.0882459709	0.6456401022
Ca	0	-1.7446174798	0.2888431102	-2.6830367935
C	-1	0.5904944450	4.5770902425	-5.5780149350
H	-1	0.6675937236	5.5055396031	-5.0316027209
H	-1	0.7863244976	4.6588149513	-6.6367198678
H	0	1.3963388644	3.9456717726	-5.1807124701
C	0	-0.7433506189	3.8591413073	-5.2956562672
H	0	-0.8885541167	3.0301621738	-5.9992706778
H	0	-1.6019197339	4.5278595857	-5.4480413088
C	0	-0.8762175173	3.2432834239	-3.8871731156
O	0	-1.8325894892	2.4385708003	-3.6917517899
O	0	-0.0159328135	3.5705923731	-3.0144019290
C	-1	-3.0562238317	-6.6249611593	-5.4270150476

H	-1	-2.1025212249	-7.1024666717	-5.5968464833
H	-1	-3.7864433463	-6.7487573072	-6.2130477915
H	0	-3.4974539818	-7.2184506535	-4.6063351937
C	0	-2.8500600232	-5.2180192150	-4.9080685115
H	0	-3.7998186867	-4.6763612745	-4.8131789190
H	0	-2.2106279789	-4.6360861255	-5.5767881162
C	0	-2.1880063526	-5.3369430530	-3.5339801181
H	0	-1.4401557093	-6.1450140988	-3.5528653378
H	0	-2.9120497787	-5.6084362957	-2.7586335758
C	0	-1.4409723873	-4.0977958542	-3.1242011255
O	0	-0.9700689955	-3.3641684839	-4.0206481544
O	0	-1.3199272677	-3.9245781204	-1.8546593933
C	-1	4.9356395972	-4.7544812079	0.9554844750
H	0	5.6286606210	-5.5674165817	1.1986065687
H	0	5.3330104023	-4.2200628510	0.0890400390
C	0	4.8097843809	-3.8257413733	2.1567606594
O	0	4.2013572552	-4.1936469363	3.1837327721
C	0	3.5453474063	-5.3983736276	0.6288514979
H	0	3.3068676743	-6.0938715709	1.4428927219
H	0	3.6355430733	-5.9903952481	-0.2860633211
C	0	2.3937975291	-4.4348189972	0.4746186329
N	0	2.1812338172	-3.4534399601	1.4297741341
H	0	2.6943092245	-3.3976609714	2.3061623166
C	0	1.3725231258	-4.2553422525	-0.4340099219
H	0	1.1449000760	-4.7951160948	-1.3392652391
C	0	1.1308484731	-2.7077268417	1.0814699239
H	0	0.8484364026	-1.8019849466	1.5796179984
N	0	0.5761189258	-3.1791726451	-0.0324673436
N	0	5.2326306340	-2.5638550021	1.9768074521
H	0	5.8134553618	-2.3617406164	1.1564623933
C	-1	4.9502123634	-1.4947590734	2.9275306034
H	0	5.8559999410	-0.8800448895	3.0098501625
H	0	4.7697633232	-1.9530787200	3.9024928866
C	0	3.7648474093	-0.6058408374	2.5244447503
H	0	3.6236527172	0.1570850925	3.3005112582
H	0	2.8478827511	-1.1959516862	2.5146617021
C	0	3.9722756904	0.0588890796	1.1653246622
H	0	4.4118593290	-0.6538752617	0.4552569983
H	0	4.6778744619	0.8945500230	1.2347491438
C	0	2.7336589707	0.5910228123	0.4611813213
O	0	2.9180685070	1.1861486235	-0.6199724111
O	0	1.5841780450	0.3231275095	0.9808747623
C	-1	-5.5631597504	-3.9557143051	2.1483859499
H	0	-5.4555277673	-3.2287785476	2.9597354254
H	0	-6.0402155534	-4.8501422378	2.5676645892
C	0	-4.1829999753	-4.3466638820	1.5823921062
H	0	-4.3024846530	-5.0487864116	0.7512546633
H	0	-3.6071189865	-4.8762833178	2.3514897760
C	0	-3.3052270823	-3.2024491808	1.0690913788
O	0	-3.7048870947	-2.0153187614	1.2537803381
O	0	-2.2002023953	-3.4905564549	0.5069524016
C	0	-6.4787001680	-3.4039693743	1.0604219998
O	0	-6.3277188776	-3.6804347010	-0.1375121484
N	0	-7.5115406655	-2.6452328538	1.4988899693
H	0	-7.5207173283	-2.3478283744	2.4650109383
C	-1	-8.5017520669	-2.0615726512	0.6009127050
H	0	-9.4248636640	-1.8901681350	1.1551457640
H	0	-8.6869659456	-2.7737015396	-0.2080938897
C	0	-8.0431349320	-0.7003753318	0.0281497442
O	0	-8.5700385416	0.3501972485	0.3994111289

N	0	-7.0454654276	-0.7704629952	-0.8868974493
H	0	-6.6165286847	-1.6663345449	-1.0984426662
C	0	-6.4334762034	0.4016364451	-1.4843071263
H	0	-6.6142119673	0.4280042557	-2.5627166476
H	0	-6.9000683034	1.2820737596	-1.0317984749
C	0	-4.9137190757	0.4680161775	-1.2672464033
O	0	-4.1839946367	0.8185002081	-2.2085748771
O	0	-4.5280066979	0.1580617320	-0.0723475453
C	-1	-3.4339280110	3.6111181249	4.9927483090
H	-1	-3.4728525209	3.3068049738	6.0282583089
H	-1	-4.2393216583	4.2709425123	4.7057877668
H	0	-2.5155637507	4.2078742174	4.8896900784
C	0	-3.4048861314	2.4826399348	3.9720777317
H	0	-3.4804303265	2.9296750777	2.9741398928
H	0	-4.2712119055	1.8201703791	4.0745794863
C	0	-2.1098245360	1.6692639744	4.0466095573
H	0	-2.1983461052	0.9157891695	4.8378056530
H	0	-1.2557597713	2.3081845012	4.2875652953
C	0	-1.8364163646	1.0049097471	2.7159803762
O	0	-0.6865975229	1.1579815491	2.2129968116
O	0	-2.7959866078	0.3506897760	2.1960605593
C	-1	-5.4169835810	9.0822055516	2.0513158450
H	-1	-5.2902285264	8.6613145645	3.0378187665
H	-1	-6.4477747061	9.3375476978	1.8547901367
H	0	-4.8413076709	10.0148798486	2.0118191816
C	0	-4.8899864862	8.0787482828	1.0195996360
H	0	-3.8058118975	7.9735349109	1.1658331075
H	0	-5.0170073347	8.4624534578	-0.0009829883
C	0	-5.5857672143	6.7139356864	1.1414129589
H	0	-6.6265326011	6.8022569393	0.8079261664
H	0	-5.6178136983	6.4029909859	2.1949332934
C	0	-4.9143003592	5.6018731064	0.3343219447
H	0	-4.8345523815	5.8958602575	-0.7225636465
H	0	-5.5140757208	4.6863943141	0.3875369475
N	0	-3.5913616001	5.3167302555	0.8908124826
H	0	-3.1263427832	6.0672563463	1.3822469140
C	0	-2.8112953952	4.2804632573	0.5204130470
N	0	-3.2163343814	3.4189265949	-0.4127412604
H	0	-2.7441238972	2.4991563689	-0.4931150336
H	0	-4.0147577175	3.6061361913	-0.9981841303
N	0	-1.6396438094	4.0790709313	1.1265981714
H	0	-1.3300797520	4.6485032836	1.9015414020
H	0	-0.9061919189	3.4905893453	0.6772681596
C	-1	-1.0729776240	-1.4132500958	7.4948786105
H	-1	-0.0778499883	-1.0301371775	7.3235304996
H	-1	-1.2580613202	-1.6266246599	8.5372712543
H	0	-1.8088962730	-0.6815722919	7.1453727042
C	0	-1.2374338982	-2.7723357976	6.7859011691
H	0	-2.2177508862	-3.1992020080	7.0387600204
H	0	-0.4914810042	-3.4742385184	7.1815486460
C	0	-1.1216820725	-2.7340630562	5.2975460781
N	0	-1.1335124846	-3.8887417990	4.5237295940
C	0	-1.0577250098	-1.7040411430	4.4002513326
H	0	-0.9859234595	-0.6468438757	4.5692316768
C	0	-1.0913458157	-3.5712176334	3.2226598267
H	0	-1.0911281610	-4.2567039001	2.3912012808
N	0	-1.0613753058	-2.2445628226	3.1296980467
H	0	-1.0646435719	-1.7163971473	2.2104743411
C	-1	3.8045148195	6.0960772285	2.4043031204
H	-1	4.6814678458	6.5804088348	2.0008288596

H	-1	3.3431002307	6.6137914426	3.2322331521
H	0	3.0518795614	6.0087079789	1.6142437801
C	0	4.2069576441	4.6747884087	2.8839504165
H	0	5.1582659608	4.6991502035	3.4260032460
H	0	3.4306332663	4.2859831870	3.5526089387
C	0	4.2737753776	3.7340263416	1.6861674660
O	0	3.1808307108	3.5077890251	1.1148174067
O	0	5.4040493990	3.2754528497	1.2998717767
C	-1	12.0305466985	-2.6164984572	-0.6435523138
H	-1	13.0809024943	-2.3695045246	-0.6898448042
H	-1	11.7949587228	-3.4976424909	-1.2218926371
H	0	11.8170224278	-2.8890376735	0.4000637334
C	0	11.1529046072	-1.4106108235	-1.0429603383
H	0	11.5979334393	-0.8984565826	-1.9084788709
H	0	10.1629553444	-1.7621995589	-1.3557132742
C	0	10.9751708341	-0.4182790272	0.1211611509
H	0	10.2656045950	-0.8508427846	0.8401720649
H	0	11.9279677857	-0.3142426388	0.6593563317
C	0	10.5289773234	0.9975890701	-0.2803648540
H	0	10.4632658163	1.6306060147	0.6152507255
H	0	11.3049713889	1.4442012619	-0.9166657675
C	0	9.2178916962	1.1206623120	-1.0573424653
H	0	9.0797670438	2.1551053080	-1.3842506350
H	0	9.2112858856	0.4835933116	-1.9453953209
N	0	8.0045668256	0.7602450640	-0.2572145395
H	0	7.1638009663	1.1880323539	-0.7038039875
H	0	7.8656187758	-0.2786997666	-0.2085198265
H	0	8.0094428034	1.1594459413	0.7112130309
O	0	2.1184474873	1.6452745623	-3.3627171326
H	0	2.9807132919	2.1546624541	-3.4675601394
O	0	0.3206100901	2.5714838516	0.0965199956
O	0	0.8828333983	3.5780449445	2.7962958181
H	0	0.4288314248	2.7535642157	2.5459960847
H	0	1.5891364462	3.6346574676	2.1137239411
O	0	-2.8962066091	-1.3033531477	-4.2030598994
H	0	-3.6187420723	-1.7436014506	-3.7099946045
H	0	-2.2249834422	-2.0094728465	-4.3255714305
O	0	-4.7522239701	-2.4540275692	-2.2404307687
H	0	-3.9742168233	-2.1013659906	-1.7266908126
H	0	-5.0971414784	-3.1780160653	-1.6882002612
O	0	2.2926294486	3.9549791958	-1.4473975429
H	0	2.7068394184	3.8287916844	-0.5619165661
O	0	5.9941366879	2.4889779715	-1.1629508263
H	0	5.5731357066	2.7124739003	-0.2753346005
H	0	6.5294472338	3.2774272108	-1.3539080794
O	0	4.1904469843	3.2699143672	-3.1850087724
H	0	4.7855946850	2.8068358990	-2.5539923078
O	0	7.5724265655	1.9919227764	2.2302207908
H	0	6.7830446003	2.5515714296	1.9970184848
H	0	7.2304048323	1.3437916893	2.8652222350
O	0	2.4908542793	-0.8937086468	-2.4951140282
H	0	2.6967464906	-0.4012556860	-1.6814113472
H	0	-1.1629879949	-4.8358605285	4.8810840523
H	0	3.5305888699	3.6945021287	-2.5574113319
Cl	0	7.4896918949	-2.3166082348	-0.3343215187
H	0	2.3472260822	0.6945160837	-3.1271917638
O	0	-0.0508363270	-1.4942612237	-2.4132738245
H	0	0.2521344524	-0.5152226339	-3.8250317022
O	0	-0.0002087761	0.1642984508	-4.5077873414
H	0	1.5061775305	-1.1373803545	-2.3758576789

H	0	0.6444685879	0.8852847077	-4.3596865542
H	0	-0.1641736083	-2.2412708877	-3.0311111229

L_S'₃c

E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.950814 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.385055 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.625313 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.782473 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.708896 au

Mn	0	1.1305453219	2.5283310286	-1.5726448972
Mn	0	-0.8888385323	-2.1360469311	-0.9568999589
Mn	0	-0.2483696622	1.0077005549	0.2529377102
Mn	0	-2.7295150828	-0.4420995452	0.3429176689
O	0	0.1808013348	0.8985180623	-1.4611751755
O	0	-2.0429406951	1.1344554813	-0.2266540410
O	0	-2.5219011082	-1.2932849273	-1.2468995097
O	0	-0.9533002978	-0.9433346556	0.6240794157
Ca	0	-1.8689176659	0.5897129513	-2.6923532765
C	-1	0.5763740361	4.3873610127	-5.7878860231
H	-1	0.6533720400	5.3342730124	-5.2741180231
H	-1	0.7689720363	4.4327800119	-6.8493600231
H	0	1.3793654317	3.7690256776	-5.3650806155
C	0	-0.7635676503	3.7264493705	-5.4217147882
H	0	-0.8909925274	2.7763703433	-5.9550707477
H	0	-1.6181764182	4.3503884328	-5.7152114647
C	0	-0.9340484387	3.3744152818	-3.9268022748
O	0	-1.9948920466	2.7570358721	-3.6004992046
O	0	-0.0075592457	3.6773467224	-3.1173556841
C	-1	-3.0494840089	-6.8090309727	-5.2390060231
H	-1	-2.0954120108	-7.2904809765	-5.3950670231
H	-1	-3.7817620095	-6.9611769698	-6.0181170231
H	0	-3.4791570190	-7.3267622016	-4.3654977728
C	0	-2.8067422596	-5.3640514733	-4.8655672457
H	0	-3.7435057374	-4.8426103615	-4.6292665647
H	0	-2.3291056524	-4.8117590300	-5.6804084457
C	0	-1.8962136803	-5.3602230149	-3.6433778098
H	0	-0.9780206357	-5.9281294387	-3.8586757677
H	0	-2.3727928049	-5.8489253036	-2.7872556337
C	0	-1.4734046277	-3.9756107868	-3.2495362554
O	0	-1.3583169208	-3.1101884201	-4.1543842675
O	0	-1.2348167175	-3.8104389303	-2.0028301632
C	-1	4.9575039996	-4.7053240049	1.0512589769
H	0	5.6411060430	-5.5085677817	1.3496631934
H	0	5.3900082720	-4.2039216364	0.1817094404
C	0	4.8027415763	-3.7325754924	2.2136827688
O	0	4.1749615730	-4.0604449929	3.2425983665
C	0	3.5840394800	-5.3503764036	0.6909846037
H	0	3.2923558379	-6.0096879640	1.5174397265
H	0	3.7049287025	-5.9750841113	-0.1981388690
C	0	2.4851245415	-4.3542351221	0.4508702224
N	0	2.1801708999	-3.4242377332	1.4334911650
H	0	2.6159824916	-3.4136117842	2.3541517376
C	0	1.6343872864	-4.0542816624	-0.5893096477
H	0	1.5176136006	-4.5323945576	-1.5494071576
C	0	1.2420829573	-2.5898630146	0.9763504635
H	0	0.9177812806	-1.7036674853	1.4833767821
N	0	0.8593836984	-2.9535451976	-0.2411974330
N	0	5.2452281085	-2.4834609710	1.9977951038
H	0	5.8324102600	-2.3145742681	1.1746932095
C	-1	4.9718800129	-1.3793670050	2.9094229769

H	0	5.8688721392	-0.7474841594	2.9358573431
H	0	4.8244799225	-1.7945323639	3.9090439954
C	0	3.7551567725	-0.5273542888	2.5025633744
H	0	3.6246062779	0.2730406358	3.2415700932
H	0	2.8506139222	-1.1353139225	2.5566374499
C	0	3.9039115606	0.0750280512	1.1059716929
H	0	4.2878589629	-0.6785193077	0.4054274160
H	0	4.6347426225	0.8920527922	1.1061953683
C	0	2.6519860586	0.6298164800	0.4389562425
O	0	2.8115869112	1.1643024511	-0.6799451045
O	0	1.5168826773	0.4595160633	1.0226261666
C	-1	-5.5392159971	-3.8838549627	2.2470399769
H	0	-5.4075245578	-3.1145697175	3.0152494564
H	0	-6.0402342947	-4.7375903626	2.7208202131
C	0	-4.1819665385	-4.3351776577	1.6944298585
H	0	-4.3269236016	-5.0860363910	0.9118229117
H	0	-3.6101283167	-4.8280950875	2.4904854758
C	0	-3.2686334832	-3.2550046762	1.0950660408
O	0	-3.6611265183	-2.0380773865	1.1824331874
O	0	-2.1831105181	-3.6275042513	0.5968398327
C	0	-6.4541011805	-3.3610032910	1.1431057281
O	0	-6.3008612585	-3.6597067403	-0.0497913098
N	0	-7.4941970484	-2.6002396733	1.5600488082
H	0	-7.5163795579	-2.2887364360	2.5215034188
C	-1	-8.4857449897	-2.0493879508	0.6437709769
H	0	-9.4222873921	-1.9025081462	1.1831345855
H	0	-8.6384051431	-2.7718568223	-0.1625106596
C	0	-8.0555186210	-0.6828339860	0.0754274629
O	0	-8.5714958870	0.3632062845	0.4725219912
N	0	-7.0870505429	-0.7438833054	-0.8705512701
H	0	-6.6512542686	-1.6346249629	-1.0845021260
C	0	-6.4800292323	0.4342667227	-1.4523669978
H	0	-6.6548819775	0.4730169025	-2.5315931724
H	0	-6.9526856898	1.3092216072	-0.9949937379
C	0	-4.9648349944	0.5116262660	-1.2270337872
O	0	-4.2548350886	0.9652900070	-2.1436032492
O	0	-4.5631687054	0.1155830703	-0.0689730310
C	-1	-3.4154969663	3.7804190288	4.8218599769
H	-1	-3.4508529674	3.5120130289	5.8673789769
H	-1	-4.2229229637	4.4285450320	4.5146629769
H	0	-2.4856328182	4.3487355837	4.6809042670
C	0	-3.4354809603	2.6036973222	3.8562293581
H	0	-3.3785187574	3.0072103984	2.8366662494
H	0	-4.3836225404	2.0576293449	3.9107026075
C	0	-2.2689597597	1.6265672193	4.0759047665
H	0	-2.5563381669	0.8582521305	4.8013204319
H	0	-1.3816622419	2.1482509046	4.4461452043
C	0	-1.9368341717	0.9992296093	2.7452628089
O	0	-0.8074621413	1.2609161397	2.2388396795
O	0	-2.8466192202	0.2847788080	2.2137033912
C	-1	-5.4170659447	9.1431510368	1.6990149769
H	-1	-5.2866739463	8.7568280363	2.6990929769
H	-1	-6.4488879437	9.3897750410	1.4968469769
H	0	-4.8688923848	10.0946337427	1.6689591316
C	0	-4.8408576616	8.2005022623	0.6352713492
H	0	-3.7604312931	8.1039110157	0.8106087103
H	0	-4.9539949596	8.6630679607	-0.3557813869
C	0	-5.4837287113	6.8076849645	0.6145749228
H	0	-6.5737616098	6.9059707986	0.5219273721
H	0	-5.2882194481	6.2899481666	1.5633131395

C	0	-4.9982914643	5.9282142216	-0.5496204474
H	0	-5.2658380606	6.3871682418	-1.5085983936
H	0	-5.4835239813	4.9517175425	-0.5064505492
N	0	-3.5467724599	5.7242752016	-0.5216110316
H	0	-2.9784532412	6.5601813136	-0.5131134677
C	0	-2.9046025125	4.5718106913	-0.2417474558
N	0	-3.5226966408	3.3911313309	-0.4084448265
H	0	-2.9661550319	2.5295867204	-0.2499133908
H	0	-4.1718158380	3.3043183548	-1.1800968787
N	0	-1.6656896236	4.6081324987	0.2495539792
H	0	-1.2559269931	5.4961976771	0.5048793068
H	0	-1.0029081151	3.8027834661	0.1678826863
C	-1	-1.0381279861	-1.1503959808	7.4891059769
H	-1	-0.0442029846	-0.7717239848	7.3016629769
H	-1	-1.2197879868	-1.3279309801	8.5387949769
H	0	-1.7736752450	-0.4291993004	7.1177023711
C	0	-1.1950921411	-2.5235091690	6.8078267527
H	0	-2.1820732462	-2.9416839845	7.0485244905
H	0	-0.4601682340	-3.2201965761	7.2328615115
C	0	-1.0504465178	-2.5197873348	5.3195885285
N	0	-1.1322584129	-3.6921933582	4.5755432548
C	0	-0.9003261180	-1.5212621030	4.3965672648
H	0	-0.7473685293	-0.4666653023	4.5349733476
C	0	-1.0546168867	-3.4162810055	3.2672889750
H	0	-1.1169678231	-4.1159511603	2.4490644647
N	0	-0.9288484049	-2.0985345889	3.1394500070
H	0	-0.9416343442	-1.6023644111	2.2097151890
C	-1	3.8108430434	6.1868669997	2.1275819769
H	-1	4.6857350453	6.6584709962	1.7050069769
H	-1	3.3508980456	6.7320950016	2.9384939769
H	0	3.0590571517	6.0349206950	1.3462618108
C	0	4.2657541702	4.8172726573	2.7088845779
H	0	5.1918038471	4.9438178185	3.2802030400
H	0	3.4919347317	4.4278182000	3.3778819262
C	0	4.4555389817	3.8073195169	1.5845894341
O	0	3.4102196550	3.3483127243	1.0651151806
O	0	5.6411857280	3.5257894253	1.1900704538
C	-1	12.0438210080	-2.6116930334	-0.6417870231
H	-1	13.0935860090	-2.3646410376	-0.6997090231
H	-1	11.8081560044	-3.5127040325	-1.1886280231
H	0	11.8338764232	-2.8484833760	0.4112685221
C	0	11.1647112928	-1.4207560768	-1.0785772087
H	0	11.6025313643	-0.9420025596	-1.9666242835
H	0	10.1712265907	-1.7817663304	-1.3689503200
C	0	11.0012589247	-0.3863375506	0.0499419909
H	0	10.3005872714	-0.7915869830	0.7931269083
H	0	11.9603269478	-0.2631751602	0.5726316178
C	0	10.5494495136	1.0132203310	-0.3978265160
H	0	10.4914144732	1.6778267327	0.4750103270
H	0	11.3174682456	1.4379551100	-1.0582832762
C	0	9.2299240978	1.1038634524	-1.1640987002
H	0	9.0785555483	2.1281856350	-1.5158990297
H	0	9.2199198251	0.4442825473	-2.0355291728
N	0	8.0282813102	0.7539513898	-0.3415535846
H	0	7.1855026396	1.1878124638	-0.7767028675
H	0	7.8831847916	-0.2836229356	-0.2818642920
H	0	8.0528683264	1.1580672149	0.6245183461
O	0	2.0759380539	1.7952787829	-3.3485663672
H	0	2.9320878596	2.3213900411	-3.4318748073
O	0	0.2357158165	2.7040882720	0.1075219309

```
O    0     1.3258292876    3.0967102429    2.9565377410
H    0     0.6260080690    2.5098107927    2.6244451985
H    0     1.9233353598    3.1859842751    2.1825922364
O    0    -3.1019418338   -0.9620669996   -4.1684789718
H    0    -3.8607682394   -1.2931183791   -3.6529361706
H    0    -2.5182620837   -1.7519534899   -4.2580802236
O    0    -4.7351589144   -2.4999967730   -2.1477172228
H    0    -3.9232627806   -2.1423481401   -1.7097186751
H    0    -5.1302479398   -3.0892124516   -1.4778517448
O    0     2.2275822524    4.0310026169   -1.3652932102
H    0     2.6636791227    3.8753264062   -0.4959788093
O    0     6.0710524701    2.5451781070   -1.2326586601
H    0     5.7614628666    2.8683848875   -0.3254982590
H    0     6.6380142280    3.2701759281   -1.5451233292
O    0     4.1456547577    3.4082004635   -3.1052769724
H    0     4.7448419790    2.9246117500   -2.4925871166
O    0     7.6565320028    2.0027918053    2.1430995077
H    0     6.9246837637    2.6293295562    1.8992436380
H    0     7.2493402157    1.3856987612    2.7706097258
O    0     2.4689101132   -0.7830286986   -2.6622399778
H    0     2.6450050969   -0.3567332720   -1.8024550836
H    0    -1.2330271803   -4.6240044693    4.9588345355
H    0     3.4856373930    3.8158024725   -2.4691256325
Cl   0     7.4929544824   -2.3219524856   -0.3465209204
H    0     2.3217224965    0.8378433330   -3.1748163949
O    0    -0.1353854213   -1.3160355119   -2.6789870392
H    0     0.1396123469   -0.1906704506   -3.9695724802
O    0    -0.1164085405    0.5670020212   -4.5547629095
H    0     1.4963503990   -1.0288270775   -2.6020185281
H    0     0.5850434730    1.2276508009   -4.3765839060
H    0    -0.4061821451   -1.9939184126   -3.3377917397
```

L_S'$_{3d}$-fixed

E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.93101434 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.366941 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.607385 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.76375998 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.69126834 au

```
Mn   0     1.0916207425    2.2037830245   -1.8485153811
Mn   0    -0.9093204723   -2.5418877367   -0.5965999816
Mn   0    -0.1691227468    0.7571826563    0.1151708145
Mn   0    -2.7958139257   -0.4537684812    0.3106144246
O    0     0.2016104095    0.5865590322   -1.6168521395
O    0    -1.9520038219    1.0155284916   -0.3393853844
O    0    -2.3572228170   -1.5107654644   -1.2676923433
O    0    -0.7648393278   -1.1436789993    0.6817341586
Ca   0    -2.0038919908    0.4310794707   -2.7002608166
C   -1     0.5558724423    4.7247190256   -5.5397076657
H   -1     0.6231977403    5.6498104296   -4.9861084456
H   -1     0.7446347515    4.8181982992   -6.5988171617
H    0     1.3551743141    4.0843299153   -5.1442396421
C    0    -0.7920891429    4.0080301687   -5.3129207250
H    0    -0.9339137003    3.2252613887   -6.0679512049
H    0    -1.6365951861    4.6990946551   -5.4454951109
C    0    -0.9729446756    3.3116531549   -3.9517217249
O    0    -1.9169078162    2.4688793055   -3.8598146896
O    0    -0.1812301232    3.6061617066   -3.0091140809
C   -1    -2.9326390547   -6.5281484807   -5.4619076511
H   -1    -1.9733760203   -6.9907789362   -5.6410320297
H   -1    -3.6655907357   -6.6556360807   -6.2448354619
```

H	0	-3.3557934832	-7.1114185414	-4.6266917992
C	0	-2.6894664255	-5.1096319842	-4.9479175459
H	0	-3.6279196182	-4.6120703432	-4.6733245259
H	0	-2.1977979814	-4.4821356994	-5.6991524692
C	0	-1.7950957631	-5.2295928338	-3.7079163792
H	0	-0.8548676638	-5.7328609708	-3.9817204067
H	0	-2.2730471041	-5.8561006974	-2.9479309109
C	0	-1.4019200222	-3.9186788278	-3.0719091886
O	0	-1.1952813110	-2.9119725048	-3.7863539839
O	0	-1.2684738234	-3.9785656957	-1.7869633745
C	-1	5.0684336392	-4.5983990125	0.8913187041
H	0	5.8718765901	-5.3302975432	1.0336750393
H	0	5.3051372125	-4.0171610822	-0.0030691788
C	0	4.9906477075	-3.6951297178	2.1200912134
O	0	4.4652165688	-4.1025833664	3.1774375524
C	0	3.7312929800	-5.3911862806	0.7111929592
H	0	3.6363311844	-6.0778447625	1.5610352872
H	0	3.8002546770	-6.0009640225	-0.1939471086
C	0	2.4927700347	-4.5346847925	0.6321812563
N	0	2.2957743983	-3.5333775526	1.5697687501
H	0	2.8628200174	-3.4257015102	2.4068841263
C	0	1.4077269497	-4.4333524389	-0.2115258342
H	0	1.1557637012	-4.9963811688	-1.0960237965
C	0	1.1967014684	-2.8417047471	1.2651583828
H	0	0.9159550685	-1.9159252551	1.7257091853
N	0	0.5936217829	-3.3794927093	0.2093657465
N	0	5.3673045049	-2.4184933415	1.9420613471
H	0	5.8903931677	-2.1887319770	1.0916552495
C	-1	5.0485701633	-1.3552128717	2.8903455473
H	0	5.9367445270	-0.7177158824	2.9910259325
H	0	4.8586198855	-1.8176532056	3.8609870520
C	0	3.8437266062	-0.5111451216	2.4439229897
H	0	3.6556891654	0.2604767996	3.2013715361
H	0	2.9522246122	-1.1388927060	2.4230549029
C	0	4.0399302313	0.1353320604	1.0711818462
H	0	4.5180929750	-0.5687181083	0.3775992688
H	0	4.7067116517	1.0030835260	1.1291997050
C	0	2.7758144990	0.5912389054	0.3472215696
O	0	2.9431511429	1.1770643763	-0.7502214575
O	0	1.6477062601	0.2884030419	0.8712927565
C	-1	-5.4337358438	-3.9572074769	2.1494130641
H	0	-5.3065855841	-3.2350413741	2.9620231026
H	0	-5.9245953223	-4.8433679243	2.5705436856
C	0	-4.0712299052	-4.3694771499	1.5705099614
H	0	-4.2053071464	-5.0770509814	0.7458903842
H	0	-3.4797666894	-4.8897748977	2.3327142003
C	0	-3.2323198000	-3.2158166263	1.0336610499
O	0	-3.6978795642	-2.0513259694	1.1393960727
O	0	-2.0938948474	-3.5078700666	0.5319657603
C	0	-6.3540942114	-3.3877237062	1.0738664533
O	0	-6.2291781351	-3.6783743268	-0.1261708737
N	0	-7.3661623593	-2.6097173128	1.5165887636
H	0	-7.3687091713	-2.3088122823	2.4815060650
C	-1	-8.4067652400	-2.0914269629	0.6341183831
H	0	-9.2958714001	-1.8855641136	1.2307217822
H	0	-8.6368047601	-2.8624984647	-0.1068823969
C	0	-8.0051248108	-0.7764534737	-0.0683990420
O	0	-8.4773329194	0.3038915485	0.2882200616
N	0	-7.1393477879	-0.9317584120	-1.0998851035
H	0	-6.6956746024	-1.8374145932	-1.2108514724

C	0	-6.5303764362	0.1874090530	-1.7905962692
H	0	-6.5366132261	0.0101036134	-2.8692533136
H	0	-7.1363130266	1.0747295467	-1.5849193446
C	0	-5.0796100138	0.4666422684	-1.3560604164
O	0	-4.3126496763	0.9707852621	-2.2146325223
O	0	-4.7774930623	0.1732968803	-0.1561605479
C	-1	-3.3945147043	3.6149985419	5.0448122236
H	-1	-3.4229316343	3.3018765640	6.0780098657
H	-1	-4.2103853096	4.2660616243	4.7679036274
H	0	-2.4931085336	4.2394237804	4.9511883435
C	0	-3.3297225784	2.5021189142	4.0023295645
H	0	-3.5218023446	2.9475881301	3.0175937022
H	0	-4.1169033729	1.7555644043	4.1534229178
C	0	-1.9598532332	1.8249334278	3.9602343900
H	0	-1.8548936265	1.1494484701	4.8192164994
H	0	-1.1577137592	2.5643970898	4.0371219143
C	0	-1.7629969345	1.0603219220	2.6637679125
O	0	-0.6324311023	1.1887913051	2.1023638823
O	0	-2.7320931945	0.3607036942	2.2387888007
C	-1	-5.4705131830	9.0818308074	2.1602646766
H	-1	-5.3321611873	8.6548367846	3.1425240802
H	-1	-6.5057749792	9.3245731156	1.9716331862
H	0	-4.9119318988	10.0250861842	2.1261774376
C	0	-4.9093084834	8.0885498903	1.1301159153
H	0	-3.8153794188	8.0702997596	1.2379308813
H	0	-5.1058337062	8.4315584677	0.1059212757
C	0	-5.4823296430	6.6746746454	1.3172186059
H	0	-6.5561145869	6.6848599562	1.0929756971
H	0	-5.3826950139	6.3694825546	2.3681238435
C	0	-4.8289440235	5.6016035857	0.4412436151
H	0	-4.8873057787	5.8905403683	-0.6187152964
H	0	-5.3677617545	4.6557517853	0.5627096950
N	0	-3.4370212583	5.3824047692	0.8404855817
H	0	-2.9265208253	6.1852978786	1.1824281426
C	0	-2.6748294924	4.3504126784	0.4079605957
N	0	-3.1643002314	3.4261615402	-0.4180739343
H	0	-2.7024257360	2.4945034274	-0.4635943869
H	0	-4.0543992943	3.5340131920	-0.8786827906
N	0	-1.4110384495	4.2412321371	0.8186197557
H	0	-1.0606277060	4.6932226391	1.6527849930
H	0	-0.7764321736	3.5277527655	0.3963158813
C	-1	-0.9491482595	-1.3960067221	7.4915985684
H	-1	0.0396656365	-0.9976177587	7.3181924406
H	-1	-1.1250939058	-1.6206298736	8.5333656018
H	0	-1.6937001975	-0.6640679376	7.1600485581
C	0	-1.1258728515	-2.7473426404	6.7754921111
H	0	-2.0935162476	-3.1825565968	7.0617358345
H	0	-0.3620420116	-3.4470156558	7.1401790860
C	0	-1.0610667422	-2.7030216319	5.2848806895
N	0	-1.0324993565	-3.8634069832	4.5221631336
C	0	-1.0733334206	-1.6799595359	4.3761928140
H	0	-1.0691820667	-0.6192522971	4.5367218477
C	0	-1.0303337876	-3.5532393875	3.2185886519
H	0	-0.9949916876	-4.2495560187	2.3981010841
N	0	-1.0710780947	-2.2280100178	3.1084685131
H	0	-1.0171984007	-1.7002803660	2.1609444821
C	-1	3.7935785274	6.2228293871	2.4369196347
H	-1	4.6616055967	6.7227027706	2.0325582324
H	-1	3.3300618910	6.7272340543	3.2717189262
H	0	3.0337743155	6.2200111486	1.6465173783

C	0	4.1413380136	4.7492025821	2.7587723411
H	0	5.0916320548	4.6647691708	3.2959654003
H	0	3.3472131980	4.3144363470	3.3766415870
C	0	4.1797193426	3.9457462067	1.4557970530
O	0	3.0938061300	3.8946057991	0.8208664382
O	0	5.2707942873	3.4187578236	1.0618184959
C	-1	12.1234659990	-2.3478680496	-0.7293891731
H	-1	13.1700132789	-2.0857770971	-0.7794594665
H	-1	11.8970041286	-3.2274397402	-1.3137130726
H	0	11.9188648669	-2.6312111011	0.3130079668
C	0	11.2151292929	-1.1595795152	-1.1236971663
H	0	11.6685997603	-0.6093290000	-1.9609085959
H	0	10.2500628763	-1.5381925258	-1.4800348313
C	0	10.9557465948	-0.2016237443	0.0546019924
H	0	10.2339269640	-0.6748674525	0.7346655109
H	0	11.8824916671	-0.0763032800	0.6322847186
C	0	10.4769466800	1.2085645552	-0.3334776708
H	0	10.3662105739	1.8210735864	0.5719919886
H	0	11.2592409922	1.6901259507	-0.9357376155
C	0	9.1867300187	1.3162731081	-1.1490367573
H	0	9.0463003808	2.3497653930	-1.4780839856
H	0	9.2137814365	0.6807227271	-2.0378543963
N	0	7.9538790912	0.9409509203	-0.3859670029
H	0	7.1151333707	1.3373536169	-0.8648742236
H	0	7.8378062075	-0.1011524318	-0.3300824644
H	0	7.9200905203	1.3507427155	0.5773031631
O	0	1.8063428562	1.5499907296	-3.5345273134
H	0	3.2903990253	2.4161821880	-3.6790942084
O	0	0.3486043711	2.4518139660	-0.1325692734
O	0	0.8836707772	3.6133498261	2.5804159751
H	0	0.4753399084	2.7646614344	2.3242047837
H	0	1.5501633172	3.7545835647	1.8722197228
O	0	-3.2566060637	-1.1097687673	-4.1867548240
H	0	-3.9568257280	-1.5095188592	-3.6301159293
H	0	-2.5919544986	-1.8297662391	-4.2528172107
O	0	-4.4719403151	-2.7392443957	-2.2316500935
H	0	-3.6610493816	-2.3433592679	-1.7910470385
H	0	-4.9783874070	-3.1525441092	-1.5089654729
O	0	2.3212815002	3.8636132537	-1.6850848314
H	0	2.7283238698	3.7892063137	-0.7720286405
O	0	5.8516719811	2.5305978557	-1.3959699309
H	0	5.4254097270	2.7898866330	-0.5259382282
H	0	6.3307059129	3.3351247953	-1.6566403996
O	0	4.0631311363	3.0296526602	-3.5228547756
H	0	4.6100135202	2.5847166388	-2.8391439624
O	0	7.4337829364	2.1968528805	2.0748226895
H	0	6.6421781791	2.7387744688	1.8080826952
H	0	7.0849872842	1.5587985889	2.7161960811
O	0	2.7423725368	-0.9564134040	-2.5499088249
H	0	2.1706602529	0.6608235294	-3.3125313240
H	0	-1.0096976474	-4.8074088681	4.8875185297
H	0	3.0524358241	3.7289884312	-2.3552215106
Cl	0	7.5154066004	-2.1395113875	-0.4744190550
H	0	3.0377046401	-0.2909204100	-1.8986518120
O	0	-0.3064431718	0.0308693140	-4.4593175544
H	0	0.0812122037	-0.8585312129	-4.4484757803
O	0	0.3214013001	-1.9638941687	-1.8014687950
H	0	1.8615482429	-1.2287821741	-2.1911434333
H	0	-0.1657284500	-1.9974938913	-2.6514669099
H	0	0.4396357754	0.6452359600	-4.1986139662

L_S'₃d

E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.94913175 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.384214 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.6242 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.78146892 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.70807017437 au

Mn	0	1.1118768679	2.1975429262	-1.9019581565
Mn	0	-0.9357205820	-2.4787774802	-0.7855505930
Mn	0	-0.1846530279	0.7814332915	0.0637845629
Mn	0	-2.7559240291	-0.4838247926	0.2905505393
O	0	0.1765449521	0.6072402125	-1.6733809025
O	0	-1.9693493537	1.0248100682	-0.3639180517
O	0	-2.2868734099	-1.6013380018	-1.5001128448
O	0	-0.9062670610	-1.1332566703	0.5549014612
Ca	0	-1.9733591097	0.4336602514	-2.7786632060
C	-1	0.5605739123	4.6533689999	-5.5940389561
H	-1	0.6325419087	5.5836990002	-5.0498839561
H	-1	0.7486839120	4.7353060006	-6.6542199561
H	0	1.3511869666	4.0075353564	-5.1906401581
C	0	-0.7934034233	3.9561685699	-5.3617146673
H	0	-0.9321387940	3.1469452194	-6.0893288028
H	0	-1.6325026914	4.6464265476	-5.5275415696
C	0	-0.9866024169	3.3109215771	-3.9799490832
O	0	-1.9586246859	2.5043751820	-3.8551667359
O	0	-0.1745177006	3.6016603441	-3.0546254461
C	-1	-2.9775380435	-6.5825810140	-5.3991569561
H	-1	-2.0205080416	-7.0512410103	-5.5745159561
H	-1	-3.7118310430	-6.7147260169	-6.1800519561
H	0	-3.3934332546	-7.1186852819	-4.5317411858
C	0	-2.6797970198	-5.1466578146	-4.9671702975
H	0	-3.5533676481	-4.6722496012	-4.5026086097
H	0	-2.3795900380	-4.5179042624	-5.8127964940
C	0	-1.5265630698	-5.2329893461	-3.9547853595
H	0	-0.6118710106	-5.5452524692	-4.4782054758
H	0	-1.7459402245	-5.9914929125	-3.1968970698
C	0	-1.2267128494	-3.9298016570	-3.2617160072
O	0	-1.0477232610	-2.8929219085	-3.9473007699
O	0	-1.1680281905	-4.0160561710	-1.9776550910
C	-1	5.0383589488	-4.6241889825	0.9265590439
H	0	5.8853849300	-5.3137817969	1.0260986086
H	0	5.1947919037	-4.0413479844	0.0156722888
C	0	4.9902389600	-3.7114135148	2.1534678345
O	0	4.4999996425	-4.1145780298	3.2285142380
C	0	3.7309897036	-5.4623640689	0.8422441755
H	0	3.6834962917	-6.1060405167	1.7284027290
H	0	3.7752379136	-6.1125081401	-0.0361794954
C	0	2.4944592436	-4.6147277691	0.7578028648
N	0	2.2613777851	-3.6137018341	1.6886972973
H	0	2.8122660545	-3.4946293619	2.5341102031
C	0	1.4655722786	-4.4924278756	-0.1479947429
H	0	1.2616937518	-5.0552250097	-1.0459798260
C	0	1.1846846471	-2.9052801667	1.3121930469
H	0	0.8743585815	-1.9829954653	1.7652065641
N	0	0.6537235814	-3.4329487842	0.2226275837
N	0	5.3610974043	-2.4349480796	1.9595754464
H	0	5.8599903470	-2.2103142460	1.0941189452
C	-1	5.0348319360	-1.3609149825	2.8927210439
H	0	5.9155696798	-0.7119140483	2.9850860844
H	0	4.8456680388	-1.8099930034	3.8694598934

C	0	3.8195773464	-0.5380151736	2.4237492144
H	0	3.6197542567	0.2479832400	3.1633562584
H	0	2.9370278041	-1.1786960558	2.4103712562
C	0	4.0137437035	0.0820477498	1.0378181016
H	0	4.4776113509	-0.6417323533	0.3547073046
H	0	4.6937054465	0.9404455097	1.0778732254
C	0	2.7566995245	0.5477536692	0.3047153688
O	0	2.9414971384	1.1586994601	-0.7767896769
O	0	1.6190319700	0.2312775652	0.7990919599
C	-1	-5.4596060539	-3.9238230238	2.1881860439
H	0	-5.3020090089	-3.1751237956	2.9713900335
H	0	-5.9769064811	-4.7749052680	2.6487410879
C	0	-4.1236086956	-4.3918472832	1.6115288115
H	0	-4.2824314411	-5.1377077050	0.8271685517
H	0	-3.5301932346	-4.8826873155	2.3921599275
C	0	-3.2642320934	-3.2868164905	1.0068951853
O	0	-3.6596814391	-2.0894702190	1.1265922484
O	0	-2.1854245174	-3.6485504626	0.4526607108
C	0	-6.3720265722	-3.3549271596	1.1055760322
O	0	-6.2256474481	-3.6193707389	-0.0975668200
N	0	-7.4032801536	-2.5995820851	1.5477351949
H	0	-7.4269623584	-2.3229798662	2.5196481010
C	-1	-8.4258840613	-2.0603020354	0.6569640439
H	0	-9.3287983210	-1.8707763435	1.2380867266
H	0	-8.6384079438	-2.8103047632	-0.1103749576
C	0	-8.0011344095	-0.7297963091	0.0061598668
O	0	-8.4639330746	0.3460571539	0.3870480042
N	0	-7.1086236448	-0.8651899219	-1.0054847863
H	0	-6.6902558150	-1.7780414834	-1.1525338333
C	0	-6.4915619700	0.2649744801	-1.6650216312
H	0	-6.5983064880	0.1820402564	-2.7501893113
H	0	-7.0165863390	1.1670730724	-1.3362661759
C	0	-4.9960786664	0.4202026722	-1.3563542937
O	0	-4.2703333261	0.9027911564	-2.2498734348
O	0	-4.6204770167	0.0493878593	-0.1882039433
C	-1	-3.3840450838	3.6681449844	5.0049420439
H	-1	-3.4128070826	3.3656069843	6.0412790439
H	-1	-4.1973090864	4.3199839812	4.7222500439
H	0	-2.4903211948	4.3059492770	4.9196644093
C	0	-3.2724026961	2.5413949973	3.9823508963
H	0	-3.5317107923	2.9422101900	2.9937061822
H	0	-3.9873104473	1.7358202489	4.1789533718
C	0	-1.8510913444	1.9801077212	3.9059776187
H	0	-1.6216817911	1.4033601669	4.8137079962
H	0	-1.1176441715	2.7899116900	3.8588956059
C	0	-1.6728737242	1.1050634872	2.6781819085
O	0	-0.5680981111	1.2266470399	2.0536019178
O	0	-2.6125292889	0.3242336700	2.3656086263
C	-1	-5.4387671052	9.1146939763	2.0672790439
H	-1	-5.3013161036	8.6970369768	3.0536710439
H	-1	-6.4731351062	9.3600999722	1.8771970439
H	0	-4.8780920427	10.0565820660	2.0261376078
C	0	-4.8820539621	8.1153892338	1.0427385825
H	0	-3.7881573552	8.0941642814	1.1498175466
H	0	-5.0785383192	8.4541662269	0.0170904935
C	0	-5.4603035291	6.7056624324	1.2381006811
H	0	-6.5351894411	6.7194110087	1.0192114573
H	0	-5.3559073129	6.4035299485	2.2893594333
C	0	-4.8144325932	5.6297387910	0.3616560403
H	0	-4.8858048820	5.9127454408	-0.6992087055

H	0	-5.3478199132	4.6824175057	0.4940463060
N	0	-3.4179710729	5.4167137197	0.7461914484
H	0	-2.8997468097	6.2221020811	1.0696988028
C	0	-2.6711192689	4.3640125942	0.3409260567
N	0	-3.1825719834	3.4268727447	-0.4574142236
H	0	-2.7204876027	2.4960595395	-0.5093480704
H	0	-4.0355680982	3.5705979520	-0.9748274404
N	0	-1.4114404181	4.2416146519	0.7579423477
H	0	-1.0510671577	4.7109284131	1.5782626620
H	0	-0.7757872977	3.5296530314	0.3376402446
C	-1	-0.9583840641	-1.3286620061	7.4999050439
H	-1	0.0320049343	-0.9364280022	7.3215320439
H	-1	-1.1342740633	-1.5419670068	8.5440580439
H	0	-1.6990401862	-0.5940402982	7.1658904265
C	0	-1.1499083898	-2.6871472663	6.7931872087
H	0	-2.1115136197	-3.1190770348	7.1035755368
H	0	-0.3794442563	-3.3839397758	7.1485240959
C	0	-1.1152841768	-2.6623240120	5.2985555109
N	0	-1.0136358009	-3.8281705232	4.5460947588
C	0	-1.2248212656	-1.6544260006	4.3809508988
H	0	-1.3329764775	-0.5977906810	4.5284963193
C	0	-1.0554569599	-3.5379662817	3.2388273491
H	0	-0.9886957765	-4.2349584274	2.4197200279
N	0	-1.1921074573	-2.2198904178	3.1206159409
H	0	-1.1789571257	-1.7133891694	2.1966636250
C	-1	3.8128769062	6.2176420127	2.3639280439
H	-1	4.6826969043	6.7095560161	1.9537020439
H	-1	3.3524319042	6.7325020109	3.1940300439
H	0	3.0523667110	6.2150251329	1.5745602855
C	0	4.1526041492	4.7430534120	2.6865372831
H	0	5.1015928461	4.6509514383	3.2247125384
H	0	3.3550051015	4.3114047070	3.3022624668
C	0	4.1874375116	3.9394456189	1.3827288513
O	0	3.1135394346	3.9350778663	0.7250205022
O	0	5.2612885436	3.3640748691	1.0118663132
C	-1	12.1016339402	-2.4214079547	-0.7235829561
H	-1	13.1492779391	-2.1644729506	-0.7773039561
H	-1	11.8707019436	-3.3058269556	-1.2987689561
H	0	11.8966846876	-2.6932788840	0.3217699100
C	0	11.1968904445	-1.2339799533	-1.1302752235
H	0	11.6570724476	-0.6879572929	-1.9665617305
H	0	10.2343250630	-1.6133589618	-1.4927102563
C	0	10.9287550583	-0.2699188110	0.0411819884
H	0	10.2000204206	-0.7384914088	0.7171065511
H	0	11.8505966485	-0.1434853314	0.6263873319
C	0	10.4560107833	1.1392139522	-0.3578739374
H	0	10.3413296664	1.7571796981	0.5433684603
H	0	11.2433146987	1.6152372682	-0.9580154893
C	0	9.1710036191	1.2456375109	-1.1818516312
H	0	9.0364230334	2.2772988081	-1.5189904792
H	0	9.2010274299	0.6038321779	-2.0660860141
N	0	7.9323318777	0.8801365057	-0.4233743732
H	0	7.0985649797	1.2797035646	-0.9075572581
H	0	7.8089503622	-0.1614850505	-0.3653086328
H	0	7.8972913262	1.2924073861	0.5388909977
O	0	1.8224906369	1.5353064384	-3.5852928357
H	0	3.3108614982	2.3942143858	-3.7549436574
O	0	0.3709340840	2.4585479328	-0.1820235172
O	0	0.9066384466	3.6660247508	2.4919133385
H	0	0.5079792676	2.8061681675	2.2542692634

```
H    0    1.5623113358    3.8052188259    1.7738958710
O    0   -3.1890131387   -1.1335664460   -4.2791173808
H    0   -3.8984052968   -1.5248330016   -3.7308827633
H    0   -2.5044518686   -1.8393478640   -4.3003668605
O    0   -4.5240346560   -2.7461144372   -2.2910406922
H    0   -3.6638276051   -2.4104999046   -1.9076405182
H    0   -4.9967789736   -3.1434115162   -1.5370610204
O    0    2.3482779530    3.8424118878   -1.7666027521
H    0    2.7574811742    3.7895514398   -0.8512905819
O    0    5.8445322405    2.4845110830   -1.4511459288
H    0    5.4114566242    2.7376756239   -0.5829945605
H    0    6.3356960812    3.2870616435   -1.6949048920
O    0    4.0870862545    3.0035694007   -3.6017990849
H    0    4.6306898882    2.5577599176   -2.9157606142
O    0    7.4212329801    2.1469040492    2.0334965408
H    0    6.6282613297    2.6866760206    1.7662151893
H    0    7.0773592393    1.5162109524    2.6846793829
O    0    2.8156253820   -0.9351799634   -2.6085701231
H    0    2.1951578059    0.6495906374   -3.3597829371
H    0   -0.9177388013   -4.7637200397    4.9213730328
H    0    3.0786454434    3.7034184198   -2.4368873027
Cl   0    7.4690888668   -2.1941606983   -0.5038607137
H    0    3.1146440798   -0.2766539137   -1.9514684535
O    0   -0.3045275437    0.0926683273   -4.5529498004
H    0    0.0383251617   -0.8118389102   -4.6329922891
O    0    0.3774247344   -1.9378469523   -1.8872079915
H    0    1.9421588469   -1.2165730096   -2.2433579040
H    0   -0.0552432332   -1.9537962645   -2.7687180972
H    0    0.4734195711    0.6608469837   -4.2751466523
```

L_S$_{3a}$-fixed

E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.93686933 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.372097 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.610575 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.773821 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.699738 au

```
Mn   0    1.2843416996    2.0173880554   -1.9554172787
Mn   0   -1.0819777546   -2.5208604426   -0.4471409625
Mn   0   -0.1145534385    0.7543331799    0.0844735907
Mn   0   -2.7052299322   -0.4124211818    0.3558535220
O    0    0.2246787070    0.3279850398   -1.6064192848
O    0   -1.9370673667    1.0104989774   -0.3746682086
O    0   -2.4931201263   -1.4481354862   -1.1312013819
O    0   -1.0144973119   -1.0762099619    0.7851056153
Ca   0   -1.9108385356    0.3841605111   -2.7930590480
C   -1    0.5649679506    4.4715952034   -5.6159420508
H   -1    0.6470390666    5.4154688321   -5.0973913122
H   -1    0.7514726131    4.5224942976   -6.6782555810
H    0    1.3461333313    3.8261840265   -5.1956986106
C    0   -0.8035599816    3.7916902912   -5.3866318326
H    0   -0.9267537970    2.9641472386   -6.0966512246
H    0   -1.6327938129    4.4816351550   -5.5961854710
C    0   -1.0517170923    3.1643889785   -4.0023056799
O    0   -2.1067851244    2.4588198474   -3.8720014729
O    0   -0.2078508638    3.3455404156   -3.0851371307
C   -1   -3.0821862207   -6.7198097199   -5.1079518783
H   -1   -2.1300985362   -7.2024462506   -5.2722524396
H   -1   -3.8193267852   -6.8660412765   -5.8836034916
H    0   -3.5075480769   -7.2269688654   -4.2270980884
C    0   -2.8288644564   -5.2542505756   -4.7374750980
```

H	0	-3.7691577184	-4.7362997800	-4.5107119964
H	0	-2.3565497687	-4.7097931601	-5.5631175240
C	0	-1.9213580717	-5.2175125374	-3.5070131081
H	0	-0.9795407645	-5.7478933789	-3.7156482138
H	0	-2.3828565240	-5.7530875757	-2.6689596311
C	0	-1.5291186230	-3.8435029774	-3.0106903191
O	0	-1.6061140020	-2.8336937448	-3.7325858149
O	0	-1.0533949862	-3.8464480915	-1.8080230075
C	-1	4.9659431292	-4.6683956435	1.1469802924
H	0	5.6699073991	-5.4693101217	1.3997215198
H	0	5.3553453455	-4.1467108824	0.2690993976
C	0	4.8433314851	-3.7125740475	2.3317689918
O	0	4.2060195681	-4.0451779025	3.3559107885
C	0	3.5844312474	-5.3309756813	0.8416638199
H	0	3.3572070658	-6.0192030716	1.6648449277
H	0	3.6727432306	-5.9313496523	-0.0678309202
C	0	2.4246075243	-4.3816689592	0.6856561058
N	0	2.1596094507	-3.4378172146	1.6678696663
H	0	2.6793399500	-3.3846078363	2.5450272353
C	0	1.4391386483	-4.1897734966	-0.2541040329
H	0	1.2507269530	-4.7053597605	-1.1817888575
C	0	1.1150215965	-2.6949692085	1.3069653278
H	0	0.7878337991	-1.8178516162	1.8280376900
N	0	0.6129272807	-3.1360527557	0.1518880536
N	0	5.3141312237	-2.4725926595	2.1417401256
H	0	5.9168091857	-2.3023348066	1.3283534633
C	-1	4.9984536294	-1.3528513658	3.0234347445
H	0	5.8898338604	-0.7160732584	3.0763926457
H	0	4.8078046900	-1.7484449812	4.0237056798
C	0	3.7965051701	-0.5294232884	2.5281930674
H	0	3.6389731688	0.3091513965	3.2184087304
H	0	2.8938143215	-1.1389895877	2.5824961639
C	0	3.9919108924	-0.0135464072	1.1025299847
H	0	4.4491353584	-0.7883731345	0.4755614079
H	0	4.6801939833	0.8395502861	1.0868552219
C	0	2.7523848894	0.4211642288	0.3295868935
O	0	2.9383758383	0.9310286508	-0.7818796564
O	0	1.5929640069	0.1901752775	0.8700940348
C	-1	-5.5217965377	-3.8308924997	2.4086138309
H	0	-5.3770382211	-3.0717011659	3.1842376092
H	0	-6.0234708293	-4.6861101870	2.8777829971
C	0	-4.1738742314	-4.2872038311	1.8400680991
H	0	-4.3213291890	-5.0389777194	1.0588169939
H	0	-3.5819974336	-4.7710624471	2.6269358562
C	0	-3.3067402732	-3.1893629751	1.2367676801
O	0	-3.6644703194	-1.9857277280	1.3583447536
O	0	-2.2252009274	-3.5572280495	0.6614528369
C	0	-6.4387851341	-3.2880091295	1.3161655595
O	0	-6.2763634602	-3.5588239604	0.1173379034
N	0	-7.4839669740	-2.5446856457	1.7448998149
H	0	-7.5182903447	-2.2604694711	2.7144792523
C	-1	-8.4735922350	-1.9811802000	0.8327841782
H	0	-9.4026854900	-1.8185385430	1.3798755206
H	0	-8.6444592499	-2.7017488150	0.0285771156
C	0	-8.0208126872	-0.6199944027	0.2646700710
O	0	-8.4739854724	0.4363363775	0.7061250255
N	0	-7.1048078609	-0.6992758257	-0.7326810988
H	0	-6.7129631107	-1.6037834714	-0.9696148017
C	0	-6.4903670742	0.4661038059	-1.3351942746
H	0	-6.7094275118	0.5137458319	-2.4057729402

H	0	-6.9209206824	1.3500594653	-0.8544414689
C	0	-4.9652743285	0.5041845182	-1.1740723586
O	0	-4.2734097223	0.9077204595	-2.1219861698
O	0	-4.5300706069	0.1192661007	-0.0209121376
C	-1	-3.3662872152	3.8143495678	5.0134232252
H	-1	-3.3961346244	3.5402162924	6.0576264380
H	-1	-4.1740663446	4.4659158729	4.7145451532
H	0	-2.4578131014	4.4219498868	4.8902549294
C	0	-3.3261903749	2.6489838034	4.0134367283
H	0	-3.6583503272	3.0213045279	3.0361561715
H	0	-4.0310419512	1.8559904993	4.2875176173
C	0	-1.9174371853	2.0789711687	3.8435681306
H	0	-1.6358594182	1.4788101945	4.7196779616
H	0	-1.1805794485	2.8863220901	3.7884981085
C	0	-1.7365722700	1.2489870073	2.5827021211
O	0	-0.6026183200	1.3265344502	2.0301310228
O	0	-2.7170440625	0.5373658176	2.1781621417
C	-1	-5.3742609433	9.1986628018	1.9321008298
H	-1	-5.2388862785	8.8065084654	2.9292424508
H	-1	-6.4067009607	9.4486368320	1.7373345378
H	0	-4.8119594919	10.1391268401	1.8748170397
C	0	-4.8130130733	8.1873668395	0.9199971675
H	0	-3.7176164710	8.1867416940	1.0128341173
H	0	-5.0319586598	8.5067951184	-0.1075790635
C	0	-5.3573553759	6.7693957638	1.1446869775
H	0	-6.4473257603	6.7744916534	1.0161008230
H	0	-5.1621330188	6.4569577488	2.1797554952
C	0	-4.7857153729	5.7088849672	0.1984054025
H	0	-4.9757819428	5.9938859917	-0.8468539649
H	0	-5.2857522757	4.7524646639	0.3804642711
N	0	-3.3524213369	5.5076051249	0.4209375849
H	0	-2.7896434214	6.3248321184	0.6143430420
C	0	-2.6736223406	4.3949851217	0.0648353646
N	0	-3.2995945683	3.3902210005	-0.5599964274
H	0	-2.8237670636	2.4786485484	-0.6242820011
H	0	-4.0974167899	3.5484240420	-1.1565112052
N	0	-1.3846293078	4.2702287229	0.3694145525
H	0	-0.9337071460	4.7701546781	1.1288725901
H	0	-0.8047419899	3.5011209165	-0.0208388151
C	-1	-0.9842294739	-1.1363350132	7.6393587576
H	-1	0.0094144883	-0.7587772755	7.4482126538
H	-1	-1.1601539131	-1.3193065411	8.6890907933
H	0	-1.7198659591	-0.4060050988	7.2856839628
C	0	-1.1853619315	-2.5137431387	6.9770485314
H	0	-2.1520646725	-2.9288367142	7.2940470481
H	0	-0.4218034833	-3.2059455680	7.3544598404
C	0	-1.1432666097	-2.5226615031	5.4847606681
N	0	-0.9979938079	-3.6966839438	4.7552239120
C	0	-1.2806792233	-1.5342582403	4.5491326283
H	0	-1.4177408644	-0.4767143730	4.6727126790
C	0	-1.0444556494	-3.4328577224	3.4429648753
H	0	-0.9607168820	-4.1460452505	2.6394533942
N	0	-1.2227119891	-2.1215391563	3.3018321615
H	0	-1.2373059726	-1.6273975474	2.3712126998
C	-1	3.8494823680	6.2201016502	2.2903430601
H	-1	4.7229269460	6.6921526429	1.8652825280
H	-1	3.3954712281	6.7618087863	3.1069388051
H	0	3.0893770808	6.1911748401	1.5006088159
C	0	4.1886536626	4.7585226810	2.6719177713
H	0	5.1313812278	4.6951396711	3.2256474936

H	0	3.3873024530	4.3535246587	3.3014032359
C	0	4.2402964787	3.8887147389	1.4073775519
O	0	3.1756971819	3.8208398415	0.7459105141
O	0	5.3342820246	3.3173633621	1.0771592026
C	-1	12.0468442135	-2.5807150277	-0.5758153875
H	-1	13.0967939045	-2.3356149598	-0.6385006221
H	-1	11.8060179065	-3.4781631760	-1.1262565335
H	0	11.8317400794	-2.8110296404	0.4770697268
C	0	11.1772292563	-1.3871219540	-1.0303605878
H	0	11.6311830761	-0.9164629169	-1.9147391021
H	0	10.1875939413	-1.7467247176	-1.3341043992
C	0	10.9972517578	-0.3438138503	0.0873142154
H	0	10.2718656994	-0.7387752142	0.8114056609
H	0	11.9444549265	-0.2268948963	0.6328234730
C	0	10.5709033829	1.0576588659	-0.3811336186
H	0	10.5106277350	1.7325285987	0.4838943266
H	0	11.3538439639	1.4648757474	-1.0352182557
C	0	9.2619108699	1.1584662339	-1.1648211376
H	0	9.1333363853	2.1770221584	-1.5420153636
H	0	9.2487993906	0.4788116992	-2.0208289275
N	0	8.0458460438	0.8517552439	-0.3483194786
H	0	7.2044995099	1.2451844741	-0.8299059849
H	0	7.9142653806	-0.1793686891	-0.2160007243
H	0	8.0440320772	1.3225991022	0.5873031291
O	0	1.9487688161	1.2732533435	-3.5854246185
H	0	2.7429077849	1.7803838061	-3.8624836668
O	0	0.4267281705	2.3651004445	-0.2640475505
O	0	0.8084362646	3.9295956843	2.2565720800
H	0	0.4516428802	3.0441869251	2.0592048160
H	0	1.5841574408	3.9777115455	1.6484919033
O	0	-3.4756914944	-0.9582244492	-4.1666215826
H	0	-4.2141457858	-1.2131331837	-3.5817393687
H	0	-2.9490609260	-1.7834995696	-4.2430913849
O	0	-4.7437936049	-2.5462453838	-2.0761380793
H	0	-3.9137427075	-2.1849523847	-1.6704161818
H	0	-5.1752952599	-3.0303524075	-1.3472141148
O	0	2.3608466439	3.5485178865	-1.9037924714
H	0	2.7350330384	3.5652893428	-0.9935204228
O	0	5.9922424213	2.4237687881	-1.3730357623
H	0	5.5587407598	2.7072009896	-0.5149675920
H	0	6.4058555041	3.2395249700	-1.6991748403
O	0	4.2574629530	2.9310702701	-3.6484368189
H	0	4.8055203906	2.4270161733	-3.0159629079
O	0	7.5814211925	2.2340625142	2.0589562109
H	0	6.7588487056	2.7320191185	1.7964591497
H	0	7.2704132843	1.5874528682	2.7112613742
O	0	2.0774794924	-1.3079675066	-2.7187734606
H	0	1.3681962386	-0.9915351713	-2.1116271825
H	0	-0.8697016805	-4.6207246309	5.1496591309
H	0	3.5759859189	3.3125409727	-3.0191614500
Cl	0	7.6038778499	-2.2469775662	-0.0958764846
H	0	2.3053254212	-0.4185181173	-3.1034104755
O	0	-0.3178621182	0.2158262920	-4.6274004855
H	0	0.0040191162	-2.6325862127	-4.6209461705
O	0	0.8437599221	-2.2573431675	-4.9458982357
H	0	0.0547163435	-0.6701987147	-4.8645309587
H	0	1.3280231099	-2.0110814273	-4.1099058907
H	0	0.4974295198	0.7281367355	-4.3689936211

L_S_{3a}

E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.960462 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.394375 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.637013 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.79678595 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.72234377 au

Mn	0	1.2168770099	2.1327254494	-1.7994862570
Mn	0	-0.9591999910	-2.3606150817	-0.7058472339
Mn	0	-0.1821818520	0.7730473436	0.1906994014
Mn	0	-2.7316257572	-0.5075822336	0.3461415175
O	0	0.1916789517	0.3888980496	-1.5035979374
O	0	-2.0032237221	0.9934675338	-0.2736940512
O	0	-2.4573171602	-1.3972369380	-1.2450335577
O	0	-1.0021352754	-1.1201159275	0.7248624547
Ca	0	-1.9468290263	0.5888275260	-2.7473320565
C	-1	0.5534800434	4.6067479400	-5.5057320104
H	-1	0.6206110627	5.5379779386	-4.9627480104
H	-1	0.7467470451	4.6869539360	-6.5650240104
H	0	1.3220438928	3.9481453380	-5.0835913040
C	0	-0.8260049663	3.9347128660	-5.3239349794
H	0	-0.9333696123	3.1149642815	-6.0461242021
H	0	-1.6428909442	4.6327298349	-5.5523857663
C	0	-1.1247785555	3.2895737988	-3.9609511954
O	0	-2.2233887193	2.6494099649	-3.8536605008
O	0	-0.2745389860	3.3782260999	-3.0360171615
C	-1	-2.9625911895	-6.6362919872	-5.3092040104
H	-1	-2.0036611992	-7.1032930070	-5.4788150104
H	-1	-3.6925091923	-6.7713719721	-6.0936570104
H	0	-3.3889507601	-7.1592733693	-4.4384338085
C	0	-2.7388256278	-5.1691966902	-4.9335265312
H	0	-3.6922150404	-4.6519112992	-4.7706529769
H	0	-2.2232701163	-4.6322463826	-5.7376895373
C	0	-1.9062139368	-5.1006913516	-3.6549648977
H	0	-0.9866604037	-5.6958804718	-3.7593764100
H	0	-2.4464666244	-5.5420959822	-2.8080737103
C	0	-1.4684941907	-3.7153364722	-3.2439940603
O	0	-1.6007620424	-2.7340954881	-3.9937384013
O	0	-0.8886647379	-3.6712122704	-2.0851502974
C	-1	5.0166328516	-4.6502991525	1.0541829896
H	0	5.7735546497	-5.4122654982	1.2755302087
H	0	5.3593727798	-4.0919550609	0.1796914999
C	0	4.8777251285	-3.7261006157	2.2619633310
O	0	4.2686523250	-4.1001717348	3.2880900375
C	0	3.6729830170	-5.3772146939	0.7606337491
H	0	3.4651984440	-6.0608446579	1.5922972380
H	0	3.7829181396	-5.9822381950	-0.1432854662
C	0	2.5127738681	-4.4409622395	0.5904115370
N	0	2.1970539379	-3.5482262794	1.6053655430
H	0	2.6758284526	-3.5362698319	2.5064650318
C	0	1.6253450641	-4.1541551673	-0.4189197351
H	0	1.5017596879	-4.6066984429	-1.3898715093
C	0	1.2190619393	-2.7397035384	1.1949257624
H	0	0.8741110795	-1.8791594103	1.7309201891
N	0	0.8199988782	-3.0912669915	-0.0227913432
N	0	5.3147672035	-2.4697509983	2.0939292776
H	0	5.9082463642	-2.2730389606	1.2807417693
C	-1	4.9963069193	-1.3835941521	3.0145899896
H	0	5.8734015303	-0.7259961209	3.0611217438
H	0	4.8441849098	-1.8119462612	4.0080608028
C	0	3.7630423076	-0.5761754100	2.5775909809
H	0	3.5938247605	0.2278900511	3.3052019466

H	0	2.8798294354	-1.2154421018	2.6175626043
C	0	3.9331050590	0.0041492764	1.1755922770
H	0	4.3535810750	-0.7521805917	0.5009732244
H	0	4.6428074032	0.8390964707	1.1842178408
C	0	2.6918595130	0.5064653927	0.4527696973
O	0	2.8766056088	1.1023122249	-0.6152096336
O	0	1.5334416158	0.2327649805	0.9767846525
C	-1	-5.4889241342	-3.9692639349	2.2605319896
H	0	-5.3249796310	-3.2112021484	3.0337233912
H	0	-6.0089677693	-4.8114673255	2.7338321384
C	0	-4.1582690545	-4.4495352919	1.6834685900
H	0	-4.3264895873	-5.1949495853	0.9006713950
H	0	-3.5750244016	-4.9499632311	2.4659536474
C	0	-3.2677635232	-3.3667784869	1.0754584253
O	0	-3.6241439366	-2.1536805674	1.2109518369
O	0	-2.2066106033	-3.7576475160	0.5095218947
C	0	-6.4011185931	-3.4039539964	1.1738436165
O	0	-6.2278864777	-3.6372742736	-0.0311592942
N	0	-7.4604964919	-2.6873940907	1.6150858000
H	0	-7.5083231944	-2.4335381444	2.5924839018
C	-1	-8.4516630958	-2.1149278735	0.7108919896
H	0	-9.3926803376	-1.9984364984	1.2497591317
H	0	-8.5919788711	-2.8082985711	-0.1223669094
C	0	-8.0244874663	-0.7238787281	0.2064108493
O	0	-8.4822349311	0.3051025312	0.7039920547
N	0	-7.1194996535	-0.7456509559	-0.8039736800
H	0	-6.7096635990	-1.6324482506	-1.0755892064
C	0	-6.5052363167	0.4531838951	-1.3329444605
H	0	-6.7085423981	0.5596414630	-2.4023994048
H	0	-6.9466757790	1.3079865813	-0.8111122350
C	0	-4.9845171386	0.4887176525	-1.1473524139
O	0	-4.2880791829	0.9845536011	-2.0469789170
O	0	-4.5594541640	-0.0017309728	-0.0311326616
C	-1	-3.4434679768	3.6319130228	5.0746379896
H	-1	-3.4772889830	3.3308740235	6.1112829896
H	-1	-4.2569069633	4.2813080396	4.7865809896
H	0	-2.5307161855	4.2359774032	4.9674326233
C	0	-3.4213296084	2.5189642990	4.0201659085
H	0	-3.5069895022	3.0005816956	3.0371785491
H	0	-4.2940625996	1.8626803295	4.1114770974
C	0	-2.1362701519	1.6821752382	4.0394147464
H	0	-2.2144488650	0.9221024919	4.8253236162
H	0	-1.2675800694	2.3078418946	4.2633439674
C	0	-1.8784476489	1.0116771265	2.6996995675
O	0	-0.7472342164	1.2065330193	2.1707422584
O	0	-2.8199013082	0.2999907950	2.2079655338
C	-1	-5.4944068642	9.0690430653	2.1168349896
H	-1	-5.3612788728	8.6551840625	3.1046309896
H	-1	-6.5283918591	9.3116920867	1.9210019896
H	0	-4.9435030283	10.0178832010	2.0907659293
C	0	-4.9245011732	8.1007824284	1.0757725309
H	0	-3.8337581158	8.0675498984	1.2077269599
H	0	-5.0968096463	8.4791093310	0.0594264409
C	0	-5.5178436087	6.6926024673	1.2069421019
H	0	-6.5950595084	6.7298239986	1.0011028262
H	0	-5.4032104227	6.3359624728	2.2397251870
C	0	-4.8925605216	5.6627311409	0.2645434834
H	0	-5.0119186350	5.9804049394	-0.7813971257
H	0	-5.3989227853	4.6999633561	0.3825830318
N	0	-3.4781597737	5.4622100907	0.5798448735

H	0	-2.9334330213	6.2740851040	0.8349011034
C	0	-2.7825962229	4.3433565054	0.2965826448
N	0	-3.3630789758	3.3435431797	-0.3786631321
H	0	-2.8786775979	2.4335989633	-0.4166015413
H	0	-4.0798804010	3.5200423611	-1.0667759096
N	0	-1.5356483412	4.1962227518	0.7361600159
H	0	-1.1348470738	4.7574157630	1.4770014864
H	0	-0.8989212381	3.4773366613	0.3352465757
C	-1	-1.0205150801	-1.3557130274	7.5909649896
H	-1	-0.0301660719	-0.9616830479	7.4167099896
H	-1	-1.2015310845	-1.5674930237	8.6343959896
H	0	-1.7652159208	-0.6327802823	7.2417912514
C	0	-1.1771620935	-2.7203061582	6.8876941958
H	0	-2.1461460204	-3.1591993123	7.1624584388
H	0	-0.4145949785	-3.4097046813	7.2735974956
C	0	-1.0941165177	-2.7009602484	5.3951273577
N	0	-1.1309009013	-3.8699786418	4.6418867808
C	0	-1.0434675215	-1.6878011481	4.4775606471
H	0	-0.9626943891	-0.6272257623	4.6231269669
C	0	-1.1151838148	-3.5783329289	3.3343748538
H	0	-1.1377018537	-4.2766705542	2.5130881735
N	0	-1.0769067962	-2.2540731775	3.2176849218
H	0	-1.0918361447	-1.7489184330	2.2936365850
C	-1	3.7616910762	6.1915028735	2.4661299896
H	-1	4.6323460864	6.6845408555	2.0595729896
H	-1	3.2955430869	6.7067808832	3.2929279896
H	0	3.0060579282	6.1690943375	1.6722512208
C	0	4.1117657239	4.7258085313	2.8255361679
H	0	5.0704499508	4.6569741186	3.3505235955
H	0	3.3293279520	4.3169270903	3.4760942334
C	0	4.1203244642	3.8641668635	1.5554398146
O	0	3.0344684235	3.8073832794	0.9284154487
O	0	5.1995437094	3.2889168917	1.1875681524
C	-1	12.0837928975	-2.4357882989	-0.5634660104
H	-1	13.1311369029	-2.1767783206	-0.6122680104
H	-1	11.8575868792	-3.3216722942	-1.1383010104
H	0	11.8716322575	-2.7046835496	0.4810276914
C	0	11.1877187811	-1.2451279075	-0.9786865864
H	0	11.6610374673	-0.6973264474	-1.8065369494
H	0	10.2289603188	-1.6202065833	-1.3540724794
C	0	10.9090002444	-0.2868640013	0.1944974982
H	0	10.1697139750	-0.7599978439	0.8553084350
H	0	11.8246342480	-0.1651068582	0.7904596159
C	0	10.4396905175	1.1234154334	-0.2026193235
H	0	10.3290283426	1.7417142104	0.6989969587
H	0	11.2238090673	1.5991525275	-0.8071955036
C	0	9.1487135741	1.2248150034	-1.0167630040
H	0	9.0007527395	2.2565834129	-1.3480738956
H	0	9.1770736617	0.5873643167	-1.9041878380
N	0	7.9219768621	0.8444352466	-0.2476632735
H	0	7.0789003864	1.2260195342	-0.7333723984
H	0	7.8267688132	-0.1966997698	-0.1639029129
H	0	7.8832884753	1.2741697783	0.7070617146
O	0	1.9469028351	1.4445940058	-3.4254446138
H	0	2.7033938856	2.0106528410	-3.6966563193
O	0	0.3059651077	2.4102128811	-0.1099775885
O	0	0.7484481101	3.7542244084	2.5662057968
H	0	0.3489593806	2.8950481340	2.3433544079
H	0	1.4843186628	3.8253116319	1.9138174411
O	0	-3.4381617164	-0.7720894235	-4.1582538926

H	0	-4.1695516008	-1.0890365763	-3.5956754107
H	0	-2.8949955350	-1.5771977625	-4.3049655283
O	0	-4.7055056114	-2.5337262873	-2.1782515958
H	0	-3.8731361709	-2.1850420708	-1.7728049846
H	0	-5.1339957276	-3.0260775171	-1.4523379169
O	0	2.2199288906	3.7068050343	-1.7064236483
H	0	2.6043536305	3.6864532588	-0.7985646135
O	0	5.8494487452	2.4257331885	-1.2721626128
H	0	5.3781538640	2.6638680373	-0.4205826656
H	0	6.3247602828	3.2443901890	-1.4912856113
O	0	4.1468943483	3.2142890007	-3.4703478177
H	0	4.7001874415	2.6840001457	-2.8620458625
O	0	7.3946021951	2.1417527223	2.1893624642
H	0	6.5860536439	2.6604229023	1.9189968175
H	0	7.0667748711	1.5076645750	2.8454349691
O	0	2.2026470457	-1.1210659787	-2.6092203668
H	0	1.4875781418	-0.8529452450	-1.9897454851
H	0	-1.1610664564	-4.8098283335	5.0183026848
H	0	3.4555960078	3.5557413258	-2.8308314056
Cl	0	7.6228142991	-2.2669633695	-0.1473241828
H	0	2.3799874839	-0.2142751265	-2.9829855339
O	0	-0.3038077520	0.4510514638	-4.5315981269
H	0	0.1086743069	-2.3773361288	-4.5776316892
O	0	0.9474820141	-1.9717078669	-4.8659242410
H	0	0.0888924370	-0.4252672690	-4.7738739247
H	0	1.4256197946	-1.7641662498	-4.0168616447
H	0	0.5049851916	0.9599370748	-4.2428018044

L_S$_{3b}$

E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.949341 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.384119 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.625083 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.784931 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.71088 au

Mn	0	1.2026567341	2.4617367670	-1.7102069123
Mn	0	-0.9403051972	-2.3114196954	-0.8411880057
Mn	0	-0.1490088652	0.9241151642	0.1678821398
Mn	0	-2.6923466744	-0.4629305833	0.2907267529
O	0	0.2609364932	0.7939227499	-1.5341224257
O	0	-1.9632058070	1.0510045249	-0.3222596139
O	0	-2.4825212832	-1.3747165100	-1.2785016114
O	0	-0.9403980361	-1.0517113613	0.6112382855
Ca	0	-1.7579741931	0.5006386424	-2.7828353421
C	-1	0.5895949528	4.5729229981	-5.5828429884
H	-1	0.6666599395	5.5019049992	-5.0373319884
H	-1	0.7852449517	4.6536600009	-6.6416569884
H	0	1.3799316290	3.9309324027	-5.1727887370
C	0	-0.7648580345	3.8917736443	-5.2987671819
H	0	-0.8671553851	2.9803061545	-5.8988637985
H	0	-1.6038580852	4.5394664240	-5.5917573704
C	0	-1.0113269944	3.4496189253	-3.8372444375
O	0	-1.9916268611	2.6527129989	-3.6458506805
O	0	-0.2502776412	3.8612626417	-2.9212253599
C	-1	-3.0556308863	-6.6294560543	-5.4205379884
H	-1	-2.1018928794	-7.1069990406	-5.5900649884
H	-1	-3.7859598845	-6.7541000648	-6.2063349884
H	0	-3.4898752248	-7.1860932724	-4.5733341500
C	0	-2.7785786731	-5.2135778675	-4.9579199965
H	0	-3.6971153306	-4.6812410335	-4.6800087824
H	0	-2.2795612425	-4.6260225986	-5.7347881344

```
C    0   -1.8625813284   -5.3352928754   -3.7389546372
H    0   -1.0042339079   -5.9762493464   -3.9910617058
H    0   -2.3787067309   -5.8084652793   -2.8983400523
C    0   -1.2948256999   -4.0196314848   -3.3014809232
O    0   -0.9475546398   -3.1941058989   -4.1866984866
O    0   -1.1882340908   -3.8592009318   -2.0357174263
C   -1    4.9370080867   -4.7518219395    0.9588890116
H    0    5.6930347923   -5.5170485781    1.1720275457
H    0    5.2680646945   -4.1985100147    0.0763051937
C    0    4.8185498728   -3.8262498465    2.1659770735
O    0    4.2337043768   -4.2047671194    3.2033677262
C    0    3.5834489250   -5.4685754517    0.6914740033
H    0    3.3722619411   -6.1292261421    1.5403729109
H    0    3.6751777855   -6.0945813570   -0.2001738234
C    0    2.4456515111   -4.5090905482    0.5084871648
N    0    2.1685312165   -3.5744663864    1.4958029257
H    0    2.6368883853   -3.5588263553    2.4006263988
C    0    1.5669451715   -4.2171617815   -0.5076660954
H    0    1.4252934936   -4.6996317071   -1.4620881905
C    0    1.2208845186   -2.7398721517    1.0604026525
H    0    0.9077410548   -1.8490337684    1.5683792777
N    0    0.8046797647   -3.1144475856   -0.1428499753
N    0    5.2373221087   -2.5646189815    1.9843627295
H    0    5.8013544653   -2.3588964054    1.1530293139
C   -1    4.9514690399   -1.4902119393    2.9278120116
H    0    5.8528590638   -0.8694345185    3.0084979460
H    0    4.7672197314   -1.9412815483    3.9052464852
C    0    3.7570748778   -0.6179450100    2.5033364550
H    0    3.5971456675    0.1521240032    3.2686597377
H    0    2.8525322540   -1.2272744874    2.4947124160
C    0    3.9619698519    0.0347072501    1.1355846924
H    0    4.4140016750   -0.6794097965    0.4349544188
H    0    4.6615333509    0.8763243725    1.2018724866
C    0    2.7272155395    0.5628297730    0.4114877309
O    0    2.9171546339    1.1206150949   -0.6838314263
O    0    1.5720026066    0.3398645452    0.9488956798
C   -1   -5.5617049247   -3.9532880903    2.1527060116
H    0   -5.4294856220   -3.2059477952    2.9424923881
H    0   -6.0706835778   -4.8153601812    2.6023884148
C    0   -4.2081520770   -4.3972950398    1.5982750472
H    0   -4.3506618303   -5.1230789392    0.7919216493
H    0   -3.6436641479   -4.9170439045    2.3823520561
C    0   -3.2896046348   -3.3054087056    1.0399355175
O    0   -3.6461252006   -2.0874737704    1.1607037792
O    0   -2.2086256481   -3.6981166421    0.5274985961
C    0   -6.4710421508   -3.3950521082    1.0621328610
O    0   -6.3138986734   -3.6580705022   -0.1392328279
N    0   -7.5082181429   -2.6429808084    1.5002115298
H    0   -7.5284825123   -2.3612847877    2.4708465222
C   -1   -8.5007929519   -2.0610131325    0.6038910116
H    0   -9.4184259094   -1.8788632598    1.1634999769
H    0   -8.6978007672   -2.7786757207   -0.1977460374
C    0   -8.0397321771   -0.7084357868    0.0129161060
O    0   -8.5643927463    0.3489027930    0.3655701126
N    0   -7.0406722434   -0.7964463328   -0.8999672912
H    0   -6.6231090291   -1.7012856734   -1.0912909640
C    0   -6.4233477112    0.3622110149   -1.5157485711
H    0   -6.6116085055    0.3792817379   -2.5932825748
H    0   -6.8792961879    1.2525075528   -1.0713830615
C    0   -4.9023347252    0.4258660002   -1.3121143341
```

O	0	-4.1858259640	0.8027284010	-2.2536476578
O	0	-4.5040588672	0.0884435542	-0.1296005510
C	-1	-3.4330100334	3.6165419403	4.9894840116
H	-1	-3.4717290291	3.3132149397	6.0252910116
H	-1	-4.2385360429	4.2759859287	4.7020210116
H	0	-2.5123700152	4.2094678502	4.8864275625
C	0	-3.4139940376	2.5000914438	3.9474173342
H	0	-3.4399097844	2.9746641272	2.9583634784
H	0	-4.3122294090	1.8757541330	4.0086707974
C	0	-2.1619438214	1.6172526066	4.0305422658
H	0	-2.3213679765	0.8299776426	4.7758910398
H	0	-1.2883355501	2.2017858400	4.3330612007
C	0	-1.8645451364	0.9997975148	2.6785258130
O	0	-0.7281577677	1.2193559138	2.1737860321
O	0	-2.7987445912	0.3107929676	2.1471514757
C	-1	-5.4172531120	9.0845519118	2.0431340116
H	-1	-5.2902851060	8.6646219136	3.0300190116
H	-1	-6.4481091156	9.3395708970	1.8465290116
H	0	-4.8635290250	10.0328516704	2.0360098651
C	0	-4.8475934225	8.1502913266	0.9747045566
H	0	-3.7649850270	8.0687911269	1.1455957030
H	0	-4.9622998029	8.5973145246	-0.0218592267
C	0	-5.4980368041	6.7614967741	0.9842298744
H	0	-6.5584468627	6.8524746017	0.7174848438
H	0	-5.4581040705	6.3361866507	1.9963392266
C	0	-4.8419404751	5.7758182122	0.0132277710
H	0	-4.8859949832	6.1649968853	-1.0136661362
H	0	-5.3706534177	4.8181080167	0.0317312873
N	0	-3.4562178387	5.5282450681	0.4066054546
H	0	-2.9317772265	6.2999332160	0.7928760347
C	0	-2.7853958150	4.3752374599	0.2388665454
N	0	-3.2989374689	3.3998939123	-0.5234245164
H	0	-2.8102969750	2.4884758168	-0.5320711599
H	0	-3.8411551328	3.6337890879	-1.3430912411
N	0	-1.6418025148	4.1658898278	0.8916517704
H	0	-1.3060103370	4.8070324939	1.5977776861
H	0	-0.9184547830	3.5223012084	0.5008562173
C	-1	-1.0710009613	-1.4051200258	7.4960440116
H	-1	-0.0759509668	-1.0220410115	7.3241700116
H	-1	-1.2558899583	-1.6175210284	8.5386700116
H	0	-1.8047323536	-0.6704275567	7.1477030935
C	0	-1.2356685426	-2.7582565145	6.7769478762
H	0	-2.2196624321	-3.1826102208	7.0193247695
H	0	-0.4960322387	-3.4661521594	7.1741146949
C	0	-1.1092577506	-2.7184302167	5.2878809475
N	0	-1.1548758401	-3.8770167262	4.5198983340
C	0	-1.0066888572	-1.6961663290	4.3845960609
H	0	-0.8984437488	-0.6399694587	4.5450336906
C	0	-1.0979429645	-3.5714147213	3.2173339608
H	0	-1.1334212951	-4.2578376385	2.3867997725
N	0	-1.0233640222	-2.2470246541	3.1163713932
H	0	-1.0248541275	-1.7308548704	2.1986998585
C	-1	3.8046929309	6.0999700442	2.3975030116
H	-1	4.6815179239	6.5840300568	1.9934250116
H	-1	3.3433429234	6.6184160376	3.2250110116
H	0	3.0497993105	6.0323468804	1.6068271962
C	0	4.1962378694	4.6640683715	2.8404529776
H	0	5.1570745870	4.6633926954	3.3663618187
H	0	3.4268310953	4.2711332699	3.5148284504
C	0	4.2312421167	3.7437466926	1.6205609018

O	0	3.1248291388	3.5353223425	1.0679008731
O	0	5.3479226254	3.2823993839	1.2014500858
C	-1	12.0313790560	-2.6144418376	-0.6433289884
H	-1	13.0816950525	-2.3673548225	-0.6900259884
H	-1	11.7958140687	-3.4961698410	-1.2207879884
H	0	11.8146047869	-2.8818159609	0.4007473863
C	0	11.1500829160	-1.4136164588	-1.0578478085
H	0	11.6090944633	-0.8972907477	-1.9135127943
H	0	10.1707355573	-1.7733788688	-1.3943500595
C	0	10.9339860383	-0.4202642285	0.0993715410
H	0	10.2067269388	-0.8546262219	0.7993142805
H	0	11.8711299621	-0.3098742256	0.6632179788
C	0	10.4931807329	0.9936297486	-0.3177252667
H	0	10.4144726823	1.6316350154	0.5732747320
H	0	11.2806121162	1.4356903655	-0.9431542677
C	0	9.1944960302	1.1184591361	-1.1168949473
H	0	9.0757074622	2.1484598248	-1.4648217206
H	0	9.1926786342	0.4652129659	-1.9932494422
N	0	7.9637600652	0.7910455572	-0.3289795373
H	0	7.1309375102	1.2209332849	-0.7930019880
H	0	7.8112305839	-0.2440993408	-0.2642921278
H	0	7.9633608620	1.2068997739	0.6330716164
O	0	1.8481570256	1.8749065620	-3.4436454021
H	0	2.6344420676	2.4076463962	-3.6955206576
O	0	0.3384509613	2.5982731587	0.0171544504
O	0	0.7970427685	3.7244742340	2.6796120598
H	0	0.3331330253	2.8987141351	2.4559348542
H	0	1.5324851702	3.7261573028	2.0245624562
O	0	-2.8917092743	-1.1481940244	-4.2492269644
H	0	-3.6365671947	-1.5350952698	-3.7498951108
H	0	-2.2722699326	-1.8979686444	-4.3819724598
O	0	-4.6691621492	-2.5462917169	-2.2480610624
H	0	-3.8831328575	-2.1774400818	-1.7710037337
H	0	-5.0761453502	-3.1586077958	-1.6078319516
O	0	2.2931827031	3.9738757303	-1.5286599905
H	0	2.6863206659	3.8473394915	-0.6343657214
O	0	5.9114316123	2.4465852007	-1.2888915448
H	0	5.4825742882	2.6780851101	-0.4123194966
H	0	6.4005066047	3.2569158341	-1.5093520248
O	0	4.1588491585	3.4794702475	-3.3598290430
H	0	4.6894888320	2.8672991582	-2.8120951395
O	0	7.5406859388	2.0663465557	2.1352985842
H	0	6.7407670921	2.6094431218	1.8910252407
H	0	7.2072264212	1.4248145984	2.7814077479
O	0	2.5276147940	-0.6148293458	-2.8832914993
H	0	2.8029054220	-0.3852251659	-1.9762146755
H	0	-1.2196429305	-4.8200424904	4.8833922637
H	0	3.5011343987	3.8115856494	-2.6797106753
Cl	0	7.4328905744	-2.2925818540	-0.3783992489
H	0	2.3093536948	0.3183137799	-3.1985488470
O	0	0.0016699353	-1.4166629987	-2.6357709607
H	0	0.2881581133	-0.2233332123	-4.7710322749
O	0	-0.1299329964	0.6495099864	-4.7114866127
H	0	0.9540909773	-1.0916301725	-2.6242260909
H	0	0.6087826121	1.2293048956	-4.3503359948
H	0	-0.1220750214	-2.1016558208	-3.3454288142

L_S$_{3c}$-fixed
E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.916203 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.350413 au

G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.587982 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.748628 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.67607 au

Mn	0	1.1890074105	2.2786129629	-1.9066518891
Mn	0	-1.0634066737	-2.5074010015	-0.6158423586
Mn	0	-0.1128450799	0.8667445760	0.0605220704
Mn	0	-2.6866099360	-0.4232910409	0.2740173476
O	0	0.3357270601	0.6514866988	-1.6235961003
O	0	-1.9056833451	1.0191642282	-0.4529558174
O	0	-2.5689817331	-1.4867387862	-1.1649268860
O	0	-0.9546680962	-1.0540602629	0.6031650247
Ca	0	-1.7265699152	0.1134653662	-2.8036103310
C	-1	0.5778431166	4.4089505099	-5.7697976905
H	-1	0.6562359091	5.3539733247	-5.2527712542
H	-1	0.7699306988	4.4578455621	-6.8312100874
H	0	1.3849237414	3.7904328818	-5.3545754018
C	0	-0.7546074036	3.6983427483	-5.4604441729
H	0	-0.8992019839	2.8471723042	-6.1362097906
H	0	-1.6132132543	4.3629820765	-5.6328336155
C	0	-0.8829600238	3.1320806006	-4.0310764494
O	0	-1.7802310588	2.2632291683	-3.8279053349
O	0	-0.0838364509	3.5624088938	-3.1417740257
C	-1	-3.0609674761	-6.7849968512	-5.2580362945
H	-1	-2.1075483226	-7.2670265004	-5.4162870317
H	-1	-3.7938383461	-6.9335583994	-6.0372813579
H	0	-3.5019769499	-7.3700174998	-4.4303356103
C	0	-2.8795146461	-5.3687621955	-4.7528091572
H	0	-3.8332539133	-4.8274082267	-4.7208602673
H	0	-2.2057961218	-4.8009364773	-5.3989631970
C	0	-2.2904341815	-5.4584452681	-3.3401980874
H	0	-1.6374191933	-6.3418855745	-3.2683074597
H	0	-3.0687066052	-5.5914552101	-2.5820394959
C	0	-1.4169172333	-4.2867015658	-2.9792703799
O	0	-0.8251154638	-3.6833110177	-3.9008625791
O	0	-1.3307259520	-4.0295210520	-1.7211430792
C	-1	4.9518480612	-4.7127103658	1.0352374957
H	0	5.6542351431	-5.5137515050	1.2910558211
H	0	5.3348046991	-4.1997933095	0.1495786783
C	0	4.8344611958	-3.7507474892	2.2125038873
O	0	4.2280006201	-4.0884144521	3.2512854171
C	0	3.5620618517	-5.3724955159	0.7491146137
H	0	3.3383234526	-6.0433896460	1.5875772212
H	0	3.6412471458	-5.9917364877	-0.1486795136
C	0	2.4068970076	-4.4172946515	0.5793491206
N	0	2.1956278141	-3.4063995079	1.5040166862
H	0	2.7143489594	-3.3215323940	2.3747979947
C	0	1.3832579355	-4.2685772487	-0.3310476309
H	0	1.1562326847	-4.8353820641	-1.2195690779
C	0	1.1426914381	-2.6733669579	1.1343615362
H	0	0.8539324743	-1.7547196424	1.6054367280
N	0	0.5883332778	-3.1821418388	0.0372131056
N	0	5.2598043205	-2.4958713673	1.9959164432
H	0	5.8550576850	-2.3228682445	1.1789245189
C	-1	4.9711473791	-1.3932762509	2.9049845171
H	0	5.8800668496	-0.7831755813	2.9841033068
H	0	4.7676855398	-1.8152553995	3.8917483594
C	0	3.7984722981	-0.5129017466	2.4457471732
H	0	3.6611192644	0.2921006698	3.1790553244
H	0	2.8757499421	-1.0937093248	2.4603846635
C	0	4.0155163893	0.0750352871	1.0525915082

H	0	4.4228831809	-0.6884391601	0.3769525098
H	0	4.7489617514	0.8888978063	1.0737140961
C	0	2.7856038757	0.6060084117	0.3281131699
O	0	2.9810857153	1.1805724882	-0.7622930844
O	0	1.6332849122	0.3572786391	0.8511461278
C	-1	-5.5432557804	-3.8830183802	2.2395015476
H	0	-5.4475621975	-3.1362823437	3.0343629015
H	0	-6.0098273633	-4.7732159715	2.6791702772
C	0	-4.1561358820	-4.2706873705	1.6905270808
H	0	-4.2638886621	-4.9975373720	0.8793061571
H	0	-3.5774686436	-4.7725460903	2.4762398242
C	0	-3.2805457190	-3.1386472026	1.1469745674
O	0	-3.6784092260	-1.9433933078	1.2831436228
O	0	-2.1727731480	-3.4498933751	0.6052278914
C	0	-6.4647592892	-3.3708827064	1.1384679423
O	0	-6.3256633302	-3.6977436073	-0.0483238667
N	0	-7.4887640839	-2.5875003831	1.5540066412
H	0	-7.4860354920	-2.2489769153	2.5064743466
C	-1	-8.4884634692	-2.0394893990	0.6442215342
H	0	-9.4005780689	-1.8311395200	1.2036431138
H	0	-8.6940934276	-2.7893301503	-0.1251452075
C	0	-8.0316559797	-0.7135922187	-0.0103156442
O	0	-8.5823472373	0.3519947926	0.2736929351
N	0	-7.0108910422	-0.8314854001	-0.8945030114
H	0	-6.5797539503	-1.7380083816	-1.0499883164
C	0	-6.4100461141	0.3038058068	-1.5699957302
H	0	-6.5984687498	0.2609292735	-2.6466376564
H	0	-6.8791382093	1.2083914926	-1.1708301647
C	0	-4.8888077393	0.3922318442	-1.3691714581
O	0	-4.1656403346	0.6712901927	-2.3391726992
O	0	-4.4943748597	0.1762737006	-0.1559298613
C	-1	-3.4091007606	3.7697107746	4.8399033336
H	-1	-3.4442189006	3.4977005294	5.8844987866
H	-1	-4.2159226275	4.4198585048	4.5354021488
H	0	-2.5005942747	4.3802481973	4.7258414114
C	0	-3.3524087921	2.6177158328	3.8444894668
H	0	-3.5325483513	3.0249726705	2.8421672523
H	0	-4.1454064655	1.8830607692	4.0211216216
C	0	-1.9845402981	1.9367058103	3.8445527789
H	0	-1.9023285994	1.2683459206	4.7105209956
H	0	-1.1820373488	2.6735267459	3.9373517727
C	0	-1.7525780210	1.1725074379	2.5590253270
O	0	-0.6078991349	1.2807018010	2.0308817244
O	0	-2.7210609808	0.4883058863	2.1005171895
C	-1	-5.4059833308	9.1456674396	1.7368585142
H	-1	-5.2755166250	8.7557035308	2.7355130198
H	-1	-6.4376200948	9.3942140769	1.5361043175
H	0	-4.8329168644	10.0782632497	1.6680753505
C	0	-4.8686888658	8.1115382390	0.7376526265
H	0	-3.7813403344	8.0323038472	0.8783947362
H	0	-5.0121811470	8.4547381941	-0.2951900634
C	0	-5.5318456102	6.7360075679	0.9135905988
H	0	-6.5855550163	6.7981744859	0.6163462966
H	0	-5.5207695647	6.4477553255	1.9739875351
C	0	-4.8740907892	5.6156205576	0.1035177066
H	0	-4.8293784702	5.8951989300	-0.9593292446
H	0	-5.4672990919	4.6982384261	0.1877365996
N	0	-3.5318984985	5.3410807545	0.6201244037
H	0	-3.0538774686	6.0989267960	1.0876322485
C	0	-2.7591783014	4.3009936392	0.2406733449

N	0	-3.1830858939	3.4263358348	-0.6735290088
H	0	-2.7157633879	2.5050826881	-0.7450282458
H	0	-4.0011239146	3.5995486282	-1.2357867306
N	0	-1.5683811420	4.1125168728	0.8094496029
H	0	-1.2358324584	4.6668722302	1.5862908233
H	0	-0.8573439021	3.4999152819	0.3582236082
C	-1	-1.0361501113	-1.1731851579	7.4886583731
H	-1	-0.0418768409	-0.7950359867	7.3020045355
H	-1	-1.2174610996	-1.3541676277	8.5378186851
H	0	-1.7722674659	-0.4485643809	7.1243529594
C	0	-1.2133269113	-2.5514337484	6.8190458458
H	0	-2.1914641864	-2.9675907486	7.0971814594
H	0	-0.4643334521	-3.2433844446	7.2256356350
C	0	-1.1130595618	-2.5577641548	5.3282976589
N	0	-1.0162516129	-3.7348825865	4.5947714863
C	0	-1.1552373979	-1.5595719556	4.3948311061
H	0	-1.2109591162	-0.4969009408	4.5259850869
C	0	-1.0065457502	-3.4617210724	3.2831829152
H	0	-0.9468651264	-4.1732403277	2.4763362122
N	0	-1.1017119300	-2.1416656176	3.1443628334
H	0	-1.1081647388	-1.6454254387	2.2121132173
C	-1	3.8186487799	6.1770061096	2.1501651375
H	-1	4.6938728037	6.6490476089	1.7287685900
H	-1	3.3597803013	6.7199438358	2.9632198821
H	0	3.0609030132	6.1068508648	1.3626310715
C	0	4.1914826319	4.7431699733	2.6066119111
H	0	5.1425664524	4.7302103527	3.1487161730
H	0	3.4041759685	4.3538710085	3.2619596024
C	0	4.2413178094	3.8377656230	1.3803384691
O	0	3.1421616765	3.6945603937	0.7817318821
O	0	5.3433252138	3.3294683997	0.9963522363
C	-1	12.0397365726	-2.6215575583	-0.6542917762
H	-1	13.0897614866	-2.3755464008	-0.7119146926
H	-1	11.8027144909	-3.5203762826	-1.2041464846
H	0	11.8188090422	-2.8491753638	0.3978775107
C	0	11.1643568317	-1.4360492748	-1.1213508989
H	0	11.6275051508	-0.9588022841	-1.9973592617
H	0	10.1850238719	-1.8083715151	-1.4429513423
C	0	10.9482308733	-0.3950926605	-0.0082931981
H	0	10.2200638918	-0.8025675273	0.7059975860
H	0	11.8849792528	-0.2579371031	0.5502934608
C	0	10.5012241329	0.9967452523	-0.4869446998
H	0	10.4240784217	1.6751076657	0.3739264206
H	0	11.2816525289	1.4134750643	-1.1379458880
C	0	9.1960793352	1.0739460993	-1.2807519663
H	0	9.0595031278	2.0874074906	-1.6683570954
H	0	9.1951277046	0.3858102726	-2.1298505791
N	0	7.9791115433	0.7604479234	-0.4657853832
H	0	7.1356791833	1.1434621761	-0.9427446777
H	0	7.8564804355	-0.2741881952	-0.3347304276
H	0	7.9784460340	1.2298367162	0.4708813688
O	0	2.0080797877	1.6198902323	-3.5213221422
H	0	3.4397541910	2.5166984154	-3.6855190500
O	0	0.3676556877	2.5494262913	-0.2060155419
O	0	0.8802732457	3.7238327842	2.4861276046
H	0	0.4716643927	2.8615458645	2.2862271221
H	0	1.5769709005	3.7862002128	1.7949823484
O	0	-2.8491845638	-1.6221380172	-4.2068971862
H	0	-3.5555567282	-2.0465686253	-3.6756428173
H	0	-2.1576637559	-2.3104780411	-4.2956595947

```
O    0   -4.7308945246   -2.5726680460   -2.1943457107
H    0   -3.9622366425   -2.1863583820   -1.6901534066
H    0   -5.0616298811   -3.2869025745   -1.6215299112
O    0    2.4087265802    3.9305739181   -1.7079085367
H    0    2.8026803329    3.7984704217   -0.7936815836
O    0    5.9502287920    2.4523787273   -1.4503532012
H    0    5.5076276743    2.6910352515   -0.5825671468
H    0    6.5008683727    3.2320757383   -1.6339635356
O    0    4.1868577456    3.1632414093   -3.5258910621
H    0    4.7636188691    2.7108055750   -2.8708677873
O    0    7.5674863228    2.1482457111    1.9417894637
H    0    6.7607798072    2.6778402855    1.7023081103
H    0    7.2575209954    1.5260525795    2.6178416955
O    0    2.5285496798   -1.1027935928   -2.4843638027
H    0    2.7028835708   -0.4348346897   -1.8003363300
H    0   -0.9554646903   -4.6671937084    4.9852855487
H    0    3.1503634030    3.8086593049   -2.3747669702
Cl   0    7.5810971952   -2.3241348716   -0.2249655491
H    0    2.3145560353    0.7115953408   -3.3001023857
O    0   -0.0743284234   -1.6527335263   -2.4193868747
H    0    0.2988513415   -0.7140468714   -3.8915751379
O    0    0.0471090740   -0.0379532101   -4.5729034914
H    0    1.5440851723   -1.2926612975   -2.3706275591
H    0    0.6708486436    0.7047806127   -4.3765377924
H    0   -0.1362628958   -2.4388742022   -2.9944217663
```

L_S$_{3c}$
E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.953008 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.386181 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.624601 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.785558 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.712237 au

```
Mn   0    1.1501573746    2.3742872103   -1.7471705410
Mn   0   -0.8470803043   -2.1917619321   -0.9109566356
Mn   0   -0.1810575837    0.9545341805    0.1976620287
Mn   0   -2.6817999190   -0.4366082865    0.3212321020
O    0    0.2728092197    0.7396198550   -1.4966280116
O    0   -1.9657827455    1.0887641722   -0.3214023139
O    0   -2.4706326794   -1.3537280167   -1.2343625088
O    0   -0.9237974782   -0.9526633338    0.6635489810
Ca   0   -1.7903932026    0.4062545437   -2.7773812887
C   -1    0.5989229613    4.4660889948   -5.6995839734
H   -1    0.6768259568    5.4066829951   -5.1744709734
H   -1    0.7953829610    4.5233949957   -6.7597749734
H    0    1.3985563195    3.8406136311   -5.2809614739
C    0   -0.7395201508    3.7800283038   -5.3746376375
H    0   -0.8595776964    2.8661332767   -5.9690098056
H    0   -1.5957628523    4.4178454646   -5.6346669944
C    0   -0.9156601342    3.3382060873   -3.9063224637
O    0   -1.9076066455    2.5887851746   -3.6482823551
O    0   -0.0664841957    3.7177264476   -3.0448470956
C   -1   -3.0608989852   -6.7253880227   -5.2948109734
H   -1   -2.1076659829   -7.2077450182   -5.4531879734
H   -1   -3.7908639845   -6.8662580262   -6.0782009734
H    0   -3.4995199032   -7.2862408882   -4.4508240218
C    0   -2.8344700503   -5.3074009303   -4.8386873970
H    0   -3.7778976646   -4.7720437493   -4.6707908486
H    0   -2.2620580065   -4.7354797885   -5.5734774473
C    0   -2.0541494413   -5.3992627651   -3.5328231850
H    0   -1.2434670766   -6.1372871105   -3.6351281111
```

```
H    0   -2.6853798034   -5.7467160022   -2.7082927905
C    0   -1.4006877112   -4.1056804771   -3.1563856366
O    0   -1.0912849703   -3.3124397527   -4.0865763588
O    0   -1.1857232955   -3.9364444694   -1.9102265691
C   -1    4.9299080052   -4.7188769845    1.0475710266
H    0    5.6615583270   -5.4954656605    1.3009581293
H    0    5.2987366303   -4.1920782883    0.1637882021
C    0    4.7966728099   -3.7652515116    2.2298299563
O    0    4.2015404091   -4.1170524048    3.2702920890
C    0    3.5693125940   -5.4104429338    0.7503376468
H    0    3.3229876271   -6.0618837306    1.5971281873
H    0    3.6723487428   -6.0439714854   -0.1347042959
C    0    2.4562786855   -4.4300854328    0.5326822734
N    0    2.1574910279   -3.5022122522    1.5204405038
H    0    2.6009007074   -3.4939793286    2.4372394870
C    0    1.6209911274   -4.1129933298   -0.5121401774
H    0    1.5054681534   -4.5806867471   -1.4771318757
C    0    1.2375469040   -2.6497193906    1.0586717390
H    0    0.9139480692   -1.7629436800    1.5657012769
N    0    0.8621294782   -3.0045382710   -0.1624635367
N    0    5.2204328870   -2.5086494356    2.0210963680
H    0    5.7980632586   -2.3271308601    1.1940069140
C   -1    4.9472739894   -1.4149989844    2.9446890266
H    0    5.8532217770   -0.7984279684    3.0062731357
H    0    4.7693333748   -1.8461779957    3.9324625247
C    0    3.7554622605   -0.5422220597    2.5197822857
H    0    3.6126945394    0.2438034984    3.2723424979
H    0    2.8453345011   -1.1430697959    2.5323151604
C    0    3.9523115220    0.0810129083    1.1388929352
H    0    4.3524370011   -0.6638313774    0.4384946536
H    0    4.6884344060    0.8924910642    1.1729093830
C    0    2.7188603091    0.6401101307    0.4416971111
O    0    2.9089209379    1.2010220609   -0.6586983947
O    0    1.5719402100    0.4354478572    0.9920823071
C   -1   -5.5685579988   -3.8809950347    2.2163400266
H    0   -5.4501789314   -3.1261743408    3.0011303314
H    0   -6.0696202565   -4.7463414676    2.6686182517
C    0   -4.2017084381   -4.3166683483    1.6741843963
H    0   -4.3349310618   -5.0513236763    0.8742640807
H    0   -3.6428643232   -4.8274890343    2.4682901589
C    0   -3.2706267584   -3.2315166560    1.1097631462
O    0   -3.6425320574   -2.0099493476    1.2096381167
O    0   -2.1833461986   -3.6153327267    0.6215932458
C    0   -6.4761194897   -3.3440788608    1.1143920763
O    0   -6.3197912082   -3.6328606147   -0.0810664704
N    0   -7.5126859252   -2.5805553909    1.5348737690
H    0   -7.5336145699   -2.2768895655    2.4987847121
C   -1   -8.5041620077   -2.0192970488    0.6244620266
H    0   -9.4259604131   -1.8335034104    1.1761404598
H    0   -8.6926148066   -2.7517788634   -0.1657316329
C    0   -8.0497827933   -0.6750376719    0.0116177373
O    0   -8.5937326533    0.3835931512    0.3308063776
N    0   -7.0343358666   -0.7713861543   -0.8811744580
H    0   -6.6026899994   -1.6748601731   -1.0469967264
C    0   -6.4186245661    0.3808700476   -1.5096561765
H    0   -6.6024421511    0.3837003612   -2.5881881069
H    0   -6.8791589531    1.2757005260   -1.0792330857
C    0   -4.8987371541    0.4489602325   -1.2998957396
O    0   -4.1824409330    0.8225672730   -2.2449095982
O    0   -4.5020894628    0.1202868536   -0.1171247751
```

C	-1	-3.4319640353	3.7463489755	4.8883350266
H	-1	-3.4717660339	3.4658029753	5.9305020266
H	-1	-4.2364450384	4.4003769716	4.5859570266
H	0	-2.5085928374	4.3317542765	4.7691767523
C	0	-3.4186095208	2.5974986704	3.8893954870
H	0	-3.4300648725	3.0325424711	2.8821425840
H	0	-4.3230250189	1.9842445665	3.9659260229
C	0	-2.1766251505	1.7060629470	4.0251444285
H	0	-2.3649082822	0.9263243021	4.7709496289
H	0	-1.3062260331	2.2863778371	4.3444087210
C	0	-1.8692547573	1.0848740279	2.6820302333
O	0	-0.7418438804	1.3387896576	2.1654241668
O	0	-2.7910066370	0.3757939623	2.1646135423
C	-1	-5.4071670611	9.1511329660	1.8217050266
H	-1	-5.2814010592	8.7527299666	2.8176280266
H	-1	-6.4375610623	9.4031079611	1.6188530266
H	0	-4.8512207284	10.0977006733	1.7934107164
C	0	-4.8460037247	8.1940748526	0.7703655941
H	0	-3.7642313030	8.1053821367	0.9426121604
H	0	-4.9552364173	8.6257436287	-0.2335292449
C	0	-5.5133775828	6.8134177413	0.8019836458
H	0	-6.5693017056	6.9108835233	0.5209740440
H	0	-5.4899762153	6.4092186053	1.8231971853
C	0	-4.8548418765	5.8014284120	-0.1391746503
H	0	-4.8846221364	6.1677119233	-1.1749902913
H	0	-5.3884817153	4.8465692565	-0.1051103423
N	0	-3.4757413266	5.5607382889	0.2793792455
H	0	-2.9690604486	6.3305914686	0.6916234317
C	0	-2.7939918338	4.4128740250	0.1255467334
N	0	-3.2717368938	3.4388775380	-0.6567698922
H	0	-2.7981915583	2.5198677835	-0.6358904828
H	0	-3.8320363728	3.6576190052	-1.4673179570
N	0	-1.6647643109	4.2130661080	0.8075981814
H	0	-1.3538559305	4.8536734099	1.5249591883
H	0	-0.9352915081	3.5693822209	0.4349959028
C	-1	-1.0781250115	-1.2222970133	7.5057800266
H	-1	-0.0824660133	-0.8443420085	7.3262590266
H	-1	-1.2639830106	-1.4116030141	8.5526740266
H	0	-1.8110714543	-0.4955605809	7.1396848441
C	0	-1.2391764066	-2.5904359965	6.8148635367
H	0	-2.2267960035	-3.0073357894	7.0554849439
H	0	-0.5055332457	-3.2911716533	7.2352573491
C	0	-1.0957303406	-2.5797249835	5.3269392104
N	0	-1.1362842810	-3.7516988409	4.5792551949
C	0	-0.9814672172	-1.5742988281	4.4064860060
H	0	-0.8719879985	-0.5157100525	4.5499116168
C	0	-1.0662293147	-3.4686525939	3.2717857691
H	0	-1.1023473394	-4.1679411959	2.4520640277
N	0	-0.9873240598	-2.1468182379	3.1478162427
H	0	-0.9897649637	-1.6424303948	2.2191255951
C	-1	3.8106719532	6.1632270101	2.2476820266
H	-1	4.6883919509	6.6372110143	1.8337220266
H	-1	3.3494409506	6.7002400079	3.0633310266
H	0	3.0559487262	6.0797424189	1.4590350426
C	0	4.1934121643	4.7401191173	2.7352900520
H	0	5.1520223995	4.7466271316	3.2640432869
H	0	3.4172143680	4.3690752024	3.4140060238
C	0	4.2266921998	3.8016284409	1.5369196445
O	0	3.1128552619	3.6128301335	0.9789101531
O	0	5.3296155760	3.3129556264	1.1298401918

```
C   -1   12.0281039952   -2.6261299505   -0.5960859734
H   -1   13.0787689941   -2.3814669455   -0.6474469734
H   -1   11.7917839995   -3.5199759517   -1.1542839734
H    0   11.8065870317   -2.8657623935    0.4535623915
C    0   11.1501670361   -1.4373316398   -1.0479645570
H    0   11.6035179325   -0.9571218328   -1.9274409777
H    0   10.1666417755   -1.8072979342   -1.3600777458
C    0   10.9478159842   -0.3992241511    0.0705910933
H    0   10.2337146313   -0.8081877629    0.7983256642
H    0   11.8927262851   -0.2606503031    0.6149271999
C    0   10.4916436295    0.9933696767   -0.3982412746
H    0   10.4149122757    1.6660057956    0.4671130584
H    0   11.2691584863    1.4168561688   -1.0483586150
C    0    9.1855068134    1.0746383359   -1.1907993665
H    0    9.0516629033    2.0904021908   -1.5731998816
H    0    9.1839481641    0.3912295324   -2.0436723629
N    0    7.9657850619    0.7586670535   -0.3801016532
H    0    7.1249187349    1.1583762807   -0.8479249944
H    0    7.8282643998   -0.2774754685   -0.2766137761
H    0    7.9695674935    1.2073496495    0.5664392868
O    0    1.9761484522    1.7972645413   -3.3846059829
H    0    3.3960333818    2.7145261072   -3.5250194495
O    0    0.3102018706    2.6369937288   -0.0660912839
O    0    0.7813112500    3.8158537530    2.6132609046
H    0    0.3222200282    2.9759810052    2.4336762953
H    0    1.5061529377    3.8021206656    1.9498492290
O    0   -2.9613385407   -1.2326900261   -4.2202855712
H    0   -3.7029547367   -1.6112365603   -3.7084142910
H    0   -2.3334569095   -1.9851665206   -4.3161766647
O    0   -4.6624858500   -2.5370460663   -2.1760067573
H    0   -3.8674539264   -2.1769160288   -1.7076307697
H    0   -5.0668589629   -3.1516092674   -1.5364057640
O    0    2.3579976218    4.0192632628   -1.4824925227
H    0    2.7511862714    3.8394271036   -0.5759899168
O    0    5.9251647334    2.4700423405   -1.3290180830
H    0    5.4898803451    2.6917881721   -0.4528049001
H    0    6.4877878901    3.2464269986   -1.4904266970
O    0    4.1429942263    3.3516939714   -3.3310969111
H    0    4.7256139329    2.8570552130   -2.7126848217
O    0    7.5575049951    2.1092153819    2.0491356930
H    0    6.7534891322    2.6459630884    1.8185058385
H    0    7.2470554092    1.4841065015    2.7222669748
O    0    2.5639561780   -0.8916772107   -2.5808626936
H    0    2.7270046562   -0.3299549825   -1.8017127288
H    0   -1.2073407748   -4.6878565710    4.9586469778
H    0    3.1014775486    3.9330400135   -2.1538262698
Cl   0    7.4860656605   -2.3174185746   -0.2837929491
H    0    2.2998004447    0.8813861019   -3.2172541424
O    0   -0.0715415451   -1.4626406748   -2.6087272955
H    0    0.2504242029   -0.3747882503   -4.0206647082
O    0   -0.0231802740    0.3945423192   -4.5723603033
H    0    1.5931188355   -1.1108117714   -2.5044085696
H    0    0.6537082105    1.0750475028   -4.3118584124
H    0   -0.2717510467   -2.1824390020   -3.2527240293
```

L_S_{3d}-fixed
E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.944638 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.380679 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.621061 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.777295 au

E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.703526 au

```
Mn   0    1.1650084234    2.1859515933   -1.9464084172
Mn   0   -0.8771705360   -2.5793470594   -0.5798445229
Mn   0   -0.1511063742    0.8686785319    0.0613915176
Mn   0   -2.8248992048   -0.4123328066    0.2292510507
O    0    0.2448398821    0.5918254958   -1.6475981601
O    0   -1.9364702993    1.0385050063   -0.4326034100
O    0   -2.2911001892   -1.5139366241   -1.2695572195
O    0   -0.7096108701   -1.1313994628    0.6389136622
Ca   0   -1.9776640030    0.4126987303   -2.7743573303
C   -1    0.6177444893    4.6205058618   -5.6574728316
H   -1    0.6868081559    5.5567468354   -5.1231675508
H   -1    0.8113264898    4.6908643995   -6.7175009232
H    0    1.4087955515    3.9829537065   -5.2427798086
C    0   -0.7364742246    3.9207358187   -5.4253059725
H    0   -0.8836702844    3.1235970470   -6.1643476807
H    0   -1.5760287207    4.6146890430   -5.5715925046
C    0   -0.9134080674    3.2573280071   -4.0507171266
O    0   -1.8740484323    2.4390313125   -3.9196322321
O    0   -0.0929461279    3.5528814616   -3.1333314273
C   -1   -2.9202409299   -6.6131807684   -5.3579142504
H   -1   -1.9622725251   -7.0835846160   -5.5231848048
H   -1   -3.6504740060   -6.7539760894   -6.1411027766
H    0   -3.3472767462   -7.1665514077   -4.5053799011
C    0   -2.6613407524   -5.1799995951   -4.8897655442
H    0   -3.5881569915   -4.6846125361   -4.5749836418
H    0   -2.2163378813   -4.5660938820   -5.6806345044
C    0   -1.6969244995   -5.2709851477   -3.6990067314
H    0   -0.7483941653   -5.7193383804   -4.0314320854
H    0   -2.1034103439   -5.9316431579   -2.9271470747
C    0   -1.3399783960   -3.9512869057   -3.0606829444
O    0   -1.1342473455   -2.9394873202   -3.7622370802
O    0   -1.2400388591   -4.0164470949   -1.7685707756
C   -1    5.0626496949   -4.5844439551    0.9873407015
H    0    5.8762531218   -5.2968520769    1.1699614306
H    0    5.3290060222   -4.0141517228    0.0940078424
C    0    4.9497887626   -3.6556299638    2.1946500529
O    0    4.4004094458   -4.0359973859    3.2510428712
C    0    3.7607480346   -5.4106987119    0.7422297435
H    0    3.6548576767   -6.1305344473    1.5631540115
H    0    3.8831528760   -5.9863185161   -0.1792428282
C    0    2.5005893449   -4.5932526684    0.6585512670
N    0    2.1871312740   -3.7567106248    1.7170474470
H    0    2.7416832283   -3.7009328411    2.5734838624
C    0    1.4846954938   -4.4003908844   -0.2502025742
H    0    1.3274089348   -4.8337485854   -1.2246652587
C    0    1.0876525451   -3.0669857626    1.4293578848
H    0    0.7027055388   -2.3039290421    2.0695988863
N    0    0.5921576930   -3.4486242498    0.2540809957
N    0    5.3729249118   -2.3956122488    2.0069769921
H    0    5.9184773157   -2.1957904339    1.1633018207
C   -1    5.0486401833   -1.2998478058    2.9176238133
H    0    5.9186794938   -0.6332795767    2.9660908816
H    0    4.8882064419   -1.7223210568    3.9117042040
C    0    3.8040154066   -0.5244956539    2.4479880677
H    0    3.5496145580    0.2346873963    3.1982719312
H    0    2.9549579161   -1.2111377641    2.3969178451
C    0    4.0130012483    0.1311010930    1.0830200882
H    0    4.4831632005   -0.5769216555    0.3879228420
H    0    4.6970711016    0.9852368958    1.1521233081
```

C	0	2.7707230610	0.6232202569	0.3487646519
O	0	2.9682983199	1.1727524071	-0.7626860713
O	0	1.6262591065	0.3953882983	0.8774765414
C	-1	-5.4417666317	-3.8719219792	2.1869399951
H	0	-5.3087489522	-3.1326567594	2.9829061523
H	0	-5.9374267475	-4.7462790338	2.6260779551
C	0	-4.0827816429	-4.3030891106	1.6128451151
H	0	-4.2253385312	-5.0275749406	0.8042486707
H	0	-3.4932483218	-4.8081397914	2.3840590176
C	0	-3.2362727335	-3.1701519839	1.0410766634
O	0	-3.7052371779	-2.0036198344	1.0818905769
O	0	-2.0967329816	-3.4905409361	0.5569901943
C	0	-6.3549599302	-3.3181302370	1.0952134569
O	0	-6.2255706671	-3.6296778250	-0.0999101824
N	0	-7.3637477449	-2.5251354590	1.5169596232
H	0	-7.3721033888	-2.2087696756	2.4768588931
C	-1	-8.4002676530	-2.0257247119	0.6200992896
H	0	-9.2854181140	-1.7909777682	1.2120502439
H	0	-8.6415137019	-2.8184018983	-0.0941895299
C	0	-7.9910838441	-0.7385835065	-0.1289590945
O	0	-8.4392604663	0.3597674928	0.2008903387
N	0	-7.1495893278	-0.9400509770	-1.1739766055
H	0	-6.7143886268	-1.8534094245	-1.2509710766
C	0	-6.5360619237	0.1488789193	-1.9080379010
H	0	-6.5477924427	-0.0669411074	-2.9795879779
H	0	-7.1344045112	1.0478108701	-1.7321582570
C	0	-5.0832467692	0.4322907272	-1.4874636715
O	0	-4.3074730906	0.9008360130	-2.3572178766
O	0	-4.7835637148	0.1742999189	-0.2778830968
C	-1	-3.3815322123	3.7507389841	4.9311241093
H	-1	-3.4156233797	3.4595556777	5.9705474167
H	-1	-4.1933861699	4.3993198087	4.6371136732
H	0	-2.4684626525	4.3542662596	4.8194917965
C	0	-3.3522632516	2.6197111606	3.8981076528
H	0	-3.4650923730	3.0807326956	2.9079195042
H	0	-4.2107565385	1.9491351324	4.0148017010
C	0	-2.0510391854	1.8068147321	3.9071971192
H	0	-2.0869772055	1.0585561810	4.7071641400
H	0	-1.1887124049	2.4530990643	4.0947524587
C	0	-1.8315710295	1.1069435642	2.5768159027
O	0	-0.6950268992	1.2631980565	2.0297094143
O	0	-2.7967639531	0.4318087775	2.1031161405
C	-1	-5.4215636744	9.1644949370	1.9234407952
H	-1	-5.2891744374	8.7576793787	2.9150420035
H	-1	-6.4549585888	9.4076464065	1.7253390529
H	0	-4.8521252167	10.0995269963	1.8636269695
C	0	-4.8825411181	8.1344869498	0.9190694352
H	0	-3.7899051134	8.0895308139	1.0310694025
H	0	-5.0668753612	8.4572304727	-0.1138885378
C	0	-5.4991246899	6.7438538024	1.1414746903
H	0	-6.5700007324	6.7784908711	0.9068890846
H	0	-5.4175120010	6.4672966918	2.2017969355
C	0	-4.8679155192	5.6281545170	0.3048255532
H	0	-4.9197035887	5.8801307290	-0.7647582814
H	0	-5.4214835788	4.6956986675	0.4601820150
N	0	-3.4793510147	5.4083776841	0.7141717940
H	0	-2.9721717013	6.2141001668	1.0543212534
C	0	-2.7106133009	4.3823312407	0.2859486319
N	0	-3.1953026856	3.4429009452	-0.5263687628
H	0	-2.7208918789	2.5183545418	-0.5667265530

H	0	-4.0997346116	3.5293986537	-0.9633119427
N	0	-1.4405210840	4.3012618449	0.6858523282
H	0	-1.0937640645	4.7580614249	1.5193093346
H	0	-0.8001359742	3.5968686973	0.2710074590
C	-1	-0.9683221411	-1.2180918262	7.4931350711
H	-1	0.0229383487	-0.8276809912	7.3156011728
H	-1	-1.1495882097	-1.4199830611	8.5386356343
H	0	-1.7172748369	-0.5122163352	7.1208404393
C	0	-1.1430087640	-2.6189202076	6.8855527985
H	0	-2.0963545000	-3.0400970758	7.2369706755
H	0	-0.3610736503	-3.2795146147	7.2871296245
C	0	-1.1194362670	-2.6551340448	5.4043754046
N	0	-1.2401996303	-3.8306058496	4.6892741353
C	0	-1.0302106407	-1.6705041194	4.4531831535
H	0	-0.8897768693	-0.6130172578	4.6019409809
C	0	-1.2229967724	-3.5254235603	3.3685595515
H	0	-1.2518486551	-4.2657231143	2.5859842563
N	0	-1.1070776828	-2.2188643216	3.1917096296
H	0	-0.8227012946	-1.3821864654	1.5980345728
C	-1	3.8287033237	6.2722804833	2.2996023355
H	-1	4.7005857548	6.7598085642	1.8885191021
H	-1	3.3639216154	6.7961246801	3.1216288577
H	0	3.0719213601	6.2700375130	1.5057465783
C	0	4.1470437831	4.7967027505	2.6393505243
H	0	5.0961810515	4.6968184106	3.1757561935
H	0	3.3447000754	4.3877385722	3.2645221674
C	0	4.1643855499	3.9717089510	1.3490704972
O	0	3.0794483298	3.9435575425	0.7084700695
O	0	5.2388298717	3.4023853240	0.9705865759
C	-1	12.1341502009	-2.3987719151	-0.6502769561
H	-1	13.1820327061	-2.1422793840	-0.7013899940
H	-1	11.9062805519	-3.2894689002	-1.2169338004
H	0	11.9243584365	-2.6608920394	0.3965129196
C	0	11.2353579939	-1.2112380107	-1.0703630926
H	0	11.7125248923	-0.6587787786	-1.8928231736
H	0	10.2819064048	-1.5902249034	-1.4553799124
C	0	10.9401838300	-0.2557686535	0.1016765464
H	0	10.1982728245	-0.7323402622	0.7572840724
H	0	11.8496561600	-0.1298243490	0.7059804615
C	0	10.4691362532	1.1536158482	-0.2977290997
H	0	10.3449111681	1.7693200522	0.6038407168
H	0	11.2595021267	1.6336075007	-0.8906295996
C	0	9.1893958562	1.2556338693	-1.1297540109
H	0	9.0490259102	2.2872407932	-1.4648045740
H	0	9.2282346793	0.6159631599	-2.0151792168
N	0	7.9503808262	0.8791108278	-0.3773281962
H	0	7.1149710133	1.2539892727	-0.8768824709
H	0	7.8505618408	-0.1633210200	-0.2974116830
H	0	7.8981236225	1.3114376204	0.5752040561
O	0	1.8833046687	1.4516002123	-3.5850071563
H	0	3.3855367050	2.3170872269	-3.7706363934
O	0	0.3630682149	2.5221531229	-0.2426683202
O	0	0.8479851665	3.7185608554	2.4746708060
H	0	0.4410082429	2.8557128591	2.2727600184
H	0	1.5154710664	3.8204947257	1.7609520865
O	0	-3.2099904216	-1.1743993510	-4.2124132630
H	0	-3.9151161264	-1.5610315937	-3.6525645110
H	0	-2.5502393306	-1.8984247384	-4.2716954158
O	0	-4.4217483711	-2.7757322916	-2.2242672785
H	0	-3.6152485071	-2.3772632053	-1.7899764780

H	0	-4.9501378808	-3.1403760009	-1.4903073452
O	0	2.4156507372	3.8260479151	-1.8173259693
H	0	2.7959553136	3.7870707670	-0.8874757032
O	0	5.8693341230	2.4555056576	-1.4505517011
H	0	5.4145646665	2.7253399512	-0.5986601211
H	0	6.3699663253	3.2524917793	-1.6934601845
O	0	4.1563361794	2.9318802176	-3.6247636062
H	0	4.6990749889	2.5012752137	-2.9278624545
O	0	7.3987811242	2.2159307138	2.0326485507
H	0	6.6057037479	2.7454751759	1.7461854124
H	0	7.0606105154	1.6214499481	2.7197487935
O	0	2.8233850246	-0.9998950065	-2.5058259586
H	0	2.2451474178	0.5704892577	-3.3243285613
H	0	-1.3224037400	-4.7578720346	5.0838916973
H	0	3.1579184239	3.6640660664	-2.4693289759
Cl	0	7.5941281046	-2.2127479357	-0.3569550819
H	0	3.1178506366	-0.3213354587	-1.8672049422
O	0	-0.2658470395	-0.0389558867	-4.4789723037
H	0	0.0850575723	-0.9411205330	-4.5439421798
O	0	0.3783248235	-2.0044759840	-1.7486246474
H	0	1.9489949039	-1.2733238651	-2.1385522960
H	0	-0.0995981950	-1.9637210359	-2.6028921023
H	0	0.5102628164	0.5427096761	-4.2326508327

L_S$_{3d}$
E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.958039 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.393233 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.63546 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.790894 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.716522 au

Mn	0	1.1118768679	2.1975429262	-1.9019581565
Mn	0	-0.9357205820	-2.4787774802	-0.7855505930
Mn	0	-0.1846530279	0.7814332915	0.0637845629
Mn	0	-2.7559240291	-0.4838247926	0.2905505393
O	0	0.1765449521	0.6072402125	-1.6733809025
O	0	-1.9693493537	1.0248100682	-0.3639180517
O	0	-2.2868734099	-1.6013380018	-1.5001128448
O	0	-0.9062670610	-1.1332566703	0.5549014612
Ca	0	-1.9733591097	0.4336602514	-2.7786632060
C	-1	0.5605739123	4.6533689999	-5.5940389561
H	-1	0.6325419087	5.5836990002	-5.0498839561
H	-1	0.7486839120	4.7353060006	-6.6542199561
H	0	1.3511869666	4.0075353564	-5.1906401581
C	0	-0.7934034233	3.9561685699	-5.3617146673
H	0	-0.9321387940	3.1469452194	-6.0893288028
H	0	-1.6325026914	4.6464265476	-5.5275415696
C	0	-0.9866024169	3.3109215771	-3.9799490832
O	0	-1.9586246859	2.5043751820	-3.8551667359
O	0	-0.1745177006	3.6016603441	-3.0546254461
C	-1	-2.9775380435	-6.5825810140	-5.3991569561
H	-1	-2.0205080416	-7.0512410103	-5.5745159561
H	-1	-3.7118310430	-6.7147260169	-6.1800519561
H	0	-3.3934332546	-7.1186852819	-4.5317411858
C	0	-2.6797970198	-5.1466578146	-4.9671702975
H	0	-3.5533676481	-4.6722496012	-4.5026086097
H	0	-2.3795900380	-4.5179042624	-5.8127964940
C	0	-1.5265630698	-5.2329893461	-3.9547853595
H	0	-0.6118710106	-5.5452524692	-4.4782054758
H	0	-1.7459402245	-5.9914929125	-3.1968970698
C	0	-1.2267128494	-3.9298016570	-3.2617160072

O	0	-1.0477232610	-2.8929219085	-3.9473007699
O	0	-1.1680281905	-4.0160561710	-1.9776550910
C	-1	5.0383589488	-4.6241889825	0.9265590439
H	0	5.8853849300	-5.3137817969	1.0260986086
H	0	5.1947919037	-4.0413479844	0.0156722888
C	0	4.9902389600	-3.7114135148	2.1534678345
O	0	4.4999996425	-4.1145780298	3.2285142380
C	0	3.7309897036	-5.4623640689	0.8422441755
H	0	3.6834962917	-6.1060405167	1.7284027290
H	0	3.7752379136	-6.1125081401	-0.0361794954
C	0	2.4944592436	-4.6147277691	0.7578028648
N	0	2.2613777851	-3.6137018341	1.6886972973
H	0	2.8122660545	-3.4946293619	2.5341102031
C	0	1.4655722786	-4.4924278756	-0.1479947429
H	0	1.2616937518	-5.0552250097	-1.0459798260
C	0	1.1846846471	-2.9052801667	1.3121930469
H	0	0.8743585815	-1.9829954653	1.7652065641
N	0	0.6537235814	-3.4329487842	0.2226275837
N	0	5.3610974043	-2.4349480796	1.9595754464
H	0	5.8599903470	-2.2103142460	1.0941189452
C	-1	5.0348319360	-1.3609149825	2.8927210439
H	0	5.9155696798	-0.7119140483	2.9850860844
H	0	4.8456680388	-1.8099930034	3.8694598934
C	0	3.8195773464	-0.5380151736	2.4237492144
H	0	3.6197542567	0.2479832400	3.1633562584
H	0	2.9370278041	-1.1786960558	2.4103712562
C	0	4.0137437035	0.0820477498	1.0378181016
H	0	4.4776113509	-0.6417323533	0.3547073046
H	0	4.6937054465	0.9404455097	1.0778732254
C	0	2.7566995245	0.5477536692	0.3047153688
O	0	2.9414971384	1.1586994601	-0.7767896769
O	0	1.6190319700	0.2312775652	0.7990919599
C	-1	-5.4596060539	-3.9238230238	2.1881860439
H	0	-5.3020090089	-3.1751237956	2.9713900335
H	0	-5.9769064811	-4.7749052680	2.6487410879
C	0	-4.1236086956	-4.3918472832	1.6115288115
H	0	-4.2824314411	-5.1377077050	0.8271685517
H	0	-3.5301932346	-4.8826873155	2.3921599275
C	0	-3.2642320934	-3.2868164905	1.0068951853
O	0	-3.6596814391	-2.0894702190	1.1265922484
O	0	-2.1854245174	-3.6485504626	0.4526607108
C	0	-6.3720265722	-3.3549271596	1.1055760322
O	0	-6.2256474481	-3.6193707389	-0.0975668200
N	0	-7.4032801536	-2.5995820851	1.5477351949
H	0	-7.4269623584	-2.3229798662	2.5196481010
C	-1	-8.4258840613	-2.0603020354	0.6569640439
H	0	-9.3287983210	-1.8707763435	1.2380867266
H	0	-8.6384079438	-2.8103047632	-0.1103749576
C	0	-8.0011344095	-0.7297963091	0.0061598668
O	0	-8.4639330746	0.3460571539	0.3870480042
N	0	-7.1086236448	-0.8651899219	-1.0054847863
H	0	-6.6902558150	-1.7780414834	-1.1525338333
C	0	-6.4915619700	0.2649744801	-1.6650216312
H	0	-6.5983064880	0.1820402564	-2.7501893113
H	0	-7.0165863390	1.1670730724	-1.3362661759
C	0	-4.9960786664	0.4202026722	-1.3563542937
O	0	-4.2703333261	0.9027911564	-2.2498734348
O	0	-4.6204770167	0.0493878593	-0.1882039433
C	-1	-3.3840450838	3.6681449844	5.0049420439
H	-1	-3.4128070826	3.3656069843	6.0412790439

H	-1	-4.1973090864	4.3199839812	4.7222500439
H	0	-2.4903211948	4.3059492770	4.9196644093
C	0	-3.2724026961	2.5413949973	3.9823508963
H	0	-3.5317107923	2.9422101900	2.9937061822
H	0	-3.9873104473	1.7358202489	4.1789533718
C	0	-1.8510913444	1.9801077212	3.9059776187
H	0	-1.6216817911	1.4033601669	4.8137079962
H	0	-1.1176441715	2.7899116900	3.8588956059
C	0	-1.6728737242	1.1050634872	2.6781819085
O	0	-0.5680981111	1.2266470399	2.0536019178
O	0	-2.6125292889	0.3242336700	2.3656086263
C	-1	-5.4387671052	9.1146939763	2.0672790439
H	-1	-5.3013161036	8.6970369768	3.0536710439
H	-1	-6.4731351062	9.3600999722	1.8771970439
H	0	-4.8780920427	10.0565820660	2.0261376078
C	0	-4.8820539621	8.1153892338	1.0427385825
H	0	-3.7881573552	8.0941642814	1.1498175466
H	0	-5.0785383192	8.4541662269	0.0170904935
C	0	-5.4603035291	6.7056624324	1.2381006811
H	0	-6.5351894411	6.7194110087	1.0192114573
H	0	-5.3559073129	6.4035299485	2.2893594333
C	0	-4.8144325932	5.6297387910	0.3616560403
H	0	-4.8858048820	5.9127454408	-0.6992087055
H	0	-5.3478199132	4.6824175057	0.4940463060
N	0	-3.4179710729	5.4167137197	0.7461914484
H	0	-2.8997468097	6.2221020811	1.0696988028
C	0	-2.6711192689	4.3640125942	0.3409260567
N	0	-3.1825719834	3.4268727447	-0.4574142236
H	0	-2.7204876027	2.4960595395	-0.5093480704
H	0	-4.0355680982	3.5705979520	-0.9748274404
N	0	-1.4114404181	4.2416146519	0.7579423477
H	0	-1.0510671577	4.7109284131	1.5782626620
H	0	-0.7757872977	3.5296530314	0.3376402446
C	-1	-0.9583840641	-1.3286620061	7.4999050439
H	-1	0.0320049343	-0.9364280022	7.3215320439
H	-1	-1.1342740633	-1.5419670068	8.5440580439
H	0	-1.6990401862	-0.5940402982	7.1658904265
C	0	-1.1499083898	-2.6871472663	6.7931872087
H	0	-2.1115136197	-3.1190770348	7.1035755368
H	0	-0.3794442563	-3.3839397758	7.1485240959
C	0	-1.1152841768	-2.6623240120	5.2985555109
N	0	-1.0136358009	-3.8281705232	4.5460947588
C	0	-1.2248212656	-1.6544260006	4.3809508988
H	0	-1.3329764775	-0.5977906810	4.5284963193
C	0	-1.0554569599	-3.5379662817	3.2388273491
H	0	-0.9886957765	-4.2349584274	2.4197200279
N	0	-1.1921074573	-2.2198904178	3.1206159409
H	0	-1.1789571257	-1.7133891694	2.1966636250
C	-1	3.8128769062	6.2176420127	2.3639280439
H	-1	4.6826969043	6.7095560161	1.9537020439
H	-1	3.3524319042	6.7325020109	3.1940300439
H	0	3.0523667110	6.2150251329	1.5745602855
C	0	4.1526041492	4.7430534120	2.6865372831
H	0	5.1015928461	4.6509514383	3.2247125384
H	0	3.3550051015	4.3114047070	3.3022624668
C	0	4.1874375116	3.9394456189	1.3827288513
O	0	3.1135394346	3.9350778663	0.7250205022
O	0	5.2612885436	3.3640748691	1.0118663132
C	-1	12.1016339402	-2.4214079547	-0.7235829561
H	-1	13.1492779391	-2.1644729506	-0.7773039561

```
H   -1   11.8707019436   -3.3058269556   -1.2987689561
H    0   11.8966846876   -2.6932788840    0.3217699100
C    0   11.1968904445   -1.2339799533   -1.1302752235
H    0   11.6570724476   -0.6879572929   -1.9665617305
H    0   10.2343250630   -1.6133589618   -1.4927102563
C    0   10.9287550583   -0.2699188110    0.0411819884
H    0   10.2000204206   -0.7384914088    0.7171065511
H    0   11.8505966485   -0.1434853314    0.6263873319
C    0   10.4560107833    1.1392139522   -0.3578739374
H    0   10.3413296664    1.7571796981    0.5433684603
H    0   11.2433146987    1.6152372682   -0.9580154893
C    0    9.1710036191    1.2456375109   -1.1818516312
H    0    9.0364230334    2.2772988081   -1.5189904792
H    0    9.2010274299    0.6038321779   -2.0660860141
N    0    7.9323318777    0.8801365057   -0.4233743732
H    0    7.0985649797    1.2797035646   -0.9075572581
H    0    7.8089503622   -0.1614850505   -0.3653086328
H    0    7.8972913262    1.2924073861    0.5388909977
O    0    1.8224906369    1.5353064384   -3.5852928357
H    0    3.3108614982    2.3942143858   -3.7549436574
O    0    0.3709340840    2.4585479328   -0.1820235172
O    0    0.9066384466    3.6660247508    2.4919133385
H    0    0.5079792676    2.8061681675    2.2542692634
H    0    1.5623113358    3.8052188259    1.7738958710
O    0   -3.1890131387   -1.1335664460   -4.2791173808
H    0   -3.8984052968   -1.5248330016   -3.7308827633
H    0   -2.5044518686   -1.8393478640   -4.3003668605
O    0   -4.5240346560   -2.7461144372   -2.2910406922
H    0   -3.6638276051   -2.4104999046   -1.9076405182
H    0   -4.9967789736   -3.1434115162   -1.5370610204
O    0    2.3482779530    3.8424118878   -1.7666027521
H    0    2.7574811742    3.7895514398   -0.8512905819
O    0    5.8445322405    2.4845110830   -1.4511459288
H    0    5.4114566242    2.7376756239   -0.5829945605
H    0    6.3356960812    3.2870616435   -1.6949048920
O    0    4.0870862545    3.0035694007   -3.6017990849
H    0    4.6306898882    2.5577599176   -2.9157606142
O    0    7.4212329801    2.1469040492    2.0334965408
H    0    6.6282613297    2.6866760206    1.7662151893
H    0    7.0773592393    1.5162109524    2.6846793829
O    0    2.8156253820   -0.9351799634   -2.6085701231
H    0    2.1951578059    0.6495906374   -3.3597829371
H    0   -0.9177388013   -4.7637200397    4.9213730328
H    0    3.0786454434    3.7034184198   -2.4368873027
Cl   0    7.4690888668   -2.1941606983   -0.5038607137
H    0    3.1146440798   -0.2766539137   -1.9514684535
O    0   -0.3045275437    0.0926683273   -4.5529498004
H    0    0.0383251617   -0.8118389102   -4.6329922891
O    0    0.3774247344   -1.9378469523   -1.8872079915
H    0    1.9421588469   -1.2165730096   -2.2433579040
H    0   -0.0552432332   -1.9537962645   -2.7687180972
H    0    0.4734195711    0.6608469837   -4.2751466523
```

15L_S3a-fixed
E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.93569 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.371075 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.610157 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.772443 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.698051 au
Mn   0   1.2724596603   2.0492099262   -1.9064989583

```
Mn   0   -1.0446926339   -2.5233661155   -0.5298789495
Mn   0   -0.1224535003    0.7407544999    0.1016708601
Mn   0   -2.6967502258   -0.4562088579    0.3218086255
O    0    0.2215860809    0.3285088330   -1.5907564374
O    0   -1.9458967567    0.9927665353   -0.3690855255
O    0   -2.4677781200   -1.4512015336   -1.1896437411
O    0   -1.0018100579   -1.1142249955    0.7438880600
Ca   0   -1.8983833121    0.4075408308   -2.8069454424
C   -1    0.5534799135    4.6067477078   -5.5057325502
H   -1    0.6206110655    5.5379777831   -4.9627474014
H   -1    0.7467476250    4.6869541607   -6.5650249435
H    0    1.3344842279    3.9570821227   -5.0934088801
C    0   -0.8120932662    3.9093444963   -5.3104475289
H    0   -0.9287727955    3.1139870990   -6.0571895681
H    0   -1.6440044496    4.6037887793   -5.4931628498
C    0   -1.0633035369    3.2237644333   -3.9545400862
O    0   -2.1041126481    2.4910532706   -3.8669056188
O    0   -0.2386221648    3.3912939755   -3.0176358498
C   -1   -2.9625902702   -6.6362927581   -5.3092037769
H   -1   -2.0036613178   -7.1032927016   -5.4788150120
H   -1   -3.6925092076   -6.7713714825   -6.0936570363
H    0   -3.3888594905   -7.1692648770   -4.4442192759
C    0   -2.7276796663   -5.1770445389   -4.9029081187
H    0   -3.6757265672   -4.6664980659   -4.6933537640
H    0   -2.2355083594   -4.6153081371   -5.7049837966
C    0   -1.8548397117   -5.1584012506   -3.6475118620
H    0   -0.9101908000   -5.6917879970   -3.8342212205
H    0   -2.3421277979   -5.7002594057   -2.8280352459
C    0   -1.4702961485   -3.7920151280   -3.1247621444
O    0   -1.5528175859   -2.7687179327   -3.8268771926
O    0   -0.9947314363   -3.8150900194   -1.9223420935
C   -1    5.0166329032   -4.6502990515    1.0541821670
H    0    5.7249148987   -5.4515313631    1.2934346208
H    0    5.4100320098   -4.1034204034    0.1936083716
C    0    4.8740145676   -3.7265470647    2.2618059607
O    0    4.2316497898   -4.0920347963    3.2714871733
C    0    3.6436358328   -5.3173669910    0.7189175274
H    0    3.4167074128   -6.0297256179    1.5213745357
H    0    3.7456418516   -5.8922415128   -0.2054854376
C    0    2.4743556163   -4.3767878862    0.5789223291
N    0    2.1912657783   -3.4633519789    1.5845636856
H    0    2.7042108383   -3.4281419881    2.4666130765
C    0    1.4930713514   -4.1704868282   -0.3623829995
H    0    1.3171395694   -4.6624717310   -1.3052110953
C    0    1.1405370037   -2.7230640844    1.2365519154
H    0    0.7995127728   -1.8646683599    1.7793213181
N    0    0.6515172164   -3.1378308379    0.0661968737
N    0    5.3323017786   -2.4769250550    2.1075049518
H    0    5.9402189107   -2.2797733478    1.3040710040
C   -1    4.9963070496   -1.3835934828    3.0145904323
H    0    5.8794826053   -0.7375630538    3.0893197678
H    0    4.8045941946   -1.8064134940    4.0035175822
C    0    3.7881010300   -0.5628672584    2.5320704650
H    0    3.6182873595    0.2586878499    3.2396030935
H    0    2.8916446865   -1.1829030545    2.5682880672
C    0    3.9856604654   -0.0140784440    1.1193603005
H    0    4.4477840992   -0.7727261212    0.4762694409
H    0    4.6701115101    0.8421761197    1.1253698699
C    0    2.7457049738    0.4323060129    0.3551981838
O    0    2.9297173961    0.9748772638   -0.7412265692
```

O	0	1.5866666366	0.1797105686	0.8858382521
C	-1	-5.4889243760	-3.9692639360	2.2605324617
H	0	-5.3626640178	-3.2273565270	3.0558555944
H	0	-5.9780828897	-4.8449541122	2.7045095371
C	0	-4.1294886698	-4.3879332819	1.6897099397
H	0	-4.2597645269	-5.1213933411	0.8882671542
H	0	-3.5353330426	-4.8830426675	2.4678083076
C	0	-3.2744758359	-3.2617996685	1.1211363674
O	0	-3.6508244382	-2.0667752676	1.2701566889
O	0	-2.1834667009	-3.5992552902	0.5451346446
C	0	-6.4081744185	-3.4164152063	1.1748545928
O	0	-6.2383505384	-3.6622263699	-0.0281703417
N	0	-7.4624698695	-2.6923813853	1.6145022738
H	0	-7.5012382021	-2.4265990475	2.5891614257
C	-1	-8.4516629551	-2.1149275579	0.7108921477
H	0	-9.3883476504	-1.9826742592	1.2532730306
H	0	-8.6039668401	-2.8125772397	-0.1167923075
C	0	-8.0129839664	-0.7305084007	0.1901873539
O	0	-8.4872185920	0.3049920388	0.6582673107
N	0	-7.0835313990	-0.7650316125	-0.7971864232
H	0	-6.6771775250	-1.6550737250	-1.0628149433
C	0	-6.4821497556	0.4279457061	-1.3578996643
H	0	-6.6988370878	0.5095127710	-2.4269344075
H	0	-6.9246662370	1.2893318423	-0.8481326418
C	0	-4.9581677041	0.4769502741	-1.1901890364
O	0	-4.2657466344	0.9055552067	-2.1264713606
O	0	-4.5243963586	0.0718182387	-0.0432066685
C	-1	-3.4434681188	3.6319134107	5.0746380335
H	-1	-3.4772896514	3.3308738266	6.1112823944
H	-1	-4.2569069957	4.2813078682	4.7865803024
H	0	-2.5419444232	4.2540025416	4.9744443836
C	0	-3.3805191117	2.4954695087	4.0449042140
H	0	-3.6986885951	2.8936422141	3.0731464010
H	0	-4.0851391525	1.6913906821	4.2850314859
C	0	-1.9656901533	1.9379610614	3.8831692186
H	0	-1.6981998421	1.3107743787	4.7444461784
H	0	-1.2315662576	2.7494145835	3.8659975740
C	0	-1.7641219303	1.1527245015	2.5979834645
O	0	-0.6323737639	1.2726789510	2.0493931222
O	0	-2.7302297309	0.4358040497	2.1684212367
C	-1	-5.4944075919	9.0690433188	2.1168353059
H	-1	-5.3612786278	8.6531833711	3.1046304726
H	-1	-6.5283921949	9.3116918571	1.9210020179
H	0	-4.9447197165	10.0183824405	2.0896820914
C	0	-4.9108505503	8.0946397191	1.0818923799
H	0	-3.8161224971	8.1101195725	1.1810272752
H	0	-5.1300600329	8.4374894128	0.0619314650
C	0	-5.4313255195	6.6622736338	1.2662377209
H	0	-6.5212797771	6.6526372827	1.1375976737
H	0	-5.2304434263	6.3240835989	2.2920694481
C	0	-4.8425566607	5.6391973019	0.2900070715
H	0	-5.0423757277	5.9484331003	-0.7465362414
H	0	-5.3236892368	4.6689770037	0.4483138291
N	0	-3.4048015092	5.4592463793	0.5018793410
H	0	-2.8556477399	6.2817055620	0.7115794876
C	0	-2.7084708950	4.3666288065	0.1182140483
N	0	-3.3210977883	3.3675945302	-0.5282880099
H	0	-2.8377064036	2.4620193864	-0.6079711365
H	0	-4.1263657483	3.5255878785	-1.1146104635
N	0	-1.4160777042	4.2565779221	0.4134267053

H	0	-0.9746404513	4.7384886207	1.1904146546
H	0	-0.8299442307	3.4928052108	0.0178238655
C	-1	-1.0205145659	-1.3557126563	7.5909656068
H	-1	-0.0301668943	-0.9616826242	7.4167098432
H	-1	-1.2015312232	-1.5674935601	8.6343962220
H	0	-1.7628761890	-0.6262818616	7.2498426022
C	0	-1.1990041567	-2.7188182729	6.8930590380
H	0	-2.1619389112	-3.1545664995	7.1934327918
H	0	-0.4285371659	-3.4099622049	7.2582135665
C	0	-1.1477065808	-2.6909748466	5.4012730985
N	0	-0.9868058183	-3.8454137239	4.6440886350
C	0	-1.2886451294	-1.6813541123	4.4892093473
H	0	-1.4360351684	-0.6284900416	4.6375275181
C	0	-1.0275078021	-3.5498619024	3.3383352937
H	0	-0.9312417443	-4.2423212981	2.5181648148
N	0	-1.2175327947	-2.2372240541	3.2282904941
H	0	-1.2310832043	-1.7194538656	2.3107871660
C	-1	3.7616906488	6.1915032604	2.4661295386
H	-1	4.6323457254	6.6845410906	2.0595735721
H	-1	3.2955425899	6.7067812083	3.2929282521
H	0	3.0071286987	6.1804125778	1.6707671736
C	0	4.1113546966	4.7213698476	2.7998887896
H	0	5.0492170553	4.6460307844	3.3603422649
H	0	3.3077851953	4.2865986978	3.4063926720
C	0	4.1840359136	3.8964144379	1.5055953160
O	0	3.1338340186	3.8611120889	0.8189505565
O	0	5.2799400781	3.3259768783	1.1802841464
C	-1	12.0837929376	-2.4357879728	-0.5634652826
H	-1	13.1311375511	-2.1767781190	-0.6122679806
H	-1	11.8575869534	-3.3216720268	-1.1383015774
H	0	11.8672338826	-2.6987208106	0.4815306638
C	0	11.2001625210	-1.2410736984	-0.9862306211
H	0	11.6548308637	-0.7334388327	-1.8495237325
H	0	10.2191495582	-1.6051006272	-1.3116421579
C	0	10.9930809640	-0.2395993376	0.1647766388
H	0	10.2638967759	-0.6690555387	0.8650985968
H	0	11.9319146705	-0.1296711653	0.7259362971
C	0	10.5535197449	1.1716193709	-0.2599851438
H	0	10.4732912813	1.8151293861	0.6270740224
H	0	11.3383556763	1.6118427167	-0.8899587331
C	0	9.2524009137	1.2807807424	-1.0552864803
H	0	9.1128162942	2.3095733779	-1.3993033280
H	0	9.2590307579	0.6304492460	-1.9338292712
N	0	8.0323503570	0.9287226961	-0.2637124002
H	0	7.1900161074	1.3197260747	-0.7459295491
H	0	7.9178880257	-0.1079478284	-0.1628885996
H	0	8.0103080597	1.3724038665	0.6849060668
O	0	1.9452273050	1.3452480777	-3.5436197348
H	0	2.7408703434	1.8577369265	-3.8072203997
O	0	0.4091148136	2.3697723433	-0.2064744565
O	0	0.7534890270	3.9082539641	2.3198185850
H	0	0.4101360864	3.0238848126	2.0960220325
H	0	1.5312615938	3.9820427961	1.7168298996
O	0	-3.4518454387	-0.9132545707	-4.2130120123
H	0	-4.1846473724	-1.1999230526	-3.6355667924
H	0	-2.9113108007	-1.7263855441	-4.3167591228
O	0	-4.7093591043	-2.5486059306	-2.1618870236
H	0	-3.8851097214	-2.1908428013	-1.7415671854
H	0	-5.1360201832	-3.0681266229	-1.4546932832
O	0	2.3403359446	3.5825753001	-1.8352540158

H	0	2.7022106764	3.5982176698	-0.9197174464
O	0	5.9626758406	2.4784979909	-1.2855385075
H	0	5.5192157926	2.7435261511	-0.4270653891
H	0	6.3629172236	3.3055815685	-1.5995943729
O	0	4.2512201406	3.0002334769	-3.5748669538
H	0	4.7965702426	2.4848280959	-2.9494091214
O	0	7.5183635418	2.2394391435	2.1721558949
H	0	6.6942291338	2.7352528352	1.9092865072
H	0	7.2065906894	1.5788143822	2.8098136728
O	0	2.1205435998	-1.2492714691	-2.7114359579
H	0	1.4007576475	-0.9571570981	-2.1042550572
H	0	-0.8539425664	-4.7781359319	5.0163019064
H	0	3.5669395971	3.3700976670	-2.9416444484
Cl	0	7.6365560490	-2.1817955214	-0.1064709368
H	0	2.3316696841	-0.3508398552	-3.0829145391
O	0	-0.2902045655	0.2746253913	-4.6273179597
H	0	0.0832332874	-2.5588715164	-4.6707967897
O	0	0.9264270499	-2.1725604477	-4.9723791425
H	0	0.1015804743	-0.6009222825	-4.8707352290
H	0	1.3933293165	-1.9370674759	-4.1237953853
H	0	0.5134732818	0.7968598881	-4.3528144242

15L_S3a

E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.959337 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.393505 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.636674 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.795651 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.720929 au

Mn	0	1.2008739220	2.1317778974	-1.8186073013
Mn	0	-0.8988272270	-2.3718430251	-0.7456053517
Mn	0	-0.1752217817	0.7549988767	0.1721440669
Mn	0	-2.7028147906	-0.5574143015	0.3218649708
O	0	0.1946234021	0.3574030874	-1.5206035147
O	0	-2.0025038653	0.9550936906	-0.2972307742
O	0	-2.4198381831	-1.4360555199	-1.2714283539
O	0	-0.9631914985	-1.1449211493	0.6973648069
Ca	0	-1.9439378040	0.5601449658	-2.7706190455
C	-1	0.4906301155	4.6270840014	-5.5140459838
H	-1	0.5454701369	5.5569130002	-4.9672939838
H	-1	0.6790911175	4.7147059971	-6.5736169838
H	0	1.2701735557	3.9782674161	-5.0971729578
C	0	-0.8781099397	3.9326985891	-5.3318085444
H	0	-0.9729628448	3.1136030810	-6.0566172595
H	0	-1.7064693738	4.6181060381	-5.5569156466
C	0	-1.1637044088	3.2776443712	-3.9706990854
O	0	-2.2562586406	2.6272732944	-3.8594335302
O	0	-0.3072741378	3.3665681822	-3.0520356504
C	-1	-2.8539871439	-6.6687249217	-5.3541809838
H	-1	-1.8886671543	-7.1204039439	-5.5289609838
H	-1	-3.5844121472	-6.8115309049	-6.1367919838
H	0	-3.2694908469	-7.2010929612	-4.4838846109
C	0	-2.6513003020	-5.1994009284	-4.9745204958
H	0	-3.6118688707	-4.6961162729	-4.8095982460
H	0	-2.1446521704	-4.6530659804	-5.7780326345
C	0	-1.8182681162	-5.1213839491	-3.6966927000
H	0	-0.8907007582	-5.7036566941	-3.8028693607
H	0	-2.3515090727	-5.5714434696	-2.8498962386
C	0	-1.3995785336	-3.7305318050	-3.2839138690
O	0	-1.5517140938	-2.7493746829	-4.0302519742
O	0	-0.8143167852	-3.6798696302	-2.1283049627

C	-1	5.1156069038	-4.5889531048	0.9912890162
H	0	5.8798573698	-5.3439011558	1.2113513887
H	0	5.4537179011	-4.0242325167	0.1190613598
C	0	4.9645186841	-3.6711442197	2.2021373089
O	0	4.3630215277	-4.0582678561	3.2279309378
C	0	3.7798475882	-5.3291179859	0.6931634092
H	0	3.5808164589	-6.0210949205	1.5200737115
H	0	3.8963937747	-5.9265426538	-0.2149801735
C	0	2.6072320414	-4.4067787826	0.5304987161
N	0	2.2787060082	-3.5272742454	1.5529608976
H	0	2.7589375485	-3.5144591449	2.4532844206
C	0	1.7143589163	-4.1256019789	-0.4756130183
H	0	1.5967886418	-4.5721657536	-1.4500572240
C	0	1.2875880338	-2.7309136618	1.1500603703
H	0	0.9299285886	-1.8803619181	1.6936258648
N	0	0.8927693476	-3.0784985290	-0.0702033929
N	0	5.3816022080	-2.4076410912	2.0376956991
H	0	5.9710613639	-2.1986532695	1.2246098306
C	-1	5.0523839787	-1.3312791033	2.9657600162
H	0	5.9192341667	-0.6600540616	3.0092354591
H	0	4.9145104496	-1.7667683307	3.9582636294
C	0	3.8033508810	-0.5412716981	2.5425873032
H	0	3.6247136522	0.2536765091	3.2778978742
H	0	2.9312273490	-1.1956155838	2.5821637059
C	0	3.9562073746	0.0531547429	1.1446246698
H	0	4.3938390669	-0.6873466658	0.4634277876
H	0	4.6458919657	0.9048282591	1.1575440640
C	0	2.7021275335	0.5311189445	0.4281331136
O	0	2.8708885883	1.1242236731	-0.6443453676
O	0	1.5507190878	0.2455747083	0.9598945262
C	-1	-5.3949420843	-4.0724638634	2.2352380162
H	0	-5.2422005607	-3.3159768991	3.0122459406
H	0	-5.8987926222	-4.9263758288	2.7050472393
C	0	-4.0575926044	-4.5263025124	1.6515934763
H	0	-4.2154887417	-5.2718979323	0.8668070044
H	0	-3.4624087555	-5.0190092590	2.4299759108
C	0	-3.1890467863	-3.4255218929	1.0433414536
O	0	-3.5688726437	-2.2195644553	1.1824439107
O	0	-2.1225944101	-3.7948934794	0.4735562388
C	0	-6.3190141300	-3.5179220064	1.1537079441
O	0	-6.1480789987	-3.7463253830	-0.0525763016
N	0	-7.3863506552	-2.8167763443	1.6010957140
H	0	-7.4323695294	-2.5645645342	2.5789798357
C	-1	-8.3906410426	-2.2567197945	0.7033660162
H	0	-9.3303572691	-2.1552490613	1.2475096812
H	0	-8.5251689969	-2.9503217149	-0.1306476767
C	0	-7.9865037241	-0.8585773238	0.1997366200
O	0	-8.4547262486	0.1625223466	0.7037411358
N	0	-7.0891312887	-0.8650434706	-0.8177210057
H	0	-6.6678635883	-1.7451502687	-1.0936596432
C	0	-6.4956719310	0.3437771661	-1.3476993863
H	0	-6.7010670996	0.4454409234	-2.4171756334
H	0	-6.9518092757	1.1912877867	-0.8266927588
C	0	-4.9756696095	0.4063877112	-1.1626375110
O	0	-4.2886539607	0.9165687978	-2.0614973463
O	0	-4.5414223246	-0.0787554542	-0.0478216416
C	-1	-3.4554389093	3.5468550921	5.0751830162
H	-1	-3.4812039163	3.2409420927	6.1106320162
H	-1	-4.2795898946	4.1850541110	4.7926040162
H	0	-2.5516068000	4.1638759191	4.9666517785

C	0	-3.4240703443	2.4398455939	4.0151536340
H	0	-3.5156333665	2.9263664362	3.0351540320
H	0	-4.2906599858	1.7751111458	4.1039803699
C	0	-2.1315577175	1.6145567206	4.0278466002
H	0	-2.2045247772	0.8451475586	4.8048864980
H	0	-1.2686525002	2.2454135196	4.2592942676
C	0	-1.8685381613	0.9624144421	2.6806870714
O	0	-0.7442509299	1.1830520380	2.1475376156
O	0	-2.7999896290	0.2402493332	2.1855306340
C	-1	-5.5984797848	8.9647531413	2.1475400162
H	-1	-5.4557407944	8.5467731380	3.1330970162
H	-1	-6.6366767796	9.1925201652	1.9561660162
H	0	-5.0620235441	9.9219021888	2.1237212652
C	0	-5.0173747140	8.0092717682	1.1011877966
H	0	-3.9261272660	7.9890597414	1.2318053109
H	0	-5.1952930391	8.3901748516	0.0867935660
C	0	-5.5935200862	6.5934969222	1.2261697768
H	0	-6.6703523055	6.6179993045	1.0165971860
H	0	-5.4782962603	6.2349702477	2.2582486746
C	0	-4.9519321214	5.5746714639	0.2831915731
H	0	-5.0666377493	5.8968676538	-0.7619400794
H	0	-5.4499627754	4.6065157214	0.3924001649
N	0	-3.5379871310	5.3854221444	0.6081179284
H	0	-3.0038733436	6.1995192736	0.8781482936
C	0	-2.8298064105	4.2773749330	0.3135900399
N	0	-3.3986290375	3.2825478498	-0.3790897474
H	0	-2.9031324041	2.3796642732	-0.4292312442
H	0	-4.1110620694	3.4635775000	-1.0705317944
N	0	-1.5852487504	4.1319725913	0.7599262705
H	0	-1.1887520323	4.6986536219	1.4987819914
H	0	-0.9349958923	3.4316192820	0.3441389253
C	-1	-0.9487270232	-1.4140789655	7.5620570162
H	-1	0.0349459862	-1.0043369881	7.3862260162
H	-1	-1.1229980283	-1.6330049615	8.6051620162
H	0	-1.7053228180	-0.7008173372	7.2186156251
C	0	-1.0870052448	-2.7778304560	6.8530737907
H	0	-2.0479840758	-3.2329286799	7.1296420057
H	0	-0.3123190276	-3.4569912108	7.2329255316
C	0	-1.0102616699	-2.7508621348	5.3601590764
N	0	-1.0316696858	-3.9171096676	4.6019488128
C	0	-0.9798825650	-1.7331845767	4.4467230558
H	0	-0.9149816906	-0.6721411117	4.5966956362
C	0	-1.0265780670	-3.6197148316	3.2956598225
H	0	-1.0413162619	-4.3146239267	2.4713026023
N	0	-1.0100156593	-2.2945253931	3.1844563588
H	0	-1.0370670910	-1.7859384695	2.2624983543
C	-1	3.7012831523	6.2264789277	2.4539080162
H	-1	4.5629931639	6.7343869079	2.0465990162
H	-1	3.2301671639	6.7311149385	3.2844460162
H	0	2.9437559680	6.1969070894	1.6621165259
C	0	4.0746544117	4.7640868081	2.8023482816
H	0	5.0328263805	4.7065092980	3.3296267163
H	0	3.2967981848	4.3365889132	3.4463674352
C	0	4.1014137998	3.9134826401	1.5249381410
O	0	3.0194556597	3.8463935624	0.8925267019
O	0	5.1904006616	3.3559027399	1.1578997603
C	-1	12.1429119573	-2.2606622662	-0.6401669838
H	-1	13.1860409636	-1.9855922902	-0.6913149838
H	-1	11.9282219370	-3.1474292613	-1.2180499838
H	0	11.9380958140	-2.5370831323	0.4038102957

C	0	11.2301374322	-1.0800786770	-1.0470801569
H	0	11.6948776975	-0.5212893911	-1.8724583794
H	0	10.2758369391	-1.4650555653	-1.4235485274
C	0	10.9420944123	-0.1322481043	0.1323239652
H	0	10.2112045752	-0.6187302394	0.7928180736
H	0	11.8579300084	-0.0018006694	0.7261230228
C	0	10.4528513192	1.2738124914	-0.2552849106
H	0	10.3372542888	1.8854832260	0.6502243305
H	0	11.2280903075	1.7634105503	-0.8602305045
C	0	9.1572497830	1.3616051675	-1.0634262782
H	0	8.9921406116	2.3932929691	-1.3868506228
H	0	9.1913050823	0.7308764391	-1.9554424146
N	0	7.9402006489	0.9571715975	-0.2915129773
H	0	7.0890088267	1.3269158948	-0.7725359213
H	0	7.8622699990	-0.0857057594	-0.2121239411
H	0	7.8983830081	1.3818529500	0.6653059554
O	0	1.9307481942	1.4634225774	-3.4467726329
H	0	2.6846325755	2.0348064700	-3.7153337090
O	0	0.2907052754	2.4063250200	-0.1206444902
O	0	0.7499987153	3.7296772177	2.5546626518
H	0	0.3593713751	2.8685612135	2.3238432362
H	0	1.4726476144	3.8223218492	1.8907191453
O	0	-3.4197840831	-0.8177589425	-4.1805808808
H	0	-4.1430816746	-1.1485440353	-3.6156276413
H	0	-2.8641428058	-1.6133478292	-4.3328198588
O	0	-4.6485831542	-2.6148865243	-2.2006432761
H	0	-3.8219471134	-2.2511478705	-1.7968869258
H	0	-5.0667067862	-3.1149402387	-1.4739083804
O	0	2.1863262095	3.7148924702	-1.7328744406
H	0	2.5696309389	3.7047179276	-0.8243767753
O	0	5.8382337341	2.5017811428	-1.3049012850
H	0	5.3757375044	2.7394302870	-0.4479728485
H	0	6.2949255635	3.3264817893	-1.5402806558
O	0	4.1162141761	3.2445776908	-3.4976192030
H	0	4.6789286673	2.7235014828	-2.8899470027
O	0	7.4023948660	2.2353178965	2.1538268697
H	0	6.5862644568	2.7436554066	1.8871277465
H	0	7.0839145340	1.5917521639	2.8052776269
O	0	2.2287299193	-1.1028967976	-2.6502775114
H	0	1.5144745682	-0.8523644632	-2.0225719485
H	0	-1.0450076189	-4.8589882094	4.9742230462
H	0	3.4238516474	3.5798222933	-2.8559131914
Cl	0	7.6845002772	-2.1580163634	-0.2014242530
H	0	2.3872972202	-0.1906801967	-3.0185905385
O	0	-0.3074021291	0.4527151207	-4.5603222116
H	0	0.1470322135	-2.3691404989	-4.6270831233
O	0	0.9788441680	-1.9476632009	-4.9129654136
H	0	0.0967951107	-0.4171891771	-4.8075171142
H	0	1.4554522030	-1.7424342132	-4.0625322262
H	0	0.4950383046	0.9706326042	-4.2705016937

15L_S3ab
E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.936942 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.371345 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.612584 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.7711 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.697189 au

Mn	0	1.3938134860	1.9138678415	-1.7649270975
Mn	0	-0.9960204827	-2.3682241579	-0.6523006077
Mn	0	-0.3089138573	0.8406161112	0.1192226297

```
Mn   0   -2.9030362821   -0.4655252851    0.0910654436
O    0    0.2685376525    0.3336573552   -1.5841461487
O    0   -2.3080017619    0.9754355254   -0.6537544988
O    0   -2.4715990746   -1.5118426723   -1.3676588687
O    0   -1.1421536093   -0.9920895842    0.6556337273
Ca   0   -1.7428316579    0.2846161570   -2.9042580367
C   -1    0.6514386360    4.5600849058   -5.5669382215
H   -1    0.7205922532    5.5000334230   -5.0394496031
H   -1    0.8564161908    4.6203122610   -6.6253530415
H    0    1.4922468964    3.9719950296   -5.1718496649
C    0   -0.6327645463    3.7912828808   -5.2183683153
H    0   -0.8055285332    2.9928090312   -5.9523665331
H    0   -1.5259481594    4.4259743224   -5.2517165245
C    0   -0.6525620317    3.0448600253   -3.8668132317
O    0   -1.7439564048    2.5227206085   -3.5137323924
O    0    0.4476994410    2.9522560854   -3.2352090778
C   -1   -2.9593325883   -6.6490469568   -5.2133326875
H   -1   -2.0025784938   -7.1266615100   -5.3646854528
H   -1   -3.6821106436   -6.7918248670   -6.0030165944
H    0   -3.3990321333   -7.1532606631   -4.3382400001
C    0   -2.7363113269   -5.1748150906   -4.8612241252
H    0   -3.6917253994   -4.6556098719   -4.7199264790
H    0   -2.2067627142   -4.6549752154   -5.6682513710
C    0   -1.9259814070   -5.0904102599   -3.5711037316
H    0   -1.0177842502   -5.7069544583   -3.6428259634
H    0   -2.4934586702   -5.5018932604   -2.7271551700
C    0   -1.4651099443   -3.7134541880   -3.1627685163
O    0   -1.6211782795   -2.7108922676   -3.8827487505
O    0   -0.8319399999   -3.6922786790   -2.0298925400
C   -1    4.9691422294   -4.6173984618    1.1988857036
H    0    5.7198988998   -5.3830573472    1.4274262175
H    0    5.3045519312   -4.0783240591    0.3093838106
C    0    4.8420887157   -3.6720041643    2.3906906138
O    0    4.2482562333   -4.0322366976    3.4299572861
C    0    3.6106158695   -5.3294203003    0.9435639750
H    0    3.4076969646   -5.9903189081    1.7944021646
H    0    3.6941556153   -5.9563083933    0.0516271943
C    0    2.4606977997   -4.3816401166    0.7665240721
N    0    2.1526043416   -3.4533474696    1.7535401335
H    0    2.6306474533   -3.4145751005    2.6528059113
C    0    1.5708493803   -4.1256278629   -0.2469130967
H    0    1.4470750030   -4.6054389813   -1.2043277888
C    0    1.1682638057   -2.6593868330    1.3203869596
H    0    0.8203991300   -1.7832661113    1.8311494724
N    0    0.7667243783   -3.0527409703    0.1173980801
N    0    5.2644697603   -2.4144711541    2.1931666829
H    0    5.8366552305   -2.2222968059    1.3642530095
C   -1    4.9553530265   -1.3170732439    3.1022101839
H    0    5.8569356520   -0.6967381415    3.1898415801
H    0    4.7437046290   -1.7404803832    4.0862426042
C    0    3.7717009833   -0.4630179882    2.6217483841
H    0    3.6255610993    0.3606309226    3.3324759687
H    0    2.8635950807   -1.0649243413    2.6692018186
C    0    3.9303172485    0.0966270583    1.2023552306
H    0    4.3262283623   -0.6654307776    0.5189986349
H    0    4.6314409819    0.9384774277    1.1750227454
C    0    2.6167148198    0.5608538138    0.5799765050
O    0    2.7409257444    1.1001937968   -0.5721448963
O    0    1.5398140342    0.3480786675    1.1916193157
C   -1   -5.5424511025   -3.8305843312    2.2820043594
```

H	0	-5.3409986306	-3.0261941301	2.9966180362
H	0	-6.0685342908	-4.6254922398	2.8268452159
C	0	-4.2431870989	-4.3796735479	1.7074113874
H	0	-4.4497685070	-5.1462367920	0.9540374085
H	0	-3.6580860660	-4.8692445645	2.4948056025
C	0	-3.3547893391	-3.3291571873	1.0501227977
O	0	-3.7482471251	-2.1253827751	1.0673882967
O	0	-2.2613921237	-3.7459811213	0.5621818381
C	0	-6.4806937937	-3.3349751948	1.1875663251
O	0	-6.4151343154	-3.7511431089	0.0206273868
N	0	-7.4425442186	-2.4683324326	1.5788049682
H	0	-7.3944165753	-2.0646930513	2.5041754224
C	-1	-8.4734101923	-1.9795509788	0.6692666700
H	0	-9.3356496489	-1.6657321079	1.2587550846
H	0	-8.7644452364	-2.8033263395	0.0115556744
C	0	-8.0071002339	-0.7687225622	-0.1575900300
O	0	-8.3630375097	0.3759652421	0.1252739024
N	0	-7.2110774824	-1.0861944153	-1.2089931453
H	0	-6.8371096262	-2.0293912897	-1.2571331062
C	0	-6.5546663812	-0.0798840363	-2.0112755228
H	0	-6.6566369238	-0.3099640271	-3.0748636944
H	0	-7.0478238707	0.8773253490	-1.8165354816
C	0	-5.0593654472	0.0720979809	-1.7107975829
O	0	-4.3063147999	0.4027305938	-2.6442540663
O	0	-4.7254684599	-0.1431045956	-0.4838759789
C	-1	-3.4637192412	3.8015418534	4.9857976879
H	-1	-3.5108543101	3.5188393300	6.0270741923
H	-1	-4.2687081309	4.4523912342	4.6779629025
H	0	-2.5267088051	4.3577018576	4.8494657511
C	0	-3.5636987912	2.6993993939	3.9130499907
H	0	-3.5759863242	3.2224138221	2.9469446179
H	0	-4.5286883586	2.1836562256	3.9820184453
C	0	-2.4327583698	1.6607732390	3.8913830938
H	0	-2.7044014892	0.8228371570	4.5404492118
H	0	-1.4986484009	2.0994267084	4.2555288635
C	0	-2.1801683491	1.1476736142	2.4781052548
O	0	-1.0732528474	1.4680863692	1.9515625789
O	0	-3.0965164273	0.4470303263	1.9312548418
C	-1	-5.4386294520	9.2028771533	1.9129093487
H	-1	-5.3192675136	8.8031761712	2.9090989315
H	-1	-6.4684700858	9.4504406017	1.7019766074
H	0	-4.8597909352	10.1311711908	1.8452497128
C	0	-4.9042437402	8.1463521800	0.9321007908
H	0	-3.8080640208	8.1281441951	1.0101941612
H	0	-5.1341615675	8.4186596705	-0.1063667034
C	0	-5.4805883898	6.7571112973	1.2463081387
H	0	-6.5721832195	6.7853245537	1.1378808361
H	0	-5.2739389423	6.5029163433	2.2950952455
C	0	-4.9567234740	5.6245017729	0.3623180026
H	0	-5.1744212517	5.8384160198	-0.6950863703
H	0	-5.4697987249	4.6946785330	0.6306200033
N	0	-3.5200589409	5.4238434253	0.5606574131
H	0	-2.9655846903	6.2553374143	0.7153429317
C	0	-2.8332870052	4.3651557002	0.0640038584
N	0	-3.4689846468	3.3760405789	-0.5616481530
H	0	-3.0281227391	2.4306376058	-0.6610528440
H	0	-4.4318085022	3.4791552608	-0.8427177822
N	0	-1.5054236794	4.3310067508	0.2067383208
H	0	-1.0429209305	4.7796222541	0.9931313129
H	0	-0.9314533718	3.5612918588	-0.1922772501

C	-1	-1.1085015274	-1.1610490240	7.6134700921
H	-1	-0.1131634712	-0.7781263965	7.4429228239
H	-1	-1.3021504010	-1.3532018355	8.6584301678
H	0	-1.8364003004	-0.4239600566	7.2569224308
C	0	-1.2795273437	-2.5109663798	6.8911340424
H	0	-2.2525659656	-2.9453158843	7.1588550367
H	0	-0.5234597078	-3.2157298610	7.2620412974
C	0	-1.2013449132	-2.4688663438	5.3958006697
N	0	-1.2703212978	-3.6342589151	4.6395493212
C	0	-1.1372758446	-1.4539339882	4.4783835462
H	0	-1.0282584879	-0.3950523609	4.6244524802
C	0	-1.2632686121	-3.3409661600	3.3335625210
H	0	-1.3048018219	-4.0373339731	2.5108013960
N	0	-1.2008042578	-2.0171895352	3.2145654105
H	0	-1.2193678858	-1.5257699080	2.2772372737
C	-1	3.7892078414	6.2570878320	2.4098563355
H	-1	4.6681083486	6.7359328026	2.0040783517
H	-1	3.3187263575	6.7904029804	3.2226431671
H	0	3.0423509379	6.2320437998	1.6072916591
C	0	4.1070346094	4.7938349803	2.8022624350
H	0	5.0354963369	4.7233258742	3.3784547770
H	0	3.2852572786	4.4015032949	3.4132671168
C	0	4.1787872700	3.9209522930	1.5446187039
O	0	3.1166827548	3.8275869935	0.8809020655
O	0	5.2876219655	3.3765781307	1.2187489981
C	-1	12.0708805218	-2.4885398457	-0.3818943159
H	-1	13.1207838722	-2.2388940447	-0.4240771428
H	-1	11.8433736129	-3.3824176889	-0.9436951705
H	0	11.8491700717	-2.7405318185	0.6651936982
C	0	11.1959096434	-1.2915367583	-0.8116569212
H	0	11.6491132917	-0.7942416259	-1.6816078308
H	0	10.2091578486	-1.6490444432	-1.1277476700
C	0	11.0067397972	-0.2799136164	0.3340647843
H	0	10.2840554767	-0.6976120404	1.0485700725
H	0	11.9519013106	-0.1726041377	0.8849670923
C	0	10.5743744538	1.1316669292	-0.0960275967
H	0	10.4860517903	1.7758897373	0.7896911461
H	0	11.3677670002	1.5692529230	-0.7170352994
C	0	9.2852747525	1.2457932491	-0.9093492481
H	0	9.1548641762	2.2764406409	-1.2513624021
H	0	9.3042829858	0.5993885919	-1.7905453854
N	0	8.0496971769	0.8935780555	-0.1418795876
H	0	7.2229896706	1.3028512896	-0.6325921550
H	0	7.9148690036	-0.1441702069	-0.0667605992
H	0	8.0117629908	1.3203676635	0.8128849973
O	0	2.2810630386	1.0574924400	-3.2206595832
H	0	3.0200704357	1.6387099242	-3.5114996144
O	0	0.3493492524	2.4694727498	-0.3457978142
O	0	0.6376120834	3.9696640740	2.2598612909
H	0	0.2158485752	3.1169760234	2.0548492943
H	0	1.4401157521	3.9585069084	1.6882601907
O	0	-3.0930777936	-0.6413197468	-4.8116083994
H	0	-3.9165925788	-0.5376714831	-4.2962537755
H	0	-2.8150893121	-1.5740433676	-4.6969291047
O	0	-4.6641547086	-2.9914648071	-2.1377287617
H	0	-3.8707484087	-2.4772453493	-1.8594121932
H	0	-5.0340207487	-3.3373378653	-1.3056663219
O	0	2.4458492741	3.4351473095	-1.7308240425
H	0	2.7725658095	3.4977042815	-0.7994343433
O	0	6.0504053607	2.5218867361	-1.1942440120

```
H    0    5.5878376517    2.8025046530    -0.3478586517
H    0    6.5071301832    3.3291857721    -1.4823546239
O    0    4.3778989921    2.9099553845    -3.4766446868
H    0    4.9645667218    2.4965433142    -2.8108410364
O    0    7.4481680376    2.1835132281    2.2882724761
H    0    6.6587777488    2.7148091169    1.9958730578
H    0    7.0821417027    1.5310256633    2.9051870127
O    0    2.2683714848    -1.4245633768   -2.2518101098
H    0    1.4908262882    -1.0244825990   -1.7949466572
H    0    -1.3159963782   -4.5743166980   5.0137442216
H    0    3.6765993049    3.2868141711    -2.8757756045
Cl   0    7.5292161394    -2.1898440998   -0.1095093765
H    0    2.5943552803    -0.5787058160   -2.6605006525
O    0    0.0653887493    0.2583991629    -4.5849266507
H    0    0.2011285326    -2.5319210322   -4.3303258351
O    0    1.1096278596    -2.2842592524   -4.5798754974
H    0    0.4122688998    -0.6485423718   -4.7714395885
H    0    1.5452236017    -2.0561476009   -3.7131439804
H    0    0.8614514643    0.6856477335    -4.1636445930
```

15L_S3d-fixed
E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.941978 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.377046 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.618136 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.774806 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.700423 au
```
Mn   0    1.1245404562    2.2198320269    -1.8802839212
Mn   0    -0.8823196406   -2.5935191656   -0.6014460480
Mn   0    -0.1680845830   0.8493111993    0.1046607479
Mn   0    -2.8317093832   -0.4470965343   0.2543839630
O    0    0.2120960969    0.6085141227    -1.6239408051
O    0    -1.9562860157   1.0245257354    -0.3814330032
O    0    -2.3000039900   -1.5145558321   -1.2617532158
O    0    -0.7100035822   -1.1678992505   0.6427075996
Ca   0    -1.9983179989   0.4457667237    -2.7375700893
C    -1   0.5540942621    4.7210336739    -5.5423230988
H    -1   0.6213303678    5.6465126827    -4.9893612651
H    -1   0.7426559722    4.8138346249    -6.6015284918
H    0    1.3496972362    4.0778802512    -5.1453279116
C    0    -0.7967614707   4.0113801303    -5.3202194358
H    0    -0.9401352257   3.2255521351    -6.0719785231
H    0    -1.6388733783   4.7044206339    -5.4564263863
C    0    -0.9742209744   3.3252999640    -3.9564743214
O    0    -1.9270418771   2.4939745095    -3.8471716344
O    0    -0.1658207673   3.6139204910    -3.0268253315
C    -1   -2.9321440410   -6.5324787420   -5.4563122277
H    -1   -1.9728197551   -6.9950377561   -5.6352904070
H    -1   -3.6652048579   -6.6606419669   -6.2390283336
H    0    -3.3528264528   -7.1055476399   -4.6136611276
C    0    -2.6764125392   -5.1086702181   -4.9584879493
H    0    -3.6034652044   -4.6251497680   -4.6271416377
H    0    -2.2391489221   -4.4754556046   -5.7383625138
C    0    -1.7041227748   -5.2212933759   -3.7756514857
H    0    -0.7559171352   -5.6581082651   -4.1239171288
H    0    -2.1030888316   -5.9001774227   -3.0159056418
C    0    -1.3482030565   -3.9144800230   -3.1106898489
O    0    -1.1434671236   -2.8884951741   -3.7918031278
O    0    -1.2478671442   -4.0045912440   -1.8201542638
C    -1   5.0696362561    -4.5968280312   0.8942272731
H    0    5.8911888430    -5.3053416777   1.0554981641
```

H	0	5.3230391410	-4.0059328466	0.0103807615
C	0	4.9597626532	-3.6935145560	2.1211384578
O	0	4.4215599381	-4.0995370380	3.1738180568
C	0	3.7734268718	-5.4294894643	0.6423465329
H	0	3.6786832078	-6.1655469008	1.4501544185
H	0	3.8942599460	-5.9864256431	-0.2907264761
C	0	2.5070864996	-4.6198482200	0.5823621969
N	0	2.1938654105	-3.8083635030	1.6602273127
H	0	2.7536203340	-3.7661342181	2.5141230461
C	0	1.4867878069	-4.4121883305	-0.3180694338
H	0	1.3283075468	-4.8242311473	-1.3014989236
C	0	1.0900215087	-3.1179071998	1.3918020246
H	0	0.7038709754	-2.3713365816	2.0503935806
N	0	0.5914140127	-3.4761739204	0.2103621172
N	0	5.3758106008	-2.4278250530	1.9570464213
H	0	5.9002252358	-2.2034831851	1.1060877665
C	-1	5.0494660131	-1.3522951942	2.8910646361
H	0	5.9182581032	-0.6853473349	2.9559500803
H	0	4.8885324914	-1.7974189392	3.8750523081
C	0	3.8036507385	-0.5702344621	2.4366025009
H	0	3.5425405912	0.1679547772	3.2053927649
H	0	2.9584585927	-1.2600580682	2.3657026532
C	0	4.0105471578	0.1229234922	1.0892244166
H	0	4.4957004689	-0.5579936737	0.3773802398
H	0	4.6806974388	0.9856972314	1.1835720653
C	0	2.7610103201	0.6156048573	0.3668920211
O	0	2.9456006298	1.1897581495	-0.7344761076
O	0	1.6212004472	0.3655173865	0.8952280012
C	-1	-5.4324452764	-3.9568930889	2.1536988387
H	0	-5.2995666625	-3.2339583981	2.9645987145
H	0	-5.9232986222	-4.8420588689	2.5763788739
C	0	-4.0744292381	-4.3708130561	1.5661453395
H	0	-4.2172324915	-5.0778516398	0.7423083258
H	0	-3.4808955114	-4.8908580109	2.3242177108
C	0	-3.2335825623	-3.2227229837	1.0172256894
O	0	-3.7033299568	-2.0581971969	1.0874243014
O	0	-2.0958273611	-3.5307572633	0.5205983167
C	0	-6.3522500260	-3.3844906835	1.0774446506
O	0	-6.2265196894	-3.6714008864	-0.1242839034
N	0	-7.3623453579	-2.6042965602	1.5193994913
H	0	-7.3685657340	-2.3086490785	2.4859152849
C	-1	-8.4061106381	-2.0927339261	0.6376555737
H	0	-9.2876047595	-1.8696027194	1.2393435813
H	0	-8.6505819299	-2.8740384913	-0.0880314847
C	0	-8.0040291773	-0.7924835313	-0.0928015523
O	0	-8.4513798152	0.2996110574	0.2584068860
N	0	-7.1685953923	-0.9754079676	-1.1460176376
H	0	-6.7330677056	-1.8870317202	-1.2400274024
C	0	-6.5587710333	0.1263107357	-1.8639416197
H	0	-6.5760639859	-0.0705186960	-2.9390540139
H	0	-7.1562249958	1.0218258073	-1.6688935569
C	0	-5.1036916102	0.4024356589	-1.4457826124
O	0	-4.3329268985	0.8884429967	-2.3101775628
O	0	-4.7981299093	0.1209084704	-0.2429296937
C	-1	-3.3942448079	3.6176785418	5.0436258728
H	-1	-3.4224203617	3.3052490526	6.0770395659
H	-1	-4.2102934237	4.2683908517	4.7664179049
H	0	-2.4843017839	4.2272075245	4.9396773294
C	0	-3.3659226019	2.5072337645	3.9881900481
H	0	-3.4911337389	2.9866368794	3.0082800317

H	0	-4.2182950183	1.8279309410	4.0999445679
C	0	-2.0579427664	1.7055105742	3.9703970238
H	0	-2.0803065682	0.9413044382	4.7557068457
H	0	-1.1996183664	2.3553105253	4.1640716295
C	0	-1.8405228501	1.0335802982	2.6255524042
O	0	-0.7045913077	1.2011771341	2.0804600688
O	0	-2.8054307547	0.3680534718	2.1380138707
C	-1	-5.4718387162	9.0821426142	2.1557412540
H	-1	-5.3332304131	8.6558395651	3.1382647203
H	-1	-6.5071815046	9.3245485270	1.9671233307
H	0	-4.9082541902	10.0217737008	2.1141867624
C	0	-4.9273494630	8.0777215674	1.1284604744
H	0	-3.8338406910	8.0409853952	1.2349647010
H	0	-5.1187405488	8.4196579703	0.1030091107
C	0	-5.5284167212	6.6762030750	1.3235100925
H	0	-6.5994221450	6.7029346856	1.0887041174
H	0	-5.4446951641	6.3795708126	2.3782779070
C	0	-4.8838245264	5.5845589086	0.4654450609
H	0	-4.9299614649	5.8618026612	-0.5980407408
H	0	-5.4325342862	4.6451696973	0.5947132036
N	0	-3.4960437953	5.3639652419	0.8786540672
H	0	-3.0019573545	6.1593692687	1.2598842133
C	0	-2.7128550206	4.3635487711	0.4174182453
N	0	-3.1816916769	3.4537313490	-0.4384517185
H	0	-2.7116396082	2.5291236521	-0.4946685474
H	0	-4.0952410799	3.5390183834	-0.8563270749
N	0	-1.4450247402	4.2766494463	0.8203489311
H	0	-1.1030722375	4.7108645298	1.6676287812
H	0	-0.8015196576	3.5832359581	0.3869752808
C	-1	-0.9474509170	-1.3911812730	7.4933783879
H	-1	0.0412522662	-0.9927108140	7.3195314249
H	-1	-1.1231717846	-1.6151346586	8.5353269171
H	0	-1.7012919249	-0.6814171170	7.1387929398
C	0	-1.1188970707	-2.7804937922	6.8589236760
H	0	-2.0683302831	-3.2128975597	7.2073017650
H	0	-0.3317714260	-3.4451659989	7.2432045717
C	0	-1.1034606697	-2.7885201562	5.3771318786
N	0	-1.2216764829	-3.9511936264	4.6408906348
C	0	-1.0250087375	-1.7859745528	4.4438067077
H	0	-0.8897299786	-0.7306087780	4.6113994730
C	0	-1.2135228080	-3.6215718157	3.3260520495
H	0	-1.2420021835	-4.3476764714	2.5302818844
N	0	-1.1058151949	-2.3113369972	3.1726569301
H	0	-0.8207755298	-1.4398825775	1.5963468398
C	-1	3.7928751552	6.2251865229	2.4327305146
H	-1	4.6607326777	6.7249612659	2.0278820845
H	-1	3.3294011907	6.7300632977	3.2672691160
H	0	3.0325555608	6.2341293708	1.6425183528
C	0	4.1229925134	4.7453167559	2.7405955924
H	0	5.0745918820	4.6413140274	3.2718086455
H	0	3.3258995353	4.3165605320	3.3590286065
C	0	4.1435881835	3.9501966746	1.4318519163
O	0	3.0584042232	3.9315149440	0.7915537648
O	0	5.2210897259	3.3954426876	1.0403498356
C	-1	12.1239371504	-2.3459777817	-0.7292194008
H	-1	13.1704230734	-2.0837102289	-0.7796468054
H	-1	11.8975516017	-3.2259902172	-1.3129087696
H	0	11.9214282173	-2.6309050329	0.3132052656
C	0	11.2137241838	-1.1575383513	-1.1189822966
H	0	11.6681568954	-0.6002278901	-1.9509646549

H	0	10.2506640841	-1.5361274739	-1.4808132758
C	0	10.9486373029	-0.2086531240	0.0655818640
H	0	10.2265504891	-0.6889645590	0.7403919631
H	0	11.8736248479	-0.0851403701	0.6463819025
C	0	10.4668520284	1.2030645810	-0.3128525728
H	0	10.3534666018	1.8088854380	0.5967922077
H	0	11.2484385032	1.6910087467	-0.9108537276
C	0	9.1771861046	1.3128603914	-1.1287227977
H	0	9.0344844676	2.3479632155	-1.4517825376
H	0	9.2062899002	0.6825548073	-2.0212283971
N	0	7.9446713315	0.9298793313	-0.3689948919
H	0	7.1057766138	1.3193395104	-0.8524734756
H	0	7.8344396207	-0.1130314830	-0.3136095705
H	0	7.9034120805	1.3418113707	0.5928863701
O	0	1.8380228901	1.5380393690	-3.5355049971
H	0	3.3413632021	2.4029541160	-3.7094331351
O	0	0.3423555667	2.5204204826	-0.1564701704
O	0	0.8462066030	3.6484217731	2.5770542743
H	0	0.4389516100	2.7918463244	2.3509694230
H	0	1.5037039409	3.7749983997	1.8580466327
O	0	-3.2232371317	-1.1227941887	-4.2010802898
H	0	-3.9271939510	-1.5194094167	-3.6472478732
H	0	-2.5629264783	-1.8447201940	-4.2762000387
O	0	-4.4313930198	-2.7650767992	-2.2363652314
H	0	-3.6257732676	-2.3708720606	-1.7977012420
H	0	-4.9535361896	-3.1481054685	-1.5073694788
O	0	2.3594641438	3.8571559823	-1.7277626698
H	0	2.7466682773	3.8035506490	-0.8011426388
O	0	5.8466046905	2.5105619268	-1.4028376466
H	0	5.3979464366	2.7619763374	-0.5416189509
H	0	6.3356508226	3.3165661840	-1.6396137936
O	0	4.1084155751	3.0187508546	-3.5502599401
H	0	4.6561930436	2.5751029298	-2.8655030277
O	0	7.3956021029	2.2064160737	2.0743552787
H	0	6.5981790461	2.7353048201	1.7993226272
H	0	7.0589599432	1.5867823201	2.7397227655
O	0	2.7874023513	-0.9356459581	-2.5312184424
H	0	2.2009486549	0.6501536064	-3.2985157295
H	0	-1.2965852892	-4.8862480788	5.0182545338
H	0	3.1017828574	3.7161643480	-2.3855417333
Cl	0	7.5084816774	-2.1466699048	-0.4812800523
H	0	3.0916261578	-0.2770267023	-1.8763714820
O	0	-0.2934925812	0.0378991540	-4.4637289425
H	0	0.0700738035	-0.8593435287	-4.5279495962
O	0	0.3684692794	-1.9921059089	-1.7610464058
H	0	1.9203081146	-1.2225461057	-2.1571032935
H	0	-0.1129231353	-1.9375693150	-2.6128061096
H	0	0.4727038042	0.6271550967	-4.2074806275

15L_S3d
E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.955082 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.390476 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.632684 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.788092 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.713116 au

Mn	0	1.0983755728	2.2205059905	-1.8635748445
Mn	0	-0.8843390591	-2.5522014339	-0.7304030240
Mn	0	-0.1906752099	0.8427355080	0.1247233078
Mn	0	-2.8269161141	-0.4884239162	0.2916300078
O	0	0.1734626503	0.6143645135	-1.6113298820

O	0	-1.9965388967	0.9888827127	-0.3508079394
O	0	-2.2511255815	-1.5481342303	-1.3214843790
O	0	-0.7223607265	-1.1622954429	0.6188740302
Ca	0	-2.0287970309	0.4890787666	-2.7339452076
C	-1	0.5257029805	4.6763420117	-5.5666300035
H	-1	0.5889839720	5.6061810123	-5.0205590035
H	-1	0.7135699797	4.7621270134	-6.6265490035
H	0	1.3216236421	4.0381289103	-5.1627766286
C	0	-0.8222301095	3.9687887754	-5.3331408239
H	0	-0.9491065933	3.1462796080	-6.0483723761
H	0	-1.6689535068	4.6458828873	-5.5119446402
C	0	-1.0058549712	3.3440047166	-3.9424879940
O	0	-1.9960880043	2.5641046075	-3.7821197935
O	0	-0.1613984802	3.6224444524	-3.0434291367
C	-1	-2.9106329168	-6.5915480196	-5.3962210035
H	-1	-1.9493159126	-7.0511690108	-5.5720520035
H	-1	-3.6433259156	-6.7287520263	-6.1777470035
H	0	-3.3220491293	-7.1311510247	-4.5290503409
C	0	-2.6425055158	-5.1466527145	-4.9680644416
H	0	-3.5337616288	-4.6878352844	-4.5222176115
H	0	-2.3425016942	-4.5182147237	-5.8140524655
C	0	-1.5060043348	-5.1966007907	-3.9337491412
H	0	-0.5718140226	-5.4854145005	-4.4356334418
H	0	-1.7183553099	-5.9568490778	-3.1761019951
C	0	-1.2491709841	-3.8833013635	-3.2402882198
O	0	-1.0878588700	-2.8356049759	-3.8999211887
O	0	-1.2066220481	-3.9849226686	-1.9481281572
C	-1	5.0841760648	-4.5734929467	0.9374239965
H	0	5.9768604730	-5.2027035572	1.0484519852
H	0	5.2328813143	-3.9724131620	0.0365677264
C	0	4.9846667880	-3.6659996633	2.1646418660
O	0	4.4851782558	-4.0751428919	3.2337606982
C	0	3.8543852460	-5.5053692449	0.7689111489
H	0	3.8170196840	-6.1944593201	1.6211384703
H	0	3.9888877536	-6.1064749613	-0.1345044216
C	0	2.5678637344	-4.7424156308	0.6840475782
N	0	2.2218096654	-3.9212577933	1.7424993387
H	0	2.7627868461	-3.8594446889	2.6051569412
C	0	1.5976840363	-4.5190283421	-0.2667486479
H	0	1.4836805172	-4.9394907056	-1.2540129525
C	0	1.1430657891	-3.2094162122	1.4090734432
H	0	0.7309469735	-2.4528838993	2.0413524336
N	0	0.7045276037	-3.5671510632	0.2113313514
N	0	5.3827985721	-2.3952248365	1.9847540836
H	0	5.8837851034	-2.1710332787	1.1204366716
C	-1	5.0501630351	-1.3143759470	2.9101779965
H	0	5.9089316146	-0.6333940333	2.9625155268
H	0	4.9013710484	-1.7513478709	3.8996158253
C	0	3.7884459876	-0.5574231511	2.4525165253
H	0	3.5107716829	0.1781622598	3.2179924796
H	0	2.9584855054	-1.2664332101	2.3811150850
C	0	3.9867228575	0.1361284626	1.1036331582
H	0	4.4748204489	-0.5427350056	0.3916963810
H	0	4.6523920998	1.0027838355	1.1958964818
C	0	2.7364310877	0.6239092002	0.3797379014
O	0	2.9196450590	1.1989297264	-0.7209429088
O	0	1.5954529378	0.3713333500	0.9051061917
C	-1	-5.4203029407	-3.9707460425	2.1952459965
H	0	-5.2699071495	-3.2272744301	2.9844965204
H	0	-5.9244857486	-4.8338221082	2.6474529337

C	0	-4.0810906585	-4.4158830358	1.6076341837
H	0	-4.2368794244	-5.1502333114	0.8113672491
H	0	-3.4798959215	-4.9108447416	2.3766831264
C	0	-3.2388633887	-3.2938496600	1.0117867436
O	0	-3.6823289032	-2.1113357145	1.0874558033
O	0	-2.1372763589	-3.6387413644	0.4865806486
C	0	-6.3406676992	-3.4067786893	1.1139415099
O	0	-6.2055924146	-3.6856949566	-0.0886257461
N	0	-7.3616189392	-2.6385623694	1.5531608547
H	0	-7.3794674839	-2.3513856789	2.5220893400
C	-1	-8.4025969575	-2.1310540696	0.6663199965
H	0	-9.2934054776	-1.9263881843	1.2610376966
H	0	-8.6294743936	-2.9072610755	-0.0703353052
C	0	-8.0083999214	-0.8187963160	-0.0428009713
O	0	-8.4542037524	0.2672481422	0.3280062232
N	0	-7.1762681706	-0.9845250967	-1.1018234637
H	0	-6.7397882449	-1.8940194872	-1.2107436394
C	0	-6.5716758134	0.1290416541	-1.8033459751
H	0	-6.6169169740	-0.0338644033	-2.8834101413
H	0	-7.1522584363	1.0257814330	-1.5671031822
C	0	-5.1045344343	0.3753806629	-1.4162840986
O	0	-4.3538858421	0.8874851217	-2.2812672488
O	0	-4.7684965536	0.0447934782	-0.2332686244
C	-1	-3.4149080100	3.6339779758	5.0283769965
H	-1	-3.4414270072	3.3290919756	6.0640849965
H	-1	-4.2339050159	4.2789989684	4.7465989965
H	0	-2.5073312426	4.2462680816	4.9200495945
C	0	-3.3772059970	2.5115558859	3.9849561526
H	0	-3.4852381373	2.9805831573	2.9981974047
H	0	-4.2351455123	1.8385090775	4.0917917415
C	0	-2.0744380148	1.6980561026	3.9937215730
H	0	-2.1151287847	0.9379822042	4.7823968965
H	0	-1.2137502703	2.3427191505	4.1938917797
C	0	-1.8479987490	1.0145154472	2.6559316188
O	0	-0.7203899083	1.2017188489	2.0990691144
O	0	-2.7999324831	0.3219698213	2.1820904576
C	-1	-5.5174500595	9.0676439567	2.1007099965
H	-1	-5.3766960557	8.6492509579	3.0863239965
H	-1	-6.5539060617	9.3040609472	1.9106099965
H	0	-4.9580740058	10.0095850656	2.0528630178
C	0	-4.9769808958	8.0620751587	1.0756285889
H	0	-3.8840477736	8.0194531232	1.1848320758
H	0	-5.1648527508	8.4055135847	0.0499685156
C	0	-5.5898622092	6.6670076605	1.2723509185
H	0	-6.6611461854	6.7032551274	1.0395722998
H	0	-5.5052128877	6.3705122888	2.3269305278
C	0	-4.9541203990	5.5721167425	0.4140522067
H	0	-5.0218074577	5.8364925415	-0.6517119294
H	0	-5.4904286449	4.6289898864	0.5631861347
N	0	-3.5592379940	5.3670026504	0.8056443009
H	0	-3.0457159774	6.1787906071	1.1200056536
C	0	-2.8048021122	4.3164769717	0.4175570873
N	0	-3.3114111678	3.3561146073	-0.3558288351
H	0	-2.8197720289	2.4456350438	-0.4218981192
H	0	-4.1556999843	3.4851903789	-0.8915639681
N	0	-1.5432533055	4.2180236588	0.8366538955
H	0	-1.1873966716	4.7155283612	1.6420070785
H	0	-0.8865308385	3.5366087857	0.4058605450
C	-1	-0.9453039646	-1.3457120017	7.5144379965
H	-1	0.0415790317	-0.9441669927	7.3373499965

H	-1	-1.1197549626	-1.5627160033	8.5580689965
H	0	-1.6978287088	-0.6333779228	7.1609272047
C	0	-1.1218471185	-2.7291995623	6.8706410187
H	0	-2.0777511481	-3.1559164175	7.2078949234
H	0	-0.3435508116	-3.4028158887	7.2576642626
C	0	-1.0927391897	-2.7316655179	5.3873418290
N	0	-1.2582310646	-3.8891052906	4.6508217814
C	0	-0.9484677948	-1.7367991348	4.4527164729
H	0	-0.7619611278	-0.6885520948	4.6191507483
C	0	-1.2114531556	-3.5644216567	3.3355263013
H	0	-1.2600889507	-4.2891236558	2.5395014514
N	0	-1.0346689049	-2.2624832500	3.1810547828
H	0	-0.7652455253	-1.4579258669	1.5718656053
C	-1	3.7598999661	6.2538650412	2.3960989965
H	-1	4.6254269616	6.7544630491	1.9873009965
H	-1	3.2944149615	6.7628530370	3.2270119965
H	0	2.9994521696	6.2484284864	1.6060462364
C	0	4.0998297856	4.7804912720	2.7262516609
H	0	5.0529637274	4.6914857661	3.2573992824
H	0	3.3063015761	4.3575058641	3.3532498135
C	0	4.1215725655	3.9641735917	1.4315487950
O	0	3.0311797403	3.9210941512	0.8010332992
O	0	5.2024966072	3.4171569678	1.0392043052
C	-1	12.1280080441	-2.3035228826	-0.7047500035
H	-1	13.1733080417	-2.0370068730	-0.7574310035
H	-1	11.9053670522	-3.1888298846	-1.2818380035
H	0	11.9269069529	-2.5812855150	0.3398891380
C	0	11.2102787341	-1.1240394864	-1.1045875056
H	0	11.6602141377	-0.5721218113	-1.9425734674
H	0	10.2491458735	-1.5122499288	-1.4616258485
C	0	10.9399769080	-0.1649369816	0.0705313375
H	0	10.2221168135	-0.6429539091	0.7514566966
H	0	11.8646954917	-0.0289601173	0.6489581076
C	0	10.4476775941	1.2394237217	-0.3216387328
H	0	10.3317272578	1.8536755413	0.5819880888
H	0	11.2249060023	1.7265232900	-0.9259770920
C	0	9.1558750947	1.3325384659	-1.1363301165
H	0	9.0056477983	2.3637288359	-1.4684115136
H	0	9.1877698177	0.6944918478	-2.0232240425
N	0	7.9270840048	0.9479643879	-0.3711688240
H	0	7.0853467764	1.3316768108	-0.8537060843
H	0	7.8200017061	-0.0954962084	-0.3124455871
H	0	7.8874547060	1.3639603810	0.5890321898
O	0	1.8177762600	1.5337674550	-3.5165086886
H	0	3.3102271867	2.4197155226	-3.7041618743
O	0	0.3013040133	2.5198542395	-0.1440642208
O	0	0.8071402181	3.6751932922	2.5728701898
H	0	0.4007182906	2.8158510133	2.3568842273
H	0	1.4723796426	3.7879155130	1.8588842611
O	0	-3.2247827455	-1.1040049852	-4.1870334578
H	0	-3.9277601926	-1.5174881386	-3.6453441744
H	0	-2.5495766004	-1.8122337680	-4.2671254255
O	0	-4.4481412399	-2.7854452877	-2.2350624191
H	0	-3.6226820471	-2.4215193581	-1.8197554110
H	0	-4.9557494103	-3.1628372479	-1.4922275532
O	0	2.3291892875	3.8585102423	-1.7106165327
H	0	2.7218911966	3.8024085312	-0.7860339880
O	0	5.8189860045	2.5218930482	-1.4042063333
H	0	5.3735577592	2.7733342511	-0.5414973823
H	0	6.3106887475	3.3267029290	-1.6396911169

O	0	4.0726853379	3.0408973301	-3.5455424346
H	0	4.6273637254	2.5974643723	-2.8660856312
O	0	7.3896717632	2.2409708350	2.0656318946
H	0	6.5881883561	2.7649165715	1.7940649648
H	0	7.0633154554	1.6292613036	2.7433307473
O	0	2.8607299414	-0.9100818483	-2.5249747006
H	0	2.1996344721	0.6545351671	-3.2775583229
H	0	-1.3838531324	-4.8182790676	5.0291965382
H	0	3.0676438461	3.7257524699	-2.3745392600
Cl	0	7.4895627905	-2.1259429791	-0.4857529123
H	0	3.1487037289	-0.2467815396	-1.8671572180
O	0	-0.3404546260	0.1176886206	-4.4664931966
H	0	-0.0251469895	-0.7838112455	-4.6376961586
O	0	0.4141736956	-1.9726056455	-1.8191066446
H	0	2.0047730283	-1.2232652662	-2.1514353754
H	0	-0.0316752407	-1.8287057592	-2.6787997151
H	0	0.4605502475	0.6579982529	-4.2014063504

1L_S3a-fixed

E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.934799 au

H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.370249 au

G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.60689 au

E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.771594 au

E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.697162 au

Mn	0	1.2760798011	2.0549734442	-1.9087717167
Mn	0	-1.0457083896	-2.5251730452	-0.5283668411
Mn	0	-0.1178300921	0.7411906559	0.0987739067
Mn	0	-2.6969177847	-0.4577280117	0.3243570749
O	0	0.2314117833	0.3366238441	-1.5968551371
O	0	-1.9388154481	0.9920317216	-0.3642185268
O	0	-2.4680831364	-1.4524114452	-1.1886936020
O	0	-1.0022571160	-1.1158444132	0.7451734194
Ca	0	-1.8933570269	0.4123029226	-2.8018203972
C	-1	0.5534799135	4.6067477078	-5.5057325502
H	-1	0.6206110655	5.5379777831	-4.9627474014
H	-1	0.7467476250	4.6869541607	-6.5650249435
H	0	1.3347516013	3.9573710986	-5.0934962631
C	0	-0.8118880265	3.9095533166	-5.3098771849
H	0	-0.9282010708	3.1127464821	-6.0551273629
H	0	-1.6439234454	4.6034629039	-5.4940195978
C	0	-1.0627864344	3.2265515602	-3.9527645866
O	0	-2.1038764195	2.4946622510	-3.8631100820
O	0	-0.2371126182	3.3950151282	-3.0167849879
C	-1	-2.9625902702	-6.6362927581	-5.3092037769
H	-1	-2.0036613178	-7.1032927016	-5.4788150120
H	-1	-3.6925092076	-6.7713714825	-6.0936570363
H	0	-3.3888169258	-7.1695389486	-4.4443564721
C	0	-2.7274815526	-5.1772990017	-4.9021782069
H	0	-3.6753750274	-4.6673155001	-4.6905604398
H	0	-2.2367221247	-4.6146138562	-5.7044347558
C	0	-1.8525648733	-5.1598631904	-3.6481449493
H	0	-0.9074715555	-5.6914839576	-3.8377233633
H	0	-2.3376730681	-5.7040620988	-2.8289791227
C	0	-1.4688615566	-3.7939657162	-3.1235113392
O	0	-1.5488222629	-2.7702518187	-3.8252603573
O	0	-0.9967364136	-3.8181235076	-1.9197263269
C	-1	5.0166329032	-4.6502990515	1.0541821670
H	0	5.7251343038	-5.4513776167	1.2933065921
H	0	5.4098606782	-4.1032836338	0.1936050025
C	0	4.8740292956	-3.7265864238	2.2618748851

O	0	4.2315228792	-4.0920738502	3.2714696945
C	0	3.6438371148	-5.3176128749	0.7189228024
H	0	3.4169429623	-6.0299244717	1.5214285535
H	0	3.7459387833	-5.8925402200	-0.2054350748
C	0	2.4745184719	-4.3771548935	0.5788611392
N	0	2.1914614244	-3.4636398062	1.5844294841
H	0	2.7045478801	-3.4283523058	2.4664195800
C	0	1.4930690096	-4.1711568444	-0.3623370972
H	0	1.3169648492	-4.6634944397	-1.3049521337
C	0	1.1404324164	-2.7237379221	1.2366262809
H	0	0.7989596109	-1.8656218198	1.7795570101
N	0	0.6512674722	-3.1388057911	0.0663842990
N	0	5.3327614296	-2.4770860838	2.1078478336
H	0	5.9405773297	-2.2798334464	1.3043383483
C	-1	4.9963070496	-1.3835934828	3.0145904323
H	0	5.8795795549	-0.7378320958	3.0903116736
H	0	4.8032462261	-1.8063031962	4.0032845622
C	0	3.7887382775	-0.5625960404	2.5305422236
H	0	3.6183655907	0.2591462067	3.2377227212
H	0	2.8921329298	-1.1824431741	2.5658023021
C	0	3.9878555248	-0.0139499242	1.1179546254
H	0	4.4489395401	-0.7733442158	0.4749374244
H	0	4.6735812589	0.8412603088	1.1243206797
C	0	2.7492300303	0.4348254925	0.3528615604
O	0	2.9347769399	0.9828757673	-0.7401998719
O	0	1.5891666962	0.1774447123	0.8798560852
C	-1	-5.4889243760	-3.9692639360	2.2605324617
H	0	-5.3621017946	-3.2266181346	3.0550812224
H	0	-5.9787603985	-4.8440318162	2.7056332834
C	0	-4.1300841193	-4.3893350401	1.6903189680
H	0	-4.2605935090	-5.1226631180	0.8887930951
H	0	-3.5363702058	-4.8847164450	2.4685740702
C	0	-3.2747844058	-3.2635663318	1.1222576651
O	0	-3.6511221808	-2.0684088275	1.2707357091
O	0	-2.1836003907	-3.6014735224	0.5471689303
C	0	-6.4082366479	-3.4169298534	1.1746952817
O	0	-6.2386739547	-3.6634136513	-0.0282169451
N	0	-7.4623864542	-2.6925995816	1.6142983747
H	0	-7.5007566529	-2.4264415340	2.5888749027
C	-1	-8.4516629551	-2.1149275579	0.7108921477
H	0	-9.3882277884	-1.9824592951	1.2534015463
H	0	-8.6042006963	-2.8125001715	-0.1168275471
C	0	-8.0129106349	-0.7304635040	0.1899555904
O	0	-8.4894203121	0.3049488843	0.6559474945
N	0	-7.0805893429	-0.7647137617	-0.7947359956
H	0	-6.6738141032	-1.6545995328	-1.0602671944
C	0	-6.4802703364	0.4285196243	-1.3561970066
H	0	-6.6975907246	0.5096219069	-2.4251478802
H	0	-6.9231538162	1.2897425283	-0.8464613987
C	0	-4.9562270033	0.4787838219	-1.1892853665
O	0	-4.2641689550	0.9055437406	-2.1265448289
O	0	-4.5215375764	0.0771133804	-0.0412924437
C	-1	-3.4434681188	3.6319134107	5.0746380335
H	-1	-3.4772896514	3.3308738266	6.1112823944
H	-1	-4.2569069957	4.2813078682	4.7865803024
H	0	-2.5422047402	4.2545316204	4.9749818824
C	0	-3.3786727292	2.4951922938	4.0450080610
H	0	-3.6978774562	2.8922732052	3.0731415311
H	0	-4.0816631811	1.6898607829	4.2856978746
C	0	-1.9628235323	1.9402087980	3.8829574756

H	0	-1.6923332636	1.3168314285	4.7461917846
H	0	-1.2305888530	2.7533123749	3.8620672698
C	0	-1.7600921657	1.1496948138	2.6008015356
O	0	-0.6258990234	1.2624105915	2.0556933363
O	0	-2.7280071060	0.4344076171	2.1720879062
C	-1	-5.4944075919	9.0690433188	2.1168353059
H	-1	-5.3612786278	8.6531833711	3.1046304726
H	-1	-6.5283921949	9.3116918571	1.9210020179
H	0	-4.9443421827	10.0181219627	2.0891205680
C	0	-4.9115220819	8.0934881596	1.0825389643
H	0	-3.8167802284	8.1085524280	1.1815570080
H	0	-5.1305719814	8.4354551608	0.0622597106
C	0	-5.4328625652	6.6615508782	1.2683661300
H	0	-6.5225276065	6.6519834853	1.1373990078
H	0	-5.2343173969	6.3252159842	2.2952688026
C	0	-4.8419984461	5.6363950164	0.2955670412
H	0	-5.0386887928	5.9438671846	-0.7421045576
H	0	-5.3239674413	4.6666193406	0.4542251220
N	0	-3.4049616912	5.4565122261	0.5121261781
H	0	-2.8567233878	6.2791852220	0.7233674244
C	0	-2.7068197975	4.3648319700	0.1290762892
N	0	-3.3159949443	3.3656347791	-0.5200562561
H	0	-2.8313382088	2.4600936744	-0.5986557266
H	0	-4.1212881157	3.5227324258	-1.1065738919
N	0	-1.4149439045	4.2559276732	0.4274374470
H	0	-0.9758425484	4.7370160616	1.2060567337
H	0	-0.8278137601	3.4939415911	0.0304321573
C	-1	-1.0205145659	-1.3557126563	7.5909656068
H	-1	-0.0301668943	-0.9616826242	7.4167098432
H	-1	-1.2015312232	-1.5674935601	8.6343962220
H	0	-1.7629065513	-0.6263902220	7.2497090056
C	0	-1.1989994004	-2.7190062068	6.8935623375
H	0	-2.1618717834	-3.1547321095	7.1941673988
H	0	-0.4284283466	-3.4099924633	7.2587925435
C	0	-1.1478147994	-2.6911764733	5.4018835772
N	0	-0.9865615537	-3.8454499885	4.6445855453
C	0	-1.2889782103	-1.6813956588	4.4900436136
H	0	-1.4368706827	-0.6286120092	4.6386374278
C	0	-1.0272253089	-3.5496424572	3.3388969522
H	0	-0.9307772453	-4.2419622144	2.5186423083
N	0	-1.2175786168	-2.2370337909	3.2290720725
H	0	-1.2309426800	-1.7190172781	2.3116197842
C	-1	3.7616906488	6.1915032604	2.4661295386
H	-1	4.6323457254	6.6845410906	2.0595735721
H	-1	3.2955425899	6.7067812083	3.2929282521
H	0	3.0071395720	6.1800244697	1.6707456052
C	0	4.1119267890	4.7215967044	2.8005775602
H	0	5.0501163461	4.6470023369	3.3605936434
H	0	3.3087958974	4.2868342280	3.4076203248
C	0	4.1842319650	3.8962686260	1.5066064327
O	0	3.1328737808	3.8585379319	0.8218132432
O	0	5.2809040734	3.3283587348	1.1795322499
C	-1	12.0837929376	-2.4357879728	-0.5634652826
H	-1	13.1311375511	-2.1767781190	-0.6122679806
H	-1	11.8575869534	-3.3216720268	-1.1383015774
H	0	11.8671653373	-2.6986448558	0.4815300215
C	0	11.2001087320	-1.2411436049	-0.9864964285
H	0	11.6551846279	-0.7332793313	-1.8494379472
H	0	10.2193770086	-1.6053422604	-1.3125745203
C	0	10.9919902991	-0.2398642424	0.1645120636

```
H   0    10.2619236452   -0.6692941608    0.8639364310
H   0    11.9302436484   -0.1302187967    0.7266927659
C   0    10.5532407721    1.1715415771   -0.2604918266
H   0    10.4725980202    1.8150444156    0.6265354781
H   0    11.3387336467    1.6114999200   -0.8898353040
C   0     9.2527661711    1.2813415885   -1.0567907649
H   0     9.1142127171    2.3101219328   -1.4012533859
H   0     9.2595489265    0.6307044392   -1.9351050457
N   0     8.0318798573    0.9304878849   -0.2659252872
H   0     7.1902008791    1.3224953019   -0.7483554312
H   0     7.9164593381   -0.1060720183   -0.1651178752
H   0     8.0098879533    1.3740645937    0.6827839427
O   0     1.9522827373    1.3540931533   -3.5451067286
H   0     2.7462113264    1.8694904867   -3.8082874590
O   0     0.4075840592    2.3711306131   -0.2057493056
O   0     0.7577951226    3.8961869742    2.3306339693
H   0     0.4142429189    3.0119467726    2.1065982346
H   0     1.5330614009    3.9723428474    1.7247501498
O   0    -3.4434571075   -0.9092126106   -4.2103718416
H   0    -4.1783506175   -1.1936692648   -3.6346457876
H   0    -2.9042066366   -1.7234219322   -4.3123486005
O   0    -4.7103318983   -2.5467044081   -2.1618292450
H   0    -3.8855543504   -2.1899916023   -1.7415700628
H   0    -5.1356889232   -3.0685645049   -1.4556037901
O   0     2.3416462065    3.5896338542   -1.8335510789
H   0     2.7040419197    3.6026672814   -0.9181181538
O   0     5.9648679305    2.4851745295   -1.2872171964
H   0     5.5194316831    2.7471274180   -0.4288263037
H   0     6.3683115723    3.3128453151   -1.5955748960
O   0     4.2536692691    3.0148329243   -3.5749414486
H   0     4.8005207992    2.4994078054   -2.9507414192
O   0     7.5190407835    2.2406815429    2.1701980120
H   0     6.6950682167    2.7370005692    1.9076670766
H   0     7.2071117300    1.5798892987    2.8076054384
O   0     2.1284103499   -1.2414856880   -2.7095458377
H   0     1.4077893467   -0.9433164401   -2.1055663468
H   0    -0.8535174875   -4.7781960853    5.0166678705
H   0     3.5689438179    3.3821749719   -2.9408031543
Cl  0     7.6355827574   -2.1800066824   -0.1073451591
H   0     2.3433900761   -0.3454000716   -3.0837243185
O   0    -0.2864228086    0.2799980725   -4.6249991078
H   0     0.0881670325   -2.5542442152   -4.6639942934
O   0     0.9303007039   -2.1668202254   -4.9672174322
H   0     0.1054600405   -0.5958278853   -4.8675786209
H   0     1.3988271480   -1.9303729133   -4.1197590853
H   0     0.5171692895    0.8027635862   -4.3520454815
```

1L_S3a
E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.958396 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.392613 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.63315 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.794703 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.719946 au

```
Mn  0     1.2057468149    2.1411273995   -1.8212082900
Mn  0    -0.9007785002   -2.3744366047   -0.7429991691
Mn  0    -0.1673039945    0.7588880583    0.1690737662
Mn  0    -2.7007082310   -0.5573993121    0.3253903203
O   0     0.2054308097    0.3709165405   -1.5266735822
O   0    -1.9930404251    0.9559411905   -0.2905607137
O   0    -2.4193306051   -1.4354906012   -1.2699985402
```

O	0	-0.9617110752	-1.1469859616	0.6972182883
Ca	0	-1.9373967465	0.5653664182	-2.7635632182
C	-1	0.4906301155	4.6270840014	-5.5140459838
H	-1	0.5454701369	5.5569130002	-4.9672939838
H	-1	0.6790911175	4.7147059971	-6.5736169838
H	0	1.2702595059	3.9784113197	-5.0971414540
C	0	-0.8781799129	3.9337129906	-5.3301836026
H	0	-0.9742156104	3.1131012449	-6.0530818890
H	0	-1.7063389755	4.6191752676	-5.5559229940
C	0	-1.1617002617	3.2829498949	-3.9666843783
O	0	-2.2532256972	2.6316750888	-3.8514204986
O	0	-0.3042467815	3.3769754049	-3.0494003977
C	-1	-2.8539871439	-6.6687249217	-5.3541809838
H	-1	-1.8886671543	-7.1204039439	-5.5289609838
H	-1	-3.5844121472	-6.8115309049	-6.1367919838
H	0	-3.2694728571	-7.2015285770	-4.4841252004
C	0	-2.6508281560	-5.1999062515	-4.9734585680
H	0	-3.6110897719	-4.6967775274	-4.8063257857
H	0	-2.1452307498	-4.6525462131	-5.7769150023
C	0	-1.8159120324	-5.1240938334	-3.6967645852
H	0	-0.8876313688	-5.7046814904	-3.8061155666
H	0	-2.3471371871	-5.5771923466	-2.8503715587
C	0	-1.3986419067	-3.7337070883	-3.2813550985
O	0	-1.5478977903	-2.7521590129	-4.0276819832
O	0	-0.8179311343	-3.6843148419	-2.1234287920
C	-1	5.1156069038	-4.5889531048	0.9912890162
H	0	5.8804171498	-5.3435600774	1.2105826075
H	0	5.4527191586	-4.0239477730	0.1188571321
C	0	4.9651051674	-3.6713815740	2.2024286429
O	0	4.3639598718	-4.0587103052	3.2283279199
C	0	3.7799538212	-5.3296459571	0.6942986503
H	0	3.5815705508	-6.0212583410	1.5216669254
H	0	3.8960810304	-5.9274624544	-0.2136417844
C	0	2.6071665454	-4.4075505924	0.5318129771
N	0	2.2795379186	-3.5268894204	1.5535580578
H	0	2.7599942580	-3.5134886373	2.4537218762
C	0	1.7133729595	-4.1275304225	-0.4738130864
H	0	1.5949299168	-4.5753846289	-1.4475684147
C	0	1.2879098125	-2.7311361666	1.1506859830
H	0	0.9302274501	-1.8802880247	1.6938020220
N	0	0.8919513490	-3.0802746661	-0.0687532219
N	0	5.3820478816	-2.4077976819	2.0380179603
H	0	5.9712321608	-2.1987165416	1.2247610837
C	-1	5.0523839787	-1.3312791033	2.9657600162
H	0	5.9200515589	-0.6612574893	3.0115145263
H	0	4.9116537015	-1.7669578527	3.9577549862
C	0	3.8053116819	-0.5394370868	2.5399884583
H	0	3.6266678894	0.2561063317	3.2746536317
H	0	2.9320992322	-1.1923562400	2.5781912854
C	0	3.9611359142	0.0544315166	1.1420367421
H	0	4.3962588570	-0.6877667322	0.4610313318
H	0	4.6536459025	0.9037354746	1.1552819014
C	0	2.7089389749	0.5366658271	0.4249665158
O	0	2.8792298725	1.1366021739	-0.6430395886
O	0	1.5565165791	0.2455048392	0.9524864269
C	-1	-5.3949420843	-4.0724638634	2.2352380162
H	0	-5.2423166935	-3.3152711917	3.0115918650
H	0	-5.8988888658	-4.9258643970	2.7059007265
C	0	-4.0576848129	-4.5267812142	1.6525356488
H	0	-4.2151412522	-5.2725101615	0.8677945424

H	0	-3.4628549160	-5.0192243065	2.4313659293
C	0	-3.1889508048	-3.4262052846	1.0447984430
O	0	-3.5678700701	-2.2199707855	1.1841631579
O	0	-2.1227182404	-3.7961973986	0.4751003369
C	0	-6.3191417201	-3.5188339364	1.1533549588
O	0	-6.1477997862	-3.7471274495	-0.0528449045
N	0	-7.3867846366	-2.8180565953	1.6007746331
H	0	-7.4325695936	-2.5658804133	2.5786853572
C	-1	-8.3906410426	-2.2567197945	0.7033660162
H	0	-9.3306005762	-2.1557032660	1.2471434319
H	0	-8.5248431328	-2.9492074111	-0.1316388479
C	0	-7.9860426930	-0.8578879857	0.2015086698
O	0	-8.4572464716	0.1625057101	0.7042078244
N	0	-7.0846296229	-0.8627874142	-0.8123707248
H	0	-6.6628776928	-1.7423003189	-1.0894866083
C	0	-6.4924441642	0.3471400238	-1.3415666102
H	0	-6.6995703557	0.4503524107	-2.4105684329
H	0	-6.9481193323	1.1936205103	-0.8184660070
C	0	-4.9722145448	0.4100446735	-1.1586763051
O	0	-4.2856961655	0.9160466450	-2.0602146173
O	0	-4.5366018304	-0.0698055719	-0.0419618936
C	-1	-3.4554389093	3.5468550921	5.0751830162
H	-1	-3.4812039163	3.2409420927	6.1106320162
H	-1	-4.2795898946	4.1850541110	4.7926040162
H	0	-2.5522334615	4.1650009456	4.9673015019
C	0	-3.4208858945	2.4388851052	4.0161827213
H	0	-3.5185583350	2.9229044985	3.0356082624
H	0	-4.2825787623	1.7683584567	4.1089188146
C	0	-2.1223335935	1.6235971850	4.0264935632
H	0	-2.1834968519	0.8604603677	4.8109094008
H	0	-1.2629893425	2.2629681358	4.2476881752
C	0	-1.8603060483	0.9612456952	2.6838314597
O	0	-0.7325097304	1.1706359599	2.1534640164
O	0	-2.7945486265	0.2410636770	2.1910416494
C	-1	-5.5984797848	8.9647531413	2.1475400162
H	-1	-5.4557407944	8.5467731380	3.1330970162
H	-1	-6.6366767796	9.1925201652	1.9561660162
H	0	-5.0611308374	9.9213003046	2.1223976601
C	0	-5.0188896499	8.0064226610	1.1028068884
H	0	-3.9276544940	7.9846985180	1.2332592993
H	0	-5.1959961633	8.3852464907	0.0875262561
C	0	-5.5980392771	6.5919924628	1.2311004256
H	0	-6.6736592502	6.6173545544	1.0156927788
H	0	-5.4891280079	6.2379013029	2.2654140489
C	0	-4.9529156646	5.5675615209	0.2967589985
H	0	-5.0575174138	5.8870179329	-0.7503005168
H	0	-5.4555897850	4.6015779782	0.4047378103
N	0	-3.5425123040	5.3741383245	0.6346411016
H	0	-3.0100792846	6.1856846520	0.9154484681
C	0	-2.8328923205	4.2680259483	0.3365138713
N	0	-3.3964095238	3.2791266390	-0.3683839522
H	0	-2.8998113453	2.3766629801	-0.4222452778
H	0	-4.1068643494	3.4651026658	-1.0604895949
N	0	-1.5920409770	4.1171603780	0.7920890709
H	0	-1.1981237699	4.6833862982	1.5324956020
H	0	-0.9379540727	3.4251044617	0.3694591458
C	-1	-0.9487270232	-1.4140789655	7.5620570162
H	-1	0.0349459862	-1.0043369881	7.3862260162
H	-1	-1.1229980283	-1.6330049615	8.6051620162
H	0	-1.7054875327	-0.7010142208	7.2185606945

C	0	-1.0869316902	-2.7780054336	6.8533735884
H	0	-2.0479410560	-3.2330414976	7.1299516627
H	0	-0.3122738507	-3.4570514582	7.2334775782
C	0	-1.0098989492	-2.7512857552	5.3604946409
N	0	-1.0288608976	-3.9176845472	4.6024429171
C	0	-0.9811344919	-1.7336886906	4.4469521464
H	0	-0.9188052670	-0.6725084142	4.5967629255
C	0	-1.0237674873	-3.6204198558	3.2961071914
H	0	-1.0370853461	-4.3155058954	2.4718764053
N	0	-1.0095839144	-2.2952145715	3.1847916256
H	0	-1.0364554381	-1.7865282643	2.2629208806
C	-1	3.7012831523	6.2264789277	2.4539080162
H	-1	4.5629931639	6.7343869079	2.0465990162
H	-1	3.2301671639	6.7311149385	3.2844460162
H	0	2.9437791518	6.1967245774	1.6621155773
C	0	4.0742572219	4.7641227166	2.8030549382
H	0	5.0329148745	4.7064676409	3.3294661960
H	0	3.2966807469	4.3374033474	3.4479096168
C	0	4.0990662996	3.9130774287	1.5260314286
O	0	3.0153889942	3.8440531836	0.8967208439
O	0	5.1880905875	3.3576196825	1.1559541721
C	-1	12.1429119573	-2.2606622662	-0.6401669838
H	-1	13.1860409636	-1.9855922902	-0.6913149838
H	-1	11.9282219370	-3.1474292613	-1.2180499838
H	0	11.9380903440	-2.5370688054	0.4038100102
C	0	11.2299933210	-1.0801610631	-1.0472072907
H	0	11.6949876710	-0.5210569325	-1.8722260356
H	0	10.2759748441	-1.4652780946	-1.4242655887
C	0	10.9410109084	-0.1326137360	0.1322132040
H	0	10.2098524621	-0.6193865968	0.7921873232
H	0	11.8564687654	-0.0020449208	0.7265658408
C	0	10.4516917166	1.2734322267	-0.2554223105
H	0	10.3355637500	1.8849547376	0.6501206503
H	0	11.2271826816	1.7632355375	-0.8598791301
C	0	9.1565055837	1.3613185851	-1.0642537712
H	0	8.9918357138	2.3929818612	-1.3879828986
H	0	9.1908617454	0.7304032268	-1.9561237549
N	0	7.9388958991	0.9573859360	-0.2929060642
H	0	7.0881160777	1.3274404085	-0.7742862613
H	0	7.8606510170	-0.0854709093	-0.2134558817
H	0	7.8966621613	1.3822676058	0.6638257907
O	0	1.9378597433	1.4743342046	-3.4479250289
H	0	2.6908324180	2.0471577774	-3.7162027942
O	0	0.2901459342	2.4118050619	-0.1190955227
O	0	0.7558003306	3.7051310032	2.5718031464
H	0	0.3655705265	2.8436898185	2.3410611000
H	0	1.4729434966	3.8028532495	1.9027870682
O	0	-3.4086128854	-0.8119558926	-4.1784309387
H	0	-4.1352566476	-1.1384114854	-3.6154764744
H	0	-2.8551004916	-1.6097436784	-4.3268924757
O	0	-4.6502807157	-2.6096334556	-2.1997413866
H	0	-3.8231067237	-2.2472706773	-1.7957725366
H	0	-5.0662072035	-3.1144028860	-1.4750498236
O	0	2.1905773466	3.7242163000	-1.7311688153
H	0	2.5742066414	3.7105542091	-0.8226933480
O	0	5.8396499819	2.5064151987	-1.3064668544
H	0	5.3734484361	2.7410364805	-0.4507549365
H	0	6.2999774905	3.3310984575	-1.5347686586
O	0	4.1206026242	3.2580093277	-3.4976305927
H	0	4.6840393948	2.7365822911	-2.8908172082

O	0	7.3995831003	2.2363911230	2.1513738695
H	0	6.5836916009	2.7450876281	1.8843824449
H	0	7.0808135495	1.5935943582	2.8034327609
O	0	2.2328512636	-1.0947988674	-2.6483403430
H	0	1.5158796498	-0.8399537072	-2.0248584529
H	0	-1.0406579898	-4.8595359583	4.9748248618
H	0	3.4282397417	3.5918853757	-2.8553118597
Cl	0	7.6834296308	-2.1577238079	-0.2027872863
H	0	2.3959135044	-0.1842064504	-3.0179274299
O	0	-0.3030326198	0.4583526831	-4.5576988233
H	0	0.1498247287	-2.3652216837	-4.6206640752
O	0	0.9808006659	-1.9431299108	-4.9082740922
H	0	0.1009151576	-0.4118879573	-4.8043477563
H	0	1.4590306159	-1.7367542164	-4.0590272640
H	0	0.4992451999	0.9769385576	-4.2696495923

1L_S3d-fixed

E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.941046 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.376143 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.614967 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.773856 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.699544 au

Mn	0	1.1270824768	2.2230150056	-1.8815928160
Mn	0	-0.8824039592	-2.5915479364	-0.6018961272
Mn	0	-0.1640216834	0.8495516501	0.1029341447
Mn	0	-2.8327972882	-0.4455786527	0.2559328530
O	0	0.2222511409	0.6087519410	-1.6244690282
O	0	-1.9484751624	1.0228638957	-0.3798627677
O	0	-2.3021482416	-1.5157488343	-1.2629398701
O	0	-0.7126231118	-1.1681924462	0.6451952403
Ca	0	-1.9940683961	0.4437077191	-2.7339452659
C	-1	0.5540942621	4.7210336739	-5.5423230988
H	-1	0.6213303678	5.6465126827	-4.9893612651
H	-1	0.7426559722	4.8138346249	-6.6015284918
H	0	1.3499280521	4.0779319836	-5.1455600084
C	0	-0.7964092430	4.0108813206	-5.3191162253
H	0	-0.9398650352	3.2246433447	-6.0704125669
H	0	-1.6389005927	4.7035091010	-5.4550862512
C	0	-0.9728502310	3.3251797758	-3.9549144556
O	0	-1.9234550384	2.4915213198	-3.8455504596
O	0	-0.1657595665	3.6164502953	-3.0248019613
C	-1	-2.9321440410	-6.5324787420	-5.4563122277
H	-1	-1.9728197551	-6.9950377561	-5.6352904070
H	-1	-3.6652048579	-6.6606419669	-6.2390283336
H	0	-3.3529897750	-7.1061442395	-4.6141140981
C	0	-2.6767944432	-5.1091115104	-4.9574234626
H	0	-3.6043979729	-4.6244473162	-4.6292840348
H	0	-2.2358863310	-4.4763365381	-5.7355880320
C	0	-1.7091629059	-5.2232550980	-3.7710863371
H	0	-0.7618368745	-5.6655962828	-4.1148156031
H	0	-2.1138393963	-5.8982261427	-3.0108429634
C	0	-1.3488854730	-3.9165700221	-3.1084999826
O	0	-1.1415317902	-2.8922988220	-3.7915791230
O	0	-1.2473852599	-4.0049993045	-1.8180141304
C	-1	5.0696362561	-4.5968280312	0.8942272731
H	0	5.8906935637	-5.3058410279	1.0558550808
H	0	5.3237603090	-4.0059782564	0.0105524126
C	0	4.9595544373	-3.6935056176	2.1211417909
O	0	4.4209664014	-4.0993898591	3.1736499114
C	0	3.7730202932	-5.4286157098	0.6417643968

H	0	3.6776514307	-6.1649107295	1.4492800107
H	0	3.8938017349	-5.9853044628	-0.2914700163
C	0	2.5071330740	-4.6183026608	0.5816657436
N	0	2.1931861963	-3.8076779626	1.6599934561
H	0	2.7525019861	-3.7660159331	2.5141804388
C	0	1.4876487126	-4.4095867561	-0.3194352676
H	0	1.3299084490	-4.8208341196	-1.3033283761
C	0	1.0896229837	-3.1167387456	1.3911830170
H	0	0.7029386979	-2.3704271541	2.0498004946
N	0	0.5921226135	-3.4737820642	0.2089288425
N	0	5.3762628676	-2.4279354866	1.9573264149
H	0	5.9008592260	-2.0036560885	1.1064182704
C	-1	5.0494660131	-1.3522951942	2.8910646361
H	0	5.9178774642	-0.6848490638	2.9557431786
H	0	4.8885136479	-1.7970422397	3.8752085819
C	0	3.8031013836	-0.5708679256	2.4359985020
H	0	3.5416779257	0.1677044740	3.2043061250
H	0	2.9582221283	-1.2610669405	2.3653343194
C	0	4.0101134954	0.1216154778	1.0881939281
H	0	4.4946579292	-0.5602100114	0.3767711267
H	0	4.6810652216	0.9837950649	1.1821243684
C	0	2.7619149563	0.6158279063	0.3644053965
O	0	2.9484805647	1.1935928154	-0.7342235222
O	0	1.6206935876	0.3623272498	0.8896246959
C	-1	-5.4324452764	-3.9568930889	2.1536988387
H	0	-5.3010147510	-3.2347087580	2.9655194318
H	0	-5.9222420086	-4.8432331728	2.5751144708
C	0	-4.0734339344	-4.3684849062	1.5666093934
H	0	-4.2149862813	-5.0758960655	0.7428776051
H	0	-3.4796258925	-4.8877040552	2.3250241836
C	0	-3.2325528108	-3.2203916877	1.0172885494
O	0	-3.7025200806	-2.0553831741	1.0869031072
O	0	-2.0953218102	-3.5288403690	0.5207404941
C	0	-6.3522197772	-3.3846253134	1.0774700697
O	0	-6.2264226441	-3.6717941931	-0.1241686103
N	0	-7.3623406970	-2.6044203267	1.5193545305
H	0	-7.3686118421	-2.3088846157	2.4859034090
C	-1	-8.4061106381	-2.0927339261	0.6376555737
H	0	-9.2877302735	-1.8699081991	1.2392455141
H	0	-8.6503277002	-2.8738621939	-0.0883263205
C	0	-8.0043948765	-0.7922478439	-0.0927067327
O	0	-8.4564114615	0.2990021007	0.2552784385
N	0	-7.1639766579	-0.9740503393	-1.1420303179
H	0	-6.7273056971	-1.8851688215	-1.2355057939
C	0	-6.5569167351	0.1279015038	-1.8619610387
H	0	-6.5753207525	-0.0700863692	-2.9368405338
H	0	-7.1557050739	1.0225306592	-1.6668417248
C	0	-5.1017608813	0.4071034623	-1.4461669704
O	0	-4.3312246372	0.8870268100	-2.3140407903
O	0	-4.7957210266	0.1346711328	-0.2411302679
C	-1	-3.3942448079	3.6176785418	5.0436258728
H	-1	-3.4224203617	3.3052490526	6.0770395659
H	-1	-4.2102934237	4.2683908517	4.7664179049
H	0	-2.4849101153	4.2283142455	4.9403986103
C	0	-3.3629897460	2.5067707045	3.9889396081
H	0	-3.4935387111	2.9840957718	3.0087437653
H	0	-4.2108536665	1.8223497377	4.1036854093
C	0	-2.0500485667	1.7136257903	3.9686922553
H	0	-2.0630637343	0.9537761188	4.7585431787
H	0	-1.1951454779	2.3700336583	4.1550214604

C	0	-1.8338454000	1.0354740731	2.6266771696
O	0	-0.6963656115	1.1970906820	2.0825714724
O	0	-2.8002449742	0.3703648352	2.1419736377
C	-1	-5.4718387162	9.0821426142	2.1557412540
H	-1	-5.3332304131	8.6558395651	3.1382647203
H	-1	-6.5071815046	9.3245485270	1.9671233307
H	0	-4.9082068314	10.0217294029	2.1140714264
C	0	-4.9269674214	8.0772803257	1.1287776569
H	0	-3.8334314840	8.0410801031	1.2352647316
H	0	-5.1185004988	8.4186834181	0.1031762686
C	0	-5.5272646719	6.6753739325	1.3243030354
H	0	-6.5981749587	6.7014350913	1.0889735266
H	0	-5.4439277454	6.3794273931	2.3792902428
C	0	-4.8818684019	5.5831527147	0.4672795945
H	0	-4.9268907903	5.8598421015	-0.5964109472
H	0	-5.4310331752	4.6440137764	0.5964267027
N	0	-3.4946236086	5.3621532694	0.8820601823
H	0	-3.0002877203	6.1583231622	1.2614006310
C	0	-2.7111016897	4.3609023581	0.4226705239
N	0	-3.1782947769	3.4493816367	-0.4318911968
H	0	-2.7063518733	2.5249178147	-0.4885819855
H	0	-4.0916927603	3.5337063073	-0.8503575004
N	0	-1.4434986531	4.2753030486	0.8271773828
H	0	-1.1025220744	4.7108659767	1.6740541155
H	0	-0.7997282338	3.5825649897	0.3943305685
C	-1	-0.9474509170	-1.3911812730	7.4933783879
H	-1	0.0412522662	-0.9927108140	7.3195314249
H	-1	-1.1231717846	-1.6151346586	8.5353269171
H	0	-1.7014294901	-0.6816637266	7.1386174239
C	0	-1.1187388022	-2.7810315701	6.8597018659
H	0	-2.0678722496	-3.2134498293	7.2089098590
H	0	-0.3312583564	-3.4451652274	7.2441804944
C	0	-1.1039840500	-2.7904611738	5.3778813905
N	0	-1.2180995690	-3.9542159012	4.6425589719
C	0	-1.0301921168	-1.7884002863	4.4437351904
H	0	-0.8995884541	-0.7323444370	4.6104347539
C	0	-1.2121065980	-3.6254625639	3.3274034774
H	0	-1.2386804733	-4.3521463358	2.5320303248
N	0	-1.1095606039	-2.3149838527	3.1730478576
H	0	-0.8251312429	-1.4402493424	1.5982679242
C	-1	3.7928751552	6.2251865229	2.4327305146
H	-1	4.6607326777	6.7249612659	2.0278820845
H	-1	3.3294011907	6.7300632977	3.2672691160
H	0	3.0325415808	6.2337198906	1.6425474179
C	0	4.1236514130	4.7455696406	2.7411633956
H	0	5.0755821935	4.6421635930	3.2718921584
H	0	3.3270912470	4.3167782574	3.3602545270
C	0	4.1438146768	3.9497824998	1.4328428254
O	0	3.0584687190	3.9313766361	0.7927357722
O	0	5.2208414730	3.3941279958	1.0414984865
C	-1	12.1239371504	-2.3459777817	-0.7292194008
H	-1	13.1704230734	-2.0837102289	-0.7796468054
H	-1	11.8975516017	-3.2259902172	-1.3129087696
H	0	11.9214853983	-2.6309062040	0.3132150311
C	0	11.2135459243	-1.1575611877	-1.1189814728
H	0	11.6681873419	-0.5998968601	-1.9506010542
H	0	10.2507496766	-1.5363305727	-1.4813301997
C	0	10.9477539690	-0.2090506301	0.0657903701
H	0	10.2250851543	-0.6894690300	0.7398826066
H	0	11.8723626448	-0.0860071887	0.6472769114

```
C   0    10.4667062688    1.2029820778   -0.3125058751
H   0    10.3529073037    1.8086065717    0.5972127009
H   0    11.2489466598    1.6907634668   -0.9097685461
C   0     9.1776252873    1.3135256862   -1.1292414461
H   0     9.0355769285    2.3487063956   -1.4523149295
H   0     9.2069049498    0.6832404452   -2.0217481744
N   0     7.9444801162    0.9311066542   -0.3701331103
H   0     7.1059210232    1.3212149669   -0.8536098225
H   0     7.8336094233   -0.1117151803   -0.3152173818
H   0     7.9033775412    1.3425919893    0.5919720140
O   0     1.8407502857    1.5458409896   -3.5375400102
H   0     3.3438564375    2.4128736871   -3.7103658766
O   0     0.3440456705    2.5197959847   -0.1553198758
O   0     0.8490639042    3.6447406223    2.5797356602
H   0     0.4429046878    2.7876296479    2.3533447032
H   0     1.5056920520    3.7729546693    1.8602386809
O   0    -3.2178262495   -1.1219585315   -4.2018096766
H   0    -3.9235112590   -1.5167758258   -3.6490293486
H   0    -2.5589572409   -1.8452653432   -4.2757842921
O   0    -4.4327860901   -2.7636759148   -2.2380616311
H   0    -3.6268049902   -2.3701132563   -1.7989061721
H   0    -4.9532734461   -3.1506169438   -1.5100068686
O   0     2.3595619862    3.8618303342   -1.7261165869
H   0     2.7468047652    3.8068306411   -0.7995198476
O   0     5.8471508700    2.5140386532   -1.4033104576
H   0     5.3977483064    2.7633664009   -0.5418971948
H   0     6.3374215992    3.3202191206   -1.6369621435
O   0     4.1100293819    3.0292734810   -3.5497838473
H   0     4.6583029048    2.5847781321   -2.8659186051
O   0     7.3974139843    2.2070807022    2.0737804557
H   0     6.5993760706    2.7354334879    1.7996794156
H   0     7.0620207850    1.5873274579    2.7396705943
O   0     2.7849690647   -0.9304270439   -2.5361281313
H   0     2.2034975058    0.6573553590   -3.3024719701
H   0    -1.2891540268   -4.8892772101    5.0206412985
H   0     3.1021970077    3.7234553356   -2.3841048085
Cl  0     7.5066361475   -2.1452345511   -0.4825762958
H   0     3.0930406096   -0.2738223552   -1.8812575599
O   0    -0.2899585156    0.0388895923   -4.4632253374
H   0     0.0776883962   -0.8568554607   -4.5250260203
O   0     0.3652713035   -1.9882031241   -1.7634237333
H   0     1.9168612376   -1.2131886373   -2.1613085789
H   0    -0.1155118123   -1.9438062313   -2.6163981677
H   0     0.4739638521    0.6313014960   -4.2085759583
```

1L_S3d
E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.954378 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.389763 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.629414 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.787283 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.712395 au
```
Mn  0     1.0981075799    2.2218793886   -1.8641281990
Mn  0    -0.8862829993   -2.5503208518   -0.7395906282
Mn  0    -0.1904829165    0.8386694329    0.1217013982
Mn  0    -2.8329753048   -0.4888078609    0.2912680160
O   0     0.1787228071    0.6134410363   -1.6137083415
O   0    -1.9945505151    0.9838929406   -0.3500187853
O   0    -2.2497953394   -1.5559918941   -1.3375835001
O   0    -0.7420117852   -1.1609071513    0.6162533895
Ca  0    -2.0237413944    0.4842313759   -2.7345245506
```

```
C   -1    0.5257029805    4.6763420117   -5.5666300035
H   -1    0.5889839720    5.6061810123   -5.0205590035
H   -1    0.7135699797    4.7621270134   -6.6265490035
H    0    1.3218094403    4.0382099856   -5.1629098772
C    0   -0.8221084638    3.9686647450   -5.3327074908
H    0   -0.9493950423    3.1464749601   -6.0481944145
H    0   -1.6689419526    4.6458570184   -5.5106647372
C    0   -1.0049432860    3.3433197987   -3.9421307247
O    0   -1.9925987678    2.5603464895   -3.7822633993
O    0   -0.1619677556    3.6246188599   -3.0424163421
C   -1   -2.9106329168   -6.5915480196   -5.3962210035
H   -1   -1.9493159126   -7.0511690108   -5.5720520035
H   -1   -3.6433259156   -6.7287520263   -6.1777470035
H    0   -3.3218097596   -7.1308388370   -4.5287682005
C    0   -2.6406649253   -5.1468507085   -4.9682653221
H    0   -3.5292331781   -4.6886082653   -4.5164813217
H    0   -2.3457929592   -4.5174807365   -5.8153603615
C    0   -1.4975989489   -5.1975781974   -3.9409141575
H    0   -0.5661887830   -5.4836336375   -4.4493689967
H    0   -1.7043604538   -5.9598144129   -3.1837120195
C    0   -1.2398181506   -3.8849031834   -3.2466894654
O    0   -1.0786745879   -2.8372209017   -3.9063776856
O    0   -1.1976882995   -3.9870128609   -1.9544767508
C   -1    5.0841760648   -4.5734929467    0.9374239965
H    0    5.9750428008   -5.2052206666    1.0485552089
H    0    5.2339670405   -3.9730241267    0.0363551149
C    0    4.9860700572   -3.6658379706    2.1646787781
O    0    4.4871704796   -4.0750004509    3.2339864969
C    0    3.8512228836   -5.5015964722    0.7711026667
H    0    3.8124330284   -6.1889303229    1.6246815682
H    0    3.9829758099   -6.1048568511   -0.1313049447
C    0    2.5669178642   -4.7349135300    0.6852574473
N    0    2.2245404951   -3.9062723451    1.7392003275
H    0    2.7648555468   -3.8427532104    2.6019310039
C    0    1.5952064924   -4.5154934290   -0.2648069649
H    0    1.4785659376   -4.9417314328   -1.2493099546
C    0    1.1457230102   -3.1950066282    1.4035573220
H    0    0.7359002872   -2.4337648100    2.0317987231
N    0    0.7042927739   -3.5595258743    0.2090891008
N    0    5.3835910187   -2.3948313454    1.9846903025
H    0    5.8843848178   -2.1703863264    1.1203364336
C   -1    5.0501630351   -1.3143759470    2.9101779965
H    0    5.9079488849   -0.6321216174    2.9618521031
H    0    4.9022286630   -1.7512055624    3.8997730676
C    0    3.7869885007   -0.5586309485    2.4531402155
H    0    3.5107497592    0.1784601063    3.2176725094
H    0    2.9570284819   -1.2677216410    2.3846312854
C    0    3.9831003547    0.1321808847    1.1025396265
H    0    4.4705897708   -0.5482450578    0.3916329501
H    0    4.6487328165    0.9990781830    1.1923196730
C    0    2.7334651362    0.6192728497    0.3768504091
O    0    2.9189119724    1.2008594485   -0.7194214906
O    0    1.5907744968    0.3588574811    0.8963359309
C   -1   -5.4203029407   -3.9707460425    2.1952459965
H    0   -5.2701829481   -3.2270980583    2.9844004182
H    0   -5.9239768987   -4.8340018672    2.6476460255
C    0   -4.0807949687   -4.4152372003    1.6075772316
H    0   -4.2360261321   -5.1524490439    0.8138820081
H    0   -3.4781999137   -4.9066736856    2.3778276064
C    0   -3.2395659136   -3.2946143214    1.0071298709
```

O	0	-3.6828468212	-2.1112038460	1.0831483323
O	0	-2.1406233762	-3.6404689100	0.4786912742
C	0	-6.3407455358	-3.4069886430	1.1139724826
O	0	-6.2053140057	-3.6853282407	-0.0886268371
N	0	-7.3622021163	-2.6394117218	1.5533577508
H	0	-7.3806373617	-2.3530868351	2.5225310850
C	-1	-8.4025969575	-2.1310540696	0.6663199965
H	0	-9.2942029985	-1.9279344699	1.2603535504
H	0	-8.6281535855	-2.9060571818	-0.0720027422
C	0	-8.0083219728	-0.8173899496	-0.0398984670
O	0	-8.4569187735	0.2675246569	0.3308286801
N	0	-7.1720529684	-0.9804242687	-1.0960910190
H	0	-6.7354940319	-1.8896336268	-1.2072355649
C	0	-6.5704735336	0.1346870072	-1.7975295446
H	0	-6.6225874515	-0.0237220960	-2.8779403249
H	0	-7.1481664089	1.0313231048	-1.5538006531
C	0	-5.1007167189	0.3774852638	-1.4196068474
O	0	-4.3520809478	0.8821528526	-2.2894979077
O	0	-4.7606642694	0.0514626696	-0.2353725097
C	-1	-3.4149080100	3.6339779758	5.0283769965
H	-1	-3.4414270072	3.3290919756	6.0640849965
H	-1	-4.2339050159	4.2789989684	4.7465989965
H	0	-2.5083552783	4.2481660882	4.9213500293
C	0	-3.3722727484	2.5110833089	3.9863346265
H	0	-3.4880958333	2.9769286523	2.9989912159
H	0	-4.2233705650	1.8301555673	4.0975423225
C	0	-2.0617406183	1.7108927032	3.9918788947
H	0	-2.0877665281	0.9587933970	4.7889419749
H	0	-1.2060886850	2.3661237810	4.1787952719
C	0	-1.8398953024	1.0157582988	2.6591501201
O	0	-0.7111616634	1.1947182109	2.1001602849
O	0	-2.7938750800	0.3226346737	2.1928398506
C	-1	-5.5174500595	9.0676439567	2.1007099965
H	-1	-5.3766960557	8.6492509579	3.0863239965
H	-1	-6.5539060617	9.3040609472	1.9106099965
H	0	-4.9580075171	10.0095302394	2.0527827507
C	0	-4.9761313161	8.0616683074	1.0760783905
H	0	-3.8832824328	8.0188775382	1.1862616118
H	0	-5.1629786250	8.4050469516	0.0502106613
C	0	-5.5889677872	6.6663330933	1.2718996155
H	0	-6.6598380924	6.7022788157	1.0371772861
H	0	-5.5062549268	6.3699145976	2.3266595739
C	0	-4.9516700487	5.5711497650	0.4147913306
H	0	-5.0151049802	5.8367771583	-0.6509242045
H	0	-5.4902153315	4.6288140875	0.5609520467
N	0	-3.5585408437	5.3628907295	0.8110830209
H	0	-3.0451965640	6.1728644478	1.1304081593
C	0	-2.8042579670	4.3114459029	0.4248540725
N	0	-3.3081147693	3.3534628131	-0.3532606729
H	0	-2.8164735132	2.4424320091	-0.4211173241
H	0	-4.1504232422	3.4854736277	-0.8914009870
N	0	-1.5453397919	4.2092372049	0.8512080315
H	0	-1.1910832805	4.7085357679	1.6560167683
H	0	-0.8871357811	3.5303024168	0.4198266928
C	-1	-0.9453039646	-1.3457120017	7.5144379965
H	-1	0.0415790317	-0.9441669927	7.3373499965
H	-1	-1.1197549626	-1.5627160033	8.5580689965
H	0	-1.6977134299	-0.6330906544	7.1612368571
C	0	-1.1216663129	-2.7287768055	6.8689647448
H	0	-2.0777946246	-3.1556923635	7.2053614390

H	0	-0.3436913256	-3.4027305458	7.2560382140
C	0	-1.0915578656	-2.7309520973	5.3853098659
N	0	-1.2523466943	-3.8889853813	4.6483224377
C	0	-0.9507273973	-1.7355285362	4.4507474261
H	0	-0.7688461198	-0.6865708768	4.6174046340
C	0	-1.2061036953	-3.5638325674	3.3329363330
H	0	-1.2526668378	-4.2883339943	2.5364765612
N	0	-1.0342739877	-2.2612821953	3.1789052897
H	0	-0.7771886542	-1.4569267104	1.5696690979
C	-1	3.7598999661	6.2538650412	2.3960989965
H	-1	4.6254269616	6.7544630491	1.9873009965
H	-1	3.2944149615	6.7628530370	3.2270119965
H	0	2.9994726142	6.2479050574	1.6060599873
C	0	4.1003496668	4.7807184959	2.7271232397
H	0	5.0538029771	4.6923628689	3.2578092400
H	0	3.3073459579	4.3580143995	3.3549868032
C	0	4.1214244580	3.9630638511	1.4332447116
O	0	3.0309936484	3.9206149892	0.8027279570
O	0	5.2015825753	3.4141349062	1.0415551849
C	-1	12.1280080441	-2.3035228826	-0.7047500035
H	-1	13.1733080417	-2.0370068730	-0.7574310035
H	-1	11.9053670522	-3.1888298846	-1.2818380035
H	0	11.9267620286	-2.5810979494	0.3399009918
C	0	11.2102288673	-1.1241880634	-1.1050637067
H	0	11.6601510504	-0.5726934460	-1.9433374444
H	0	10.2491033220	-1.5126144072	-1.4619032819
C	0	10.9398934083	-0.1644871348	0.0695348874
H	0	10.2221454898	-0.6421866008	0.7508026962
H	0	11.8646478706	-0.0280517646	0.6477945256
C	0	10.4473687990	1.2395970025	-0.3234129890
H	0	10.3316574324	1.8544355002	0.5798424557
H	0	11.2243783793	1.7263544596	-0.9283037587
C	0	9.1552932813	1.3320763127	-1.1377759980
H	0	9.0049529753	2.3629769325	-1.4707001562
H	0	9.1868759354	0.6932682457	-2.0241306572
N	0	7.9267680601	0.9481173062	-0.3718354830
H	0	7.0848716858	1.3316965708	-0.8540296150
H	0	7.8194993360	-0.0953534209	-0.3127724104
H	0	7.8877431442	1.3644288034	0.5882916082
O	0	1.8192567822	1.5395229696	-3.5174603134
H	0	3.3106306440	2.4283193215	-3.7042785019
O	0	0.3000804726	2.5155395132	-0.1418843799
O	0	0.8107667099	3.6648968806	2.5774443453
H	0	0.4062358346	2.8048129313	2.3600710646
H	0	1.4741671123	3.7816852456	1.8625340808
O	0	-3.2181401480	-1.1054268060	-4.1946784486
H	0	-3.9228251111	-1.5172485610	-3.6542089496
H	0	-2.5424672780	-1.8136942281	-4.2707122153
O	0	-4.4527514087	-2.7852568740	-2.2407550780
H	0	-3.6237466875	-2.4245249744	-1.8288754662
H	0	-4.9565935383	-3.1648568782	-1.4965498377
O	0	2.3267741094	3.8608092502	-1.7073652551
H	0	2.7203438630	3.8033067081	-0.7831351919
O	0	5.8176581882	2.5229905807	-1.4034717814
H	0	5.3719763214	2.7723345123	-0.5403164481
H	0	6.3107570620	3.3278677235	-1.6358363659
O	0	4.0714335129	3.0509538820	-3.5438074158
H	0	4.6274845656	2.6067264838	-2.8659439971
O	0	7.3920499618	2.2415769607	2.0650359679
H	0	6.5891770733	2.7641500356	1.7949385581

H	0	7.0683214881	1.6301654461	2.7442573575
O	0	2.8619522112	-0.9050942370	-2.5307574555
H	0	2.2018635876	0.6601501332	-3.2801004552
H	0	-1.3745807538	-4.8187333418	5.0263802411
H	0	3.0651165452	3.7309287543	-2.3721652631
Cl	0	7.4877269547	-2.1250301101	-0.4878568643
H	0	3.1516394056	-0.2439551272	-1.8717985935
O	0	-0.3366068513	0.1184306198	-4.4697092487
H	0	-0.0187585221	-0.7819706494	-4.6420370388
O	0	0.4150523162	-1.9673694485	-1.8229209684
H	0	2.0058693485	-1.2177256536	-2.1569619388
H	0	-0.0277978337	-1.8260202792	-2.6844961460
H	0	0.4628788836	0.6608782798	-4.2050732765

3L_S3a-fixed

E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.938759 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.374043 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.611543 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.775497 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.701608 au

Mn	0	1.2760892425	2.0528554576	-1.9104263332
Mn	0	-1.0451066720	-2.5279627528	-0.5273265048
Mn	0	-0.1229078197	0.7442513105	0.0974853499
Mn	0	-2.6935716204	-0.4560213464	0.3174472323
O	0	0.2256259952	0.3476042712	-1.5969390456
O	0	-1.9449857282	0.9946990405	-0.3729399071
O	0	-2.4652026171	-1.4507872246	-1.1853683909
O	0	-1.0071259648	-1.1162654827	0.7437628986
Ca	0	-1.9006518698	0.4145326121	-2.8102976091
C	-1	0.5534799135	4.6067477078	-5.5057325502
H	-1	0.6206110655	5.5379777831	-4.9627474014
H	-1	0.7467476250	4.6869541607	-6.5650249435
H	0	1.3343293248	3.9570716562	-5.0931511229
C	0	-0.8122086540	3.9104694802	-5.3100169013
H	0	-0.9294522877	3.1140778585	-6.0556250797
H	0	-1.6439589159	4.6049203053	-5.4931098044
C	0	-1.0626020950	3.2261670914	-3.9537325884
O	0	-2.1080143431	2.5009509368	-3.8616602618
O	0	-0.2317877946	3.3864683453	-3.0207614840
C	-1	-2.9625902702	-6.6362927581	-5.3092037769
H	-1	-2.0036613178	-7.1032927016	-5.4788150120
H	-1	-3.6925092076	-6.7713714825	-6.0936570363
H	0	-3.3886420850	-7.1688520992	-4.4438972464
C	0	-2.7268988888	-5.1771391746	-4.9035130977
H	0	-3.6741987748	-4.6680526322	-4.6870571484
H	0	-2.2406388526	-4.6139801686	-5.7081875168
C	0	-1.8457759675	-5.1593829589	-3.6539213250
H	0	-0.8988324051	-5.6852026963	-3.8503087164
H	0	-2.3238884862	-5.7089034632	-2.8342522756
C	0	-1.4672436090	-3.7931222707	-3.1269258126
O	0	-1.5488079075	-2.7689370913	-3.8278536267
O	0	-0.9979691378	-3.8172184341	-1.9221735239
C	-1	5.0166329032	-4.6502990515	1.0541821670
H	0	5.7249677363	-5.4515335306	1.2933112606
H	0	5.4101056239	-4.1032103440	0.1937638467
C	0	4.8740891539	-3.7267068311	2.2620417460
O	0	4.2315100025	-4.0922927496	3.2715949204
C	0	3.6438346943	-5.3168352265	0.7187176629
H	0	3.4160113928	-6.0289146223	1.5211544851
H	0	3.7456303745	-5.8917694536	-0.2056711446

C	0	2.4760504893	-4.3748793151	0.5782324294
N	0	2.1912506367	-3.4633714367	1.5852814780
H	0	2.7029192399	-3.4300215353	2.4682203626
C	0	1.4980127940	-4.1651780253	-0.3654620332
H	0	1.3239418212	-4.6552585940	-1.3096499463
C	0	1.1424331448	-2.7210196965	1.2359309702
H	0	0.7997938755	-1.8639325794	1.7799118603
N	0	0.6565689925	-3.1326695483	0.0631231203
N	0	5.3326203370	-2.4772055906	2.1079598575
H	0	5.9406391730	-2.2801165829	1.3045514614
C	-1	4.9963070496	-1.3835934828	3.0145904323
H	0	5.8796730653	-0.7379175576	3.0899572288
H	0	4.8034055441	-1.8060963199	4.0034096335
C	0	3.7887297775	-0.5623232487	2.5307169907
H	0	3.6189910840	0.2596076470	3.2378443774
H	0	2.8919949582	-1.1819109260	2.5668392434
C	0	3.9870889580	-0.0142992744	1.1177170843
H	0	4.4505909642	-0.7730219102	0.4757247342
H	0	4.6710603544	0.8423675668	1.1238712398
C	0	2.7474921305	0.4306777019	0.3511650859
O	0	2.9344489506	0.9706033927	-0.7463183246
O	0	1.5883389729	0.1789180598	0.8810910317
C	-1	-5.4889243760	-3.9692639360	2.2605324617
H	0	-5.3622337444	-3.2270939694	3.0555396110
H	0	-5.9791910762	-4.8441734038	2.7049057083
C	0	-4.1301896692	-4.3890488246	1.6903823858
H	0	-4.2605893751	-5.1217394532	0.8882483817
H	0	-3.5365499978	-4.8850969906	2.4682697206
C	0	-3.2749619163	-3.2625609708	1.1235705100
O	0	-3.6520299306	-2.0679538338	1.2717638619
O	0	-2.1826254290	-3.6021510635	0.5507127659
C	0	-6.4077490866	-3.4159575770	1.1747509151
O	0	-6.2378401123	-3.6614886152	-0.0283844384
N	0	-7.4620825450	-2.6920188084	1.6143674690
H	0	-7.5014112393	-2.4271386371	2.5892414660
C	-1	-8.4516629551	-2.1149275579	0.7108921477
H	0	-9.3880880489	-1.9824063554	1.2536484495
H	0	-8.6043979573	-2.8129579862	-0.1164036897
C	0	-8.0132652458	-0.7307508492	0.1892648733
O	0	-8.4884004142	0.3049733698	0.6559526942
N	0	-7.0829881324	-0.7658675737	-0.7972454150
H	0	-6.6769143031	-1.6563105236	-1.0618579111
C	0	-6.4821018669	0.4267478955	-1.3594821064
H	0	-6.6992534286	0.5069344084	-2.4285269683
H	0	-6.9249147446	1.2884542458	-0.8505473047
C	0	-4.9579908924	0.4762086268	-1.1921672800
O	0	-4.2662358829	0.9022642074	-2.1306034200
O	0	-4.5231724428	0.0747202772	-0.0450187338
C	-1	-3.4434681188	3.6319134107	5.0746380335
H	-1	-3.4772896514	3.3308738266	6.1112823944
H	-1	-4.2569069957	4.2813078682	4.7865803024
H	0	-2.5420033124	4.2541182467	4.9745647447
C	0	-3.3802909678	2.4953299862	4.0447829769
H	0	-3.7023057104	2.8923956863	3.0738666485
H	0	-4.0822198810	1.6895288390	4.2869922195
C	0	-1.9646052807	1.9413498067	3.8783360317
H	0	-1.6915404535	1.3154932098	4.7389040315
H	0	-1.2327353592	2.7547990923	3.8582949926
C	0	-1.7652257199	1.1551762431	2.5931642691
O	0	-0.6313809868	1.2694021227	2.0461854291

O	0	-2.7338146323	0.4436771448	2.1619257705
C	-1	-5.4944075919	9.0690433188	2.1168353059
H	-1	-5.3612786278	8.6531833711	3.1046304726
H	-1	-6.5283921949	9.3116918571	1.9210020179
H	0	-4.9441477832	10.0179643658	2.0886594093
C	0	-4.9116698999	8.0923768428	1.0834340164
H	0	-3.8167573462	8.1094915608	1.1801833920
H	0	-5.1333885158	8.4313709795	0.0627502540
C	0	-5.4302345720	6.6600941118	1.2742358846
H	0	-6.5201815920	6.6484265489	1.1458457956
H	0	-5.2288335223	6.3268498798	2.3015952174
C	0	-4.8402177429	5.6332112664	0.3029827855
H	0	-5.0389384818	5.9381458218	-0.7350687075
H	0	-5.3213216770	4.6635061578	0.4648281158
N	0	-3.4025669913	5.4546568635	0.5173005590
H	0	-2.8546471305	6.2778524277	0.7274730131
C	0	-2.7046038785	4.3651003170	0.1279318652
N	0	-3.3151719336	3.3676006334	-0.5218587462
H	0	-2.8326919678	2.4608250532	-0.6009735774
H	0	-4.1257106158	3.5240851908	-1.1012158740
N	0	-1.4108199765	4.2576590189	0.4200049643
H	0	-0.9699444973	4.7325296885	1.2017417104
H	0	-0.8254541760	3.4971102017	0.0201913993
C	-1	-1.0205145659	-1.3557126563	7.5909656068
H	-1	-0.0301668943	-0.9616826242	7.4167098432
H	-1	-1.2015312232	-1.5674935601	8.6343962220
H	0	-1.7628661744	-0.6262954934	7.2498079478
C	0	-1.1991441948	-2.7190071049	6.8936469262
H	0	-2.1618891094	-3.1547383639	7.1946475065
H	0	-0.4284284356	-3.4099270814	7.2586435141
C	0	-1.1485490355	-2.6915855475	5.4019268951
N	0	-0.9832992182	-3.8457473821	4.6452979404
C	0	-1.2941356674	-1.6829330296	4.4895144821
H	0	-1.4465265462	-0.6306042089	4.6370701739
C	0	-1.0258892686	-3.5511786115	3.3394346914
H	0	-0.9277651005	-4.2436532068	2.5195148636
N	0	-1.2211356320	-2.2393331420	3.2289642649
H	0	-1.2371964623	-1.7223651020	2.3118186027
C	-1	3.7616906488	6.1915032604	2.4661295386
H	-1	4.6323457254	6.6845410906	2.0595735721
H	-1	3.2955425899	6.7067812083	3.2929282521
H	0	3.0071792087	6.1794256688	1.6706672110
C	0	4.1124450756	4.7218232875	2.8020286582
H	0	5.0508608368	4.6484993213	3.3618326950
H	0	3.3097116654	4.2878534035	3.4101267434
C	0	4.1846993602	3.8946961260	1.5091596106
O	0	3.1312737650	3.8497283953	0.8279991224
O	0	5.2833961570	3.3327454505	1.1785885238
C	-1	12.0837929376	-2.4357879728	-0.5634652826
H	-1	13.1311375511	-2.1767781190	-0.6122679806
H	-1	11.8575869534	-3.3216720268	-1.1383015774
H	0	11.8669103817	-2.6983140456	0.4815354793
C	0	11.2002487083	-1.2412647083	-0.9871666729
H	0	11.6549958173	-0.7345162255	-1.8509411170
H	0	10.2191775428	-1.6054552639	-1.3122579575
C	0	10.9932492231	-0.2386276051	0.1628094772
H	0	10.2640609314	-0.6673438816	0.8635742027
H	0	11.9321185810	-0.1280934492	0.7238006766
C	0	10.5537458530	1.1721352949	-0.2635204229
H	0	10.4735280463	1.8166115427	0.6228422713

```
H    0    11.3386687656    1.6116303978    -0.8939045033
C    0    9.2527190070    1.2806801466    -1.0591060878
H    0    9.1135815585    2.3090937050    -1.4044420743
H    0    9.2592302823    0.6292359683    -1.9368294500
N    0    8.0324821390    0.9300605816    -0.2671731843
H    0    7.1902200766    1.3211335510    -0.7494853580
H    0    7.9176838474    -0.1064544979    -0.1652552893
H    0    8.0109480060    1.3745983700    0.6810505440
O    0    1.9503280584    1.3444297082    -3.5517476223
H    0    2.7425609528    1.8605410887    -3.8174036933
O    0    0.4124011222    2.3649302095    -0.2156470975
O    0    0.7532601253    3.8956222032    2.3276003588
H    0    0.4102974893    3.0100012901    2.1080179235
H    0    1.5314924472    3.9683439004    1.7248750220
O    0    -3.4482025823    -0.9143053451    -4.2131434413
H    0    -4.1819336064    -1.1992039796    -3.6360361091
H    0    -2.9076708403    -1.7277601381    -4.3147555331
O    0    -4.7056830158    -2.5527579685    -2.1623067616
H    0    -3.8825059476    -2.1941425326    -1.7419926404
H    0    -5.1340204173    -3.0689779133    -1.4536151073
O    0    2.3424145350    3.5892580101    -1.8321097380
H    0    2.7067511240    3.6005161442    -0.9177293220
O    0    5.9635298003    2.4818152881    -1.2876236915
H    0    5.5202963584    2.7467005651    -0.4291215780
H    0    6.3644813701    3.3088629538    -1.6008543502
O    0    4.2511182122    3.0121800913    -3.5782805564
H    0    4.7973521977    2.4942974939    -2.9558017283
O    0    7.5200753203    2.2413972206    2.1688418918
H    0    6.6969940125    2.7391396760    1.9062399233
H    0    7.2064788208    1.5798626722    2.8046800663
O    0    2.1165390539    -1.2453438446    -2.7226698133
H    0    1.4006164303    -0.9528547177    -2.1120618713
H    0    -0.8465816180    -4.7777109953    5.0180387931
H    0    3.5665598689    3.3783058500    -2.9431419624
Cl   0    7.6366735731    -2.1801241118    -0.1053902785
H    0    2.3284006245    -0.3458541500    -3.0932433878
O    0    -0.2920958805    0.2853057844    -4.6295507643
H    0    0.0783972928    -2.5518707509    -4.6832758777
O    0    0.9200093440    -2.1624029802    -4.9853981495
H    0    0.0962265366    -0.5904622991    -4.8778423945
H    0    1.3875585487    -1.9286499627    -4.1366734399
H    0    0.5145733298    0.8036678805    -4.3549900212
```

3L_S3a
E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.96209 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.396107 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.637621 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.798428 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.724112 au

```
Mn   0    1.2052853219    2.1409399227    -1.8211912895
Mn   0    -0.9013419347    -2.3777587637    -0.7388959338
Mn   0    -0.1722853204    0.7606452070    0.1681047736
Mn   0    -2.6962581294    -0.5572000365    0.3194884914
O    0    0.1983039087    0.3821963859    -1.5270975304
O    0    -1.9990714754    0.9578830750    -0.2981665482
O    0    -2.4187693671    -1.4355630625    -1.2660290787
O    0    -0.9654064349    -1.1495522248    0.6961832234
Ca   0    -1.9452119399    0.5658380932    -2.7719574293
C    -1    0.4906301155    4.6270840014    -5.5140459838
H    -1    0.5454701369    5.5569130002    -4.9672939838
```

H	-1	0.6790911175	4.7147059971	-6.5736169838
H	0	1.2698688175	3.9780865890	-5.0968145119
C	0	-0.8785464159	3.9348690799	-5.3299024222
H	0	-0.9762705565	3.1150079640	-6.0534119122
H	0	-1.7063570926	4.6213250371	-5.5538739256
C	0	-1.1610930690	3.2830232693	-3.9669697413
O	0	-2.2540691583	2.6342724809	-3.8510745545
O	0	-0.3019375999	3.3739135022	-3.0509952450
C	-1	-2.8539871439	-6.6687249217	-5.3541809838
H	-1	-1.8886671543	-7.1204039439	-5.5289609838
H	-1	-3.5844121472	-6.8115309049	-6.1367919838
H	0	-3.2694780704	-7.2013708064	-4.4840352443
C	0	-2.6509865037	-5.1998466072	-4.9739161815
H	0	-3.6113092929	-4.6967401230	-4.8069928585
H	0	-2.1453895793	-4.6526652577	-5.7774929872
C	0	-1.8161884465	-5.1237436811	-3.6972553955
H	0	-0.8877881151	-5.7041400522	-3.8065420975
H	0	-2.3473462046	-5.5769358074	-2.8508549377
C	0	-1.3993486861	-3.7332252603	-3.2819386132
O	0	-1.5488038788	-2.7519492239	-4.0287936277
O	0	-0.8190214555	-3.6832091142	-2.1241107074
C	-1	5.1156069038	-4.5889531048	0.9912890162
H	0	5.8809246867	-5.3431769120	1.2102146533
H	0	5.4520576432	-4.0237646131	0.1187114620
C	0	4.9653105543	-3.6714275904	2.2025119275
O	0	4.3649298253	-4.0591568676	3.2287587690
C	0	3.7802515489	-5.3299386858	0.6949560105
H	0	3.5823298225	-6.0217746382	1.5222284767
H	0	3.8959168408	-5.9273951179	-0.2132778407
C	0	2.6079152245	-4.4073806096	0.5334276320
N	0	2.2786448351	-3.5294430917	1.5570512914
H	0	2.7589562979	-3.5173821525	2.4573599404
C	0	1.7165100828	-4.1241309249	-0.4732721440
H	0	1.5998418427	-4.5693392500	-1.4484597973
C	0	1.2881850995	-2.7321014541	1.1542343374
H	0	0.9292325191	-1.8827740137	1.6990664014
N	0	0.8947966492	-3.0776746365	-0.0670390775
N	0	5.3817410805	-2.4077507645	2.0379005569
H	0	5.9703884709	-2.1983932181	1.2243403013
C	-1	5.0523839787	-1.3312791033	2.9657600162
H	0	5.9202160874	-0.6614739263	3.0118730933
H	0	4.9112869526	-1.7671794414	3.9576007063
C	0	3.8052985710	-0.5393228018	2.5397751155
H	0	3.6254325208	0.2549645267	3.2755234401
H	0	2.9326300623	-1.1930511559	2.5764255259
C	0	3.9611251116	0.0566091542	1.1425700096
H	0	4.4024324839	-0.6823798030	0.4621410817
H	0	4.6488727654	0.9098219104	1.1580473025
C	0	2.7076157561	0.5325176343	0.4225408690
O	0	2.8791493196	1.1250513078	-0.6498843695
O	0	1.5559163600	0.2446370586	0.9519760028
C	-1	-5.3949420843	-4.0724638634	2.2352380162
H	0	-5.2427367799	-3.3161046455	3.0124766793
H	0	-5.8992380466	-4.9263508093	2.7046693012
C	0	-4.0575448410	-4.5261733976	1.6526869579
H	0	-4.2147212663	-5.2706066481	0.8666458302
H	0	-3.4633119621	-5.0200715970	2.4310391477
C	0	-3.1881437695	-3.4248036452	1.0474147374
O	0	-3.5674748302	-2.2190049900	1.1864814954
O	0	-2.1203108352	-3.7957937112	0.4803629000

C	0	-6.3186538025	-3.5177693984	1.1534713204
O	0	-6.1469732467	-3.7453444265	-0.0528530459
N	0	-7.3865622887	-2.8175142930	1.6009176317
H	0	-7.4328921123	-2.5659799692	2.5789630082
C	-1	-8.3906410426	-2.2567197945	0.7033660162
H	0	-9.3308436054	-2.1567242646	1.2469273305
H	0	-8.5240193680	-2.9490692303	-0.1318675049
C	0	-7.9868513980	-0.8574789538	0.2023068772
O	0	-8.4573246929	0.1625060386	0.7065214098
N	0	-7.0870325691	-0.8617275375	-0.8129189528
H	0	-6.6652917290	-1.7411846772	-1.0901773137
C	0	-6.4941051076	0.3484062277	-1.3409189974
H	0	-6.7021471557	0.4532658802	-2.4095792718
H	0	-6.9484975621	1.1945772855	-0.8162415715
C	0	-4.9734901363	0.4089318976	-1.1592806375
O	0	-4.2880572567	0.9163859225	-2.0613995779
O	0	-4.5371189857	-0.0742348408	-0.0451200666
C	-1	-3.4554389093	3.5468550921	5.0751830162
H	-1	-3.4812039163	3.2409420927	6.1106320162
H	-1	-4.2795898946	4.1850541110	4.7926040162
H	0	-2.5521994256	4.1648787679	4.9671022532
C	0	-3.4220557081	2.4396567765	4.0152150578
H	0	-3.5222641253	2.9246911003	3.0353351156
H	0	-4.2832224559	1.7685749639	4.1089062774
C	0	-2.1230707147	1.6249288634	4.0215220505
H	0	-2.1828901471	0.8602052303	4.8044180627
H	0	-1.2635585651	2.2640371375	4.2427923451
C	0	-1.8634566232	0.9660000588	2.6767260010
O	0	-0.7368963950	1.1791272300	2.1440604228
O	0	-2.7971901832	0.2467480572	2.1830038536
C	-1	-5.5984797848	8.9647531413	2.1475400162
H	-1	-5.4557407944	8.5467731380	3.1330970162
H	-1	-6.6366767796	9.1925201652	1.9561660162
H	0	-5.0614694326	9.9215115938	2.1227315306
C	0	-5.0183818439	8.0071530167	1.1024980188
H	0	-3.9268721190	7.9883640297	1.2310408264
H	0	-5.1986502444	8.3846745211	0.0872704618
C	0	-5.5930866067	6.5912610347	1.2334591742
H	0	-6.6701304951	6.6138576130	1.0248288415
H	0	-5.4765608311	6.2369776247	2.2668598376
C	0	-4.9513619187	5.5692712583	0.2942245163
H	0	-5.0672334089	5.8871609201	-0.7521415107
H	0	-5.4483600616	4.6010388217	0.4078219815
N	0	-3.5369535580	5.3830118484	0.6189660937
H	0	-3.0041118669	6.1988172763	0.8864495371
C	0	-2.8257320839	4.2786985000	0.3175059928
N	0	-3.3924758568	3.2844094296	-0.3766391065
H	0	-2.8975215695	2.3809112617	-0.4271014336
H	0	-4.1127236175	3.4629120577	-1.0605148730
N	0	-1.5781293159	4.1382451806	0.7576771707
H	0	-1.1831543043	4.6965688404	1.5037672711
H	0	-0.9292738699	3.4393097165	0.3406913224
C	-1	-0.9487270232	-1.4140789655	7.5620570162
H	-1	0.0349459862	-1.0043369881	7.3862260162
H	-1	-1.1229980283	-1.6330049615	8.6051620162
H	0	-1.7058514249	-0.7016300514	7.2182196497
C	0	-1.0865869880	-2.7791031763	6.8551505126
H	0	-2.0470009904	-3.2343904886	7.1334187811
H	0	-0.3111102448	-3.4569841640	7.2356001814
C	0	-1.0111806338	-2.7548801468	5.3622342420

N	0	-1.0247417655	-3.9226137744	4.6060941553
C	0	-0.9895806500	-1.7386377393	4.4470745059
H	0	-0.9339606377	-0.6768561478	4.5949440358
C	0	-1.0232212975	-3.6277229511	3.2992773729
H	0	-1.0340001082	-4.3241041632	2.4761037232
N	0	-1.0165885524	-2.3025598897	3.1860122834
H	0	-1.0454612705	-1.7953789319	2.2648203066
C	-1	3.7012831523	6.2264789277	2.4539080162
H	-1	4.5629931639	6.7343869079	2.0465990162
H	-1	3.2301671639	6.7311149385	3.2844460162
H	0	2.9436728824	6.1951311017	1.6622195599
C	0	4.0758514927	4.7649011302	2.8059039461
H	0	5.0355359612	4.7098554240	3.3307015590
H	0	3.3001374085	4.3395558717	3.4538634247
C	0	4.0996692888	3.9100990772	1.5313420954
O	0	3.0131682806	3.8302610181	0.9080388038
O	0	5.1911343670	3.3626247602	1.1565923491
C	-1	12.1429119573	-2.2606622662	-0.6401669838
H	-1	13.1860409636	-1.9855922902	-0.6913149838
H	-1	11.9282219370	-3.1474292613	-1.2180499838
H	0	11.9379579114	-2.5368967436	0.4038256869
C	0	11.2300739754	-1.0802267196	-1.0475102890
H	0	11.6947233580	-0.5219336566	-1.8732749067
H	0	10.2757113433	-1.4654253725	-1.4236201937
C	0	10.9420862144	-0.1317096064	0.1313632265
H	0	10.2108450209	-0.6175948350	0.7918986280
H	0	11.8578156698	-0.0012259115	0.7253265703
C	0	10.4534740614	1.2743344428	-0.2571323171
H	0	10.3379181277	1.8865725141	0.6480012931
H	0	11.2291273883	1.7632432504	-0.8621125383
C	0	9.1581769998	1.3624151138	-1.0657636513
H	0	8.9941079378	2.3939404109	-1.3902319839
H	0	9.1919860790	0.7308038181	-1.9571645882
N	0	7.9404865979	0.9598331771	-0.2939011398
H	0	7.0898116095	1.3301775041	-0.7753168923
H	0	7.8615460240	-0.0829205588	-0.2137267241
H	0	7.8987638650	1.3854741572	0.6625088404
O	0	1.9354472687	1.4688770152	-3.4541038805
H	0	2.6864624168	2.0429196459	-3.7238806265
O	0	0.2976624840	2.4047147233	-0.1278623795
O	0	0.7405331002	3.7268323517	2.5610764057
H	0	0.3550844390	2.8625247596	2.3330098691
H	0	1.4687771512	3.8180644784	1.9026156990
O	0	-3.4152718294	-0.8183926837	-4.1796093009
H	0	-4.1404924502	-1.1473836301	-3.6161079909
H	0	-2.8595022757	-1.6145417146	-4.3289307803
O	0	-4.6488513845	-2.6129818210	-2.2000048033
H	0	-3.8228849374	-2.2497353937	-1.7955078831
H	0	-5.0674136535	-3.1138153692	-1.4739969656
O	0	2.1909202773	3.7255959064	-1.7262527109
H	0	2.5742649031	3.7097673719	-0.8180155336
O	0	5.8405347355	2.5078935859	-1.3066023406
H	0	5.3757228764	2.7431579398	-0.4504893897
H	0	6.2981941245	3.3332014073	-1.5379282065
O	0	4.1186200002	3.2597285040	-3.4970871338
H	0	4.6815986800	2.7356892129	-2.8922778501
O	0	7.4032829642	2.2403659071	2.1504032949
H	0	6.5879121163	2.7497881512	1.8833243575
H	0	7.0829812589	1.5961018720	2.8002922382
O	0	2.2277828621	-1.0955065642	-2.6559095658

```
H    0     1.5152294450   -0.8438744651   -2.0274024114
H    0    -1.0309950605   -4.8638835150    4.9801043110
H    0     3.4262302165    3.5912669650   -2.8535561596
Cl   0     7.6838933125   -2.1553562632   -0.2016622536
H    0     2.3873948178   -0.1829850843   -3.0244832438
O    0    -0.3073769460    0.4603306337   -4.5607578568
H    0     0.1451923759   -2.3647442126   -4.6301949546
O    0     0.9755649444   -1.9411331492   -4.9173560279
H    0     0.0950681376   -0.4097068202   -4.8103853882
H    0     1.4530959736   -1.7352586569   -4.0676010553
H    0     0.4966106133    0.9766740867   -4.2713848163
```

3L_S3d-fixed

E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.943285 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.378026 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.618133 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.776159 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.702338 au

```
Mn   0     1.1424065887    2.2075258425   -1.8875764000
Mn   0    -0.8810942767   -2.5935629103   -0.6022212068
Mn   0    -0.1648644301    0.8524673388    0.1011646912
Mn   0    -2.8348345443   -0.4432889334    0.2604846742
O    0     0.2236825264    0.6080439476   -1.6147506970
O    0    -1.9543146117    1.0265882256   -0.3763702614
O    0    -2.2962885820   -1.5077481020   -1.2566122410
O    0    -0.7057478155   -1.1644103801    0.6374480756
Ca   0    -2.0026746749    0.4462948508   -2.7278709934
C   -1     0.5540942621    4.7210336739   -5.5423230988
H   -1     0.6213303678    5.6465126827   -4.9893612651
H   -1     0.7426559722    4.8138346249   -6.6015284918
H    0     1.3503197172    4.0795012049   -5.1455297807
C    0    -0.7948832251    4.0099450220   -5.3161048284
H    0    -0.9414485641    3.2240786710   -6.0674995423
H    0    -1.6398638868    4.7005442281   -5.4453297331
C    0    -0.9553544670    3.3221020344   -3.9519957464
O    0    -1.9192914418    2.5082976658   -3.8183002234
O    0    -0.1147592719    3.5950130167   -3.0459561381
C   -1    -2.9321440410   -6.5324787420   -5.4563122277
H   -1    -1.9728197551   -6.9950377561   -5.6352904070
H   -1    -3.6652048579   -6.6606419669   -6.2390283336
H    0    -3.3527569150   -7.1053831314   -4.6135269657
C    0    -2.6766964169   -5.1085508610   -4.9590235935
H    0    -3.6036552167   -4.6256667458   -4.6263973304
H    0    -2.2409742149   -4.4750507410   -5.7395299979
C    0    -1.7026752538   -5.2204171942   -3.7776192353
H    0    -0.7540247666   -5.6549041667   -4.1275703876
H    0    -2.0993553343   -5.9007581227   -3.0179926591
C    0    -1.3489921674   -3.9132580566   -3.1123521877
O    0    -1.1437404693   -2.8876171280   -3.7936237863
O    0    -1.2517780500   -4.0028588243   -1.8214331143
C   -1     5.0696362561   -4.5968280312    0.8942272731
H    0     5.8911156198   -5.3055383412    1.0548060566
H    0     5.3216429416   -4.0065766057    0.0095847088
C    0     4.9608128718   -3.6931037354    2.1207850410
O    0     4.4246831867   -4.0994222538    3.1743816670
C    0     3.7723347900   -5.4291894615    0.6457459947
H    0     3.6786823417   -6.1637552459    1.4550095923
H    0     3.8910594982   -5.9877086291   -0.2866450157
C    0     2.5064431461   -4.6186546446    0.5864098264
N    0     2.1961086760   -3.8029106951    1.6620084830
```

H	0	2.7561447645	-3.7599253107	2.5156022382
C	0	1.4854341550	-4.4119322891	-0.3133802859
H	0	1.3250232092	-4.8263303676	-1.2954881860
C	0	1.0937923558	-3.1103493319	1.3925472047
H	0	0.7104819779	-2.3596567835	2.0481568943
N	0	0.5931722034	-3.4719539769	0.2132358899
N	0	5.3735458336	-2.4265689990	1.9550526871
H	0	5.8991711066	-2.2023962029	1.1047855125
C	-1	5.0494660131	-1.3522951942	2.8910646361
H	0	5.9175666693	-0.6840840660	2.9527707255
H	0	4.8938163520	-1.7985223260	3.8754523602
C	0	3.8013858125	-0.5710638530	2.4433261452
H	0	3.5411711047	0.1645868856	3.2147877987
H	0	2.9567950603	-1.2614103773	2.3717002010
C	0	4.0081319013	0.1250737106	1.0983110274
H	0	4.4983654120	-0.5521665269	0.3866131921
H	0	4.6743809141	0.9905610618	1.1960247900
C	0	2.7610849254	0.6145376526	0.3714364480
O	0	2.9528257813	1.1792357041	-0.7332982464
O	0	1.6192461206	0.3725125846	0.8995135478
C	-1	-5.4324452764	-3.9568930889	2.1536988387
H	0	-5.3011317255	-3.2351860600	2.9659454914
H	0	-5.9231507819	-4.8431375682	2.5742480432
C	0	-4.0729711512	-4.3691369322	1.5674678340
H	0	-4.2140494567	-5.0764499557	0.7435501787
H	0	-3.4795906658	-4.8883737749	2.3262681745
C	0	-3.2324558231	-3.2203209415	1.0191701737
O	0	-3.7040469091	-2.0564176791	1.0903995751
O	0	-2.0938965199	-3.5272220662	0.5235634503
C	0	-6.3511554400	-3.3833996199	1.0770654124
O	0	-6.2245119961	-3.6695816698	-0.1247462387
N	0	-7.3615337567	-2.6035379997	1.5189861470
H	0	-7.3685307652	-2.3090980960	2.4858556133
C	-1	-8.4061106381	-2.0927339261	0.6376555737
H	0	-9.2870209172	-1.8693297545	1.2401140032
H	0	-8.6513938017	-2.8748535509	-0.0869288272
C	0	-8.0053990210	-0.7937286699	-0.0948484922
O	0	-8.4536920189	0.2987807386	0.2539247158
N	0	-7.1703807464	-0.9788612688	-1.1477607603
H	0	-6.7341306194	-1.8904395821	-1.2391105624
C	0	-6.5617924831	0.1212806565	-1.8685667062
H	0	-6.5763417689	-0.0799713703	-2.9428675830
H	0	-7.1616822801	1.0162193761	-1.6783104769
C	0	-5.1085025353	0.4024617364	-1.4484756501
O	0	-4.3374122128	0.8830013850	-2.3158193147
O	0	-4.8036925289	0.1318094191	-0.2431696563
C	-1	-3.3942448079	3.6176785418	5.0436258728
H	-1	-3.4224203617	3.3052490526	6.0770395659
H	-1	-4.2102934237	4.2683908517	4.7664179049
H	0	-2.4845932607	4.2276782660	4.9398884322
C	0	-3.3645461777	2.5068710144	3.9883919284
H	0	-3.4913286989	2.9854236175	3.0082803172
H	0	-4.2155282714	1.8259329286	4.1008785973
C	0	-2.0549249133	1.7075462547	3.9704115101
H	0	-2.0755795333	0.9438877241	4.7562874859
H	0	-1.1977584949	2.3590929679	4.1634365625
C	0	-1.8357708670	1.0349883125	2.6260344652
O	0	-0.7011590161	1.2043110459	2.0802442294
O	0	-2.8004689147	0.3659572904	2.1408967534
C	-1	-5.4718387162	9.0821426142	2.1557412540

H	-1	-5.3332304131	8.6558395651	3.1382647203
H	-1	-6.5071815046	9.3245485270	1.9671233307
H	0	-4.9066159760	10.0205354697	2.1112713182
C	0	-4.9324849206	8.0718928540	1.1318165568
H	0	-3.8382884370	8.0373527448	1.2313860226
H	0	-5.1316720692	8.4048969604	0.1049333065
C	0	-5.5314735453	6.6723090652	1.3452782453
H	0	-6.6047472984	6.6969957401	1.1206647931
H	0	-5.4372863841	6.3860754871	2.4019997415
C	0	-4.8955169938	5.5723606629	0.4924916209
H	0	-4.9590961502	5.8345491376	-0.5740183631
H	0	-5.4382226095	4.6327576867	0.6432011402
N	0	-3.5008684394	5.3624537747	0.8872503964
H	0	-2.9991565790	6.1692539993	1.2329798657
C	0	-2.7257391399	4.3550089957	0.4268447737
N	0	-3.2146288651	3.4249955796	-0.3929333594
H	0	-2.7317697486	2.5057228886	-0.4615764991
H	0	-4.1291091679	3.5092070914	-0.8088082691
N	0	-1.4466696774	4.2838613389	0.8000665871
H	0	-1.0931067725	4.7204303712	1.6416076123
H	0	-0.8107504774	3.5860301829	0.3675537560
C	-1	-0.9474509170	-1.3911812730	7.4933783879
H	-1	0.0412522662	-0.9927108140	7.3195314249
H	-1	-1.1231717846	-1.6151346586	8.5353269171
H	0	-1.7012682996	-0.6813988583	7.1387665932
C	0	-1.1186013895	-2.7803751536	6.8585856113
H	0	-2.0684361028	-3.2126782537	7.2060156946
H	0	-0.3319510802	-3.4452079836	7.2435708700
C	0	-1.1015610999	-2.7881529737	5.3767723962
N	0	-1.2171943087	-3.9507752717	4.6401075452
C	0	-1.0236401105	-1.7852734328	4.4436967202
H	0	-0.8901831007	-0.7297780178	4.6118753576
C	0	-1.2082536841	-3.6206539073	3.3252909052
H	0	-1.2357155247	-4.3466659386	2.5293968406
N	0	-1.1023713355	-2.3102471047	3.1722541067
H	0	-0.8169297730	-1.4360339439	1.5905120784
C	-1	3.7928751552	6.2251865229	2.4327305146
H	-1	4.6607326777	6.7249612659	2.0278820845
H	-1	3.3294011907	6.7300632977	3.2672691160
H	0	3.0329072728	6.2295222977	1.6421501395
C	0	4.1256454183	4.7475674471	2.7501204067
H	0	5.0746010305	4.6501994031	3.2872847953
H	0	3.3263445970	4.3209328439	3.3672138364
C	0	4.1555232496	3.9431738021	1.4476724447
O	0	3.0720186699	3.9090306898	0.8052089125
O	0	5.2388630462	3.3954062773	1.0619928080
C	-1	12.1239371504	-2.3459777817	-0.7292194008
H	-1	13.1704230734	-2.0837102289	-0.7796468054
H	-1	11.8975516017	-3.2259902172	-1.3129087696
H	0	11.9216321012	-2.6310375974	0.3132498347
C	0	11.2152717225	-1.1566419619	-1.1173785206
H	0	11.6642639113	-0.6055424768	-1.9564467423
H	0	10.2473169081	-1.5333011736	-1.4679511294
C	0	10.9660712083	-0.2010741462	0.0650358758
H	0	10.2503995544	-0.6759515476	0.7504790114
H	0	11.8976848081	-0.0771303393	0.6350554712
C	0	10.4831598171	1.2095493868	-0.3152734789
H	0	10.3771084875	1.8190712032	0.5927762308
H	0	11.2602531375	1.6944998391	-0.9214896359
C	0	9.1873616971	1.3156754233	-1.1213956755

```
H    0    9.0387018576    2.3503883614   -1.4430601988
H    0    9.2119525605    0.6857877918   -2.0143255633
N    0    7.9619335515    0.9280236984   -0.3529356440
H    0    7.1190600315    1.3161541240   -0.8309229935
H    0    7.8540307800   -0.1150295113   -0.2981211941
H    0    7.9254344378    1.3396307495    0.6090987448
O    0    1.8595916750    1.5010527775   -3.5376441885
H    0    3.3684205795    2.3610401049   -3.6987907320
O    0    0.3410862692    2.5123343750   -0.1761707592
O    0    0.8417252852    3.6557517891    2.5668985222
H    0    0.4359222804    2.7969826054    2.3464443213
H    0    1.5112224304    3.7726121553    1.8571687277
O    0   -3.2204414427   -1.1183625193   -4.2018782743
H    0   -3.9258751817   -1.5133771932   -3.6487774988
H    0   -2.5609866753   -1.8413173010   -4.2747579010
O    0   -4.4257210018   -2.7594159353   -2.2362009433
H    0   -3.6197528789   -2.3641950389   -1.7983624079
H    0   -4.9466912854   -3.1430143611   -1.5067506290
O    0    2.3962795946    3.8491906005   -1.7259662753
H    0    2.7772978045    3.7890054385   -0.7984749014
O    0    5.8621049312    2.5018562116   -1.3770999934
H    0    5.4165930976    2.7589446626   -0.5157476294
H    0    6.3454665777    3.3078350504   -1.6251338147
O    0    4.1403596302    2.9710971914   -3.5411647612
H    0    4.6783541631    2.5317704564   -2.8463281070
O    0    7.4178596901    2.2057170036    2.0916524199
H    0    6.6198761076    2.7344037292    1.8189812122
H    0    7.0829266420    1.5852905918    2.7571547793
O    0    2.8084099177   -0.9685243490   -2.5085687445
H    0    2.2208953754    0.6149534848   -3.2935335722
H    0   -1.2911739219   -4.8860634664    5.0170709661
H    0    3.1389067000    3.6943127529   -2.3792741417
Cl   0    7.5188298957   -2.1482813766   -0.4706846342
H    0    3.1045571260   -0.3013719101   -1.8589874919
O    0   -0.2988079356    0.0360385649   -4.4520178463
H    0    0.0451523290   -0.8671768629   -4.5368115774
O    0    0.3735196717   -1.9977715228   -1.7620939686
H    0    1.9376508447   -1.2533691495   -2.1413337234
H    0   -0.1072675938   -1.9330430350   -2.6131185529
H    0    0.4820563647    0.6072937765   -4.1970172635
```

7L_S3a-fixed
E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.936699 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.372138 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.610744 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.773441 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.699187 au

```
Mn   0    1.2753821693    2.0528789159   -1.9081969088
Mn   0   -1.0446535181   -2.5284069705   -0.5276376255
Mn   0   -0.1210427806    0.7427682230    0.0978121004
Mn   0   -2.6930229604   -0.4566714348    0.3181676146
O    0    0.2237747122    0.3361946377   -1.5970402821
O    0   -1.9430606606    0.9949221863   -0.3708627814
O    0   -2.4649513101   -1.4509734733   -1.1848210110
O    0   -1.0072155704   -1.1176997724    0.7445665976
Ca   0   -1.8973118326    0.4143906857   -2.8085625512
C   -1    0.5534799135    4.6067477078   -5.5057325502
H   -1    0.6206110655    5.5379777831   -4.9627474014
H   -1    0.7467476250    4.6869541607   -6.5650249435
H    0    1.3344125921    3.9570293087   -5.0934666449
```

C	0	-0.8121297450	3.9100866692	-5.3104941224
H	0	-0.9279302650	3.1127140982	-6.0552394906
H	0	-1.6438204247	4.6040416282	-5.4959596067
C	0	-1.0648177850	3.2280376316	-3.9532963347
O	0	-2.1076201181	2.4983200289	-3.8642320040
O	0	-0.2390466955	3.3939283662	-3.0170333941
C	-1	-2.9625902702	-6.6362927581	-5.3092037769
H	-1	-2.0036613178	-7.1032927016	-5.4788150120
H	-1	-3.6925092076	-6.7713714825	-6.0936570363
H	0	-3.3886680242	-7.1688735333	-4.4439142918
C	0	-2.7269476678	-5.1771825027	-4.9035629395
H	0	-3.6742794799	-4.6678411677	-4.6878580455
H	0	-2.2399410449	-4.6142156147	-5.7079051928
C	0	-1.8467572994	-5.1595342965	-3.6533841698
H	0	-0.9003731712	-5.6868222268	-3.8485861184
H	0	-2.3261690531	-5.7076206250	-2.8335144910
C	0	-1.4665488194	-3.7933379186	-3.1275880472
O	0	-1.5473308997	-2.7696189077	-3.8292502529
O	0	-0.9967728056	-3.8170639448	-1.9230124901
C	-1	5.0166329032	-4.6502990515	1.0541821670
H	0	5.7254965906	-5.5511812118	1.2929356517
H	0	5.4094471346	-4.1030118790	0.1935963571
C	0	4.8742446192	-3.7268032662	2.2621469562
O	0	4.2315733044	-4.0923877048	3.2716305311
C	0	3.6440439519	-5.3175131878	0.7193635680
H	0	3.4168448634	-6.0295327015	1.5220249632
H	0	3.7457417478	-5.8925418743	-0.2049735562
C	0	2.4759225202	-4.3759858789	0.5791855460
N	0	2.1910821892	-3.4645774030	1.5862990974
H	0	2.7029583873	-3.4311066206	2.4691141461
C	0	1.4977399738	-4.1664438976	-0.3643969462
H	0	1.3236116460	-4.6565207537	-1.3085734423
C	0	1.1419419489	-2.7225569304	1.2371553200
H	0	0.7989093651	-1.8658443170	1.7814663328
N	0	0.6561093517	-3.1341718027	0.0643554216
N	0	5.3329352267	-2.4773140003	2.1081920466
H	0	5.9407950074	-2.2801425264	1.3046957138
C	-1	4.9963070496	-1.3835934828	3.0145904323
H	0	5.8796832757	-0.7379798471	3.0904524532
H	0	4.8027875637	-1.8060707454	4.0032886960
C	0	3.7889910474	-0.5624786079	2.5298917723
H	0	3.6190794261	0.2598483588	3.2365179250
H	0	2.8922177076	-1.1820275335	2.5659809892
C	0	3.9875219884	-0.0149864036	1.1166977747
H	0	4.4488746999	-0.7747099024	0.4742735342
H	0	4.6729895468	0.8404493961	1.1222373635
C	0	2.7479493540	0.4324717413	0.3519503195
O	0	2.9328102053	0.9772565431	-0.7432941573
O	0	1.5885447488	0.1782414836	0.8806199977
C	-1	-5.4889243760	-3.9692639360	2.2605324617
H	0	-5.3620166665	-3.2269615299	3.0553818446
H	0	-5.9791303510	-4.8440844380	2.7051288895
C	0	-4.1302940179	-4.3891906089	1.6900570857
H	0	-4.2609514475	-5.1218855612	0.8879754825
H	0	-3.5365739417	-4.8852763931	2.4678494086
C	0	-3.2749133481	-3.2628763709	1.1230164496
O	0	-3.6515755506	-2.0681490492	1.2718504288
O	0	-2.1829565777	-3.6025572756	0.5496113630
C	0	-6.4078560908	-3.4160625877	1.1747947144
O	0	-6.2379775658	-3.6615939535	-0.0283434029

```
N    0   -7.4622309368   -2.6922053918    1.6144155750
H    0   -7.5013484145   -2.4270097462    2.5892152355
C   -1   -8.4516629551   -2.1149275579    0.7108921477
H    0   -9.3880391283   -1.9821128514    1.2536503366
H    0   -8.6045824378   -2.8130026163   -0.1163371002
C    0   -8.0129939635   -0.7308721762    0.1890113282
O    0   -8.4885613709    0.3049529624    0.6550317839
N    0   -7.0820427934   -0.7661833652   -0.7968972996
H    0   -6.6758665263   -1.6567118757   -1.0610771580
C    0   -6.4810236387    0.4263243540   -1.3592524300
H    0   -6.6979276191    0.5062910154   -2.4283660868
H    0   -6.9239904503    1.2881318407   -0.8506172259
C    0   -4.9569330713    0.4760794460   -1.1916007753
O    0   -4.2649289524    0.9026303355   -2.1295782200
O    0   -4.5223127409    0.0743577226   -0.0444370460
C   -1   -3.4434681188    3.6319134107    5.0746380335
H   -1   -3.4772896514    3.3308738266    6.1112823944
H   -1   -4.2569069957    4.2813078682    4.7865803024
H    0   -2.5419950401    4.2540903305    4.9745250833
C    0   -3.3802375020    2.4949769047    4.0450956624
H    0   -3.7025409081    2.8914581495    3.0740482701
H    0   -4.0819258610    1.6891153232    4.2878190475
C    0   -1.9644737614    1.9412721456    3.8786367681
H    0   -1.6906616038    1.3164728907    4.7397779457
H    0   -1.2328465413    2.7549296942    3.8572912860
C    0   -1.7646626945    1.1538097405    2.5942602515
O    0   -0.6300192903    1.2660058301    2.0488307378
O    0   -2.7337462949    0.4431725192    2.1624426242
C   -1   -5.4944075919    9.0690433188    2.1168353059
H   -1   -5.3612786278    8.6531833711    3.1046304726
H   -1   -6.5283921949    9.3116918571    1.9210020179
H    0   -4.9444171839   10.0181753627    2.0892323271
C    0   -4.9113953010    8.0937446924    1.0824587050
H    0   -3.8166310236    8.1091652610    1.1811601463
H    0   -5.1309484029    8.4355681941    0.0622346184
C    0   -5.4321159199    6.6617156108    1.2686673664
H    0   -6.5219632777    6.6518524489    1.1391953907
H    0   -5.2320515650    6.3251720649    2.2952053720
C    0   -4.8424142978    5.6370862533    0.2947424193
H    0   -5.0409398454    5.9447206217   -0.7425337268
H    0   -5.3238568686    4.6671773852    0.4540651880
N    0   -3.4049334335    5.4574602922    0.5087340055
H    0   -2.8562409151    6.2802608315    0.7183303222
C    0   -2.7079269666    4.3656035405    0.1240677913
N    0   -3.3195589380    3.3667630119   -0.5232861274
H    0   -2.8358258263    2.4610041572   -0.6025901297
H    0   -4.1261955698    3.5240766739   -1.1078642346
N    0   -1.4153222009    4.2562779117    0.4191253968
H    0   -0.9744573917    4.7371830898    1.1970028079
H    0   -0.8288286104    3.4936930872    0.0222558250
C   -1   -1.0205145659   -1.3557126563    7.5909656068
H   -1   -0.0301668943   -0.9616826242    7.4167098432
H   -1   -1.2015312232   -1.5674935601    8.6343962220
H    0   -1.7629220659   -0.6264171078    7.2496969255
C    0   -1.1990574329   -2.7192048914    6.8939996347
H    0   -2.1616671991   -3.1550304269    7.1952987383
H    0   -0.4281540731   -3.4098971178    7.2590357155
C    0   -1.1487677050   -2.6921024909    5.4022989092
N    0   -0.9837014604   -3.8463964962    4.6458382262
C    0   -1.2944731626   -1.6835716466    4.4897699089
```

H	0	-1.4467866257	-0.6312006480	4.6371988355
C	0	-1.0265295065	-3.5520133633	3.3399369262
H	0	-0.9284514476	-4.2445696140	2.5200741997
N	0	-1.2217488168	-2.2401856624	3.2293164943
H	0	-1.2376996640	-1.7233651393	2.3120639550
C	-1	3.7616906488	6.1915032604	2.4661295386
H	-1	4.6323457254	6.6845410906	2.0595735721
H	-1	3.2955425899	6.7067812083	3.2929282521
H	0	3.0071161180	6.1802532523	1.6707772005
C	0	4.1118152379	4.7213981596	2.7999203264
H	0	5.0498196398	4.6464187568	3.3601879359
H	0	3.3084477570	4.2864358858	3.4064972684
C	0	4.1845064882	3.8969812823	1.5053744149
O	0	3.1334664800	3.8599992735	0.8200900925
O	0	5.2811601263	3.3290779568	1.1781500909
C	-1	12.0837929376	-2.4357879728	-0.5634652826
H	-1	13.1311375511	-2.1767781190	-0.6122679806
H	-1	11.8575869534	-3.3216720268	-1.1383015774
H	0	11.8672551896	-2.6987305122	0.4815193633
C	0	11.2000069686	-1.2411111024	-0.9862001996
H	0	11.6548696392	-0.7331644443	-1.8492039303
H	0	10.2191785752	-1.6052703833	-1.3120429540
C	0	10.9922589967	-0.2399726851	0.1649844755
H	0	10.2626726175	-0.6696683609	0.8647445565
H	0	11.9307828293	-0.1301248164	0.7266758177
C	0	10.5529010486	1.1713251743	-0.2596738785
H	0	10.4721459921	1.8146226266	0.6274966486
H	0	11.3381009235	1.6117312989	-0.8890773287
C	0	9.2522730249	1.2807242892	-1.0557426948
H	0	9.1131642055	2.3095265805	-1.3999132312
H	0	9.2592661890	0.6303205898	-1.9342304071
N	0	8.0316801087	0.9289915124	-0.2648330308
H	0	7.1897453077	1.3202901829	-0.7474408949
H	0	7.9170582981	-0.1076407709	-0.1639630410
H	0	8.0093305085	1.3726393432	0.6837957042
O	0	1.9487181466	1.3517280584	-3.5460434802
H	0	2.7439535457	1.8651561923	-3.8090594817
O	0	0.4112254505	2.3713184961	-0.2061256382
O	0	0.7556994087	3.9011823906	2.3240833343
H	0	0.4127185281	3.0169824740	2.0990376793
H	0	1.5324583210	3.9769370113	1.7200727033
O	0	-3.4457917602	-0.9128286460	-4.2123593064
H	0	-4.1798896833	-1.1976225998	-3.6357388036
H	0	-2.9055731471	-1.7264462783	-4.3144040206
O	0	-4.7048586577	-2.5536360885	-2.1627120832
H	0	-3.8820205240	-2.1945671535	-1.7422010755
H	0	-5.1332683286	-3.0697342866	-1.4539839840
O	0	2.3419348147	3.5869784746	-1.8350135393
H	0	2.7034499473	3.6017822816	-0.9193348269
O	0	5.9644846315	2.4818133878	-1.2873266943
H	0	5.5200467960	2.7460481816	-0.4290944971
H	0	6.3670358496	3.3087662054	-1.5987617996
O	0	4.2531051758	3.0083677274	-3.5760616275
H	0	4.7997329839	2.4931390358	-2.9515569023
O	0	7.5171976332	2.2393708545	2.1712107628
H	0	6.6937360490	2.7362025211	1.9079608619
H	0	7.2043648612	1.5790554113	2.8086687649
O	0	2.1206032922	-1.2439177923	-2.7167853473
H	0	1.4013429051	-0.9493144516	-2.1100628521
H	0	-0.8469015400	-4.7782947204	5.0187132789

H	0	3.5689000680	3.3768830493	-2.9420393286
Cl	0	7.6365056519	-2.1814853056	-0.1064820528
H	0	2.3344125991	-0.3459923827	-3.0878491578
O	0	-0.2896455234	0.2837602834	-4.6298843136
H	0	0.0840385109	-2.5522158945	-4.6774393035
O	0	0.9257672955	-2.1628010813	-4.9792913647
H	0	0.1011050105	-0.5918978436	-4.8749375781
H	0	1.3931858472	-1.9285881853	-4.1306378205
H	0	0.5146539263	0.8046488744	-4.3550143951

7L_S3a

E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.96014 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.394317 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.63679 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.796426 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.721779 au

Mn	0	1.2045160789	2.1374759530	-1.8204403234
Mn	0	-0.9001885836	-2.3746403678	-0.7410676698
Mn	0	-0.1710049141	0.7589549259	0.1689010133
Mn	0	-2.6966476908	-0.5573647967	0.3201776910
O	0	0.1972467460	0.3674131100	-1.5259996448
O	0	-1.9974908700	0.9584409372	-0.2963097029
O	0	-2.4196385810	-1.4342670557	-1.2655989924
O	0	-0.9662294515	-1.1502337446	0.6969148676
Ca	0	-1.9419940634	0.5672689695	-2.7691091965
C	-1	0.4906301155	4.6270840014	-5.5140459838
H	-1	0.5454701369	5.5569130002	-4.9672939838
H	-1	0.6790911175	4.7147059971	-6.5736169838
H	0	1.2697549824	3.9778854643	-5.0970725368
C	0	-0.8787824604	3.9346561324	-5.3309168631
H	0	-0.9754544447	3.1149610067	-6.0547709721
H	0	-1.7062482783	4.6211100615	-5.5561598398
C	0	-1.1638050935	3.2824124381	-3.9684920206
O	0	-2.2571423882	2.6336827069	-3.8547884841
O	0	-0.3065084787	3.3722037246	-3.0507023042
C	-1	-2.8539871439	-6.6687249217	-5.3541809838
H	-1	-1.8886671543	-7.1204039439	-5.5289609838
H	-1	-3.5844121472	-6.8115309049	-6.1367919838
H	0	-3.2694674692	-7.2013427208	-4.4840164384
C	0	-2.6510563051	-5.1998280979	-4.9741031629
H	0	-3.6114087828	-4.6967029715	-4.8074171937
H	0	-2.1454447173	-4.6528097999	-5.7777742449
C	0	-1.8163221433	-5.1231593973	-3.6974298879
H	0	-0.8880223558	-5.7038247673	-3.8063115692
H	0	-2.3475889862	-5.5755923188	-2.8507137004
C	0	-1.3991746877	-3.7323422263	-3.2834753603
O	0	-1.5482115438	-2.7520396318	-4.0316750385
O	0	-0.8191436719	-3.6810406794	-2.1255379053
C	-1	5.1156069038	-4.5889531048	0.9912890162
H	0	5.8803146968	-5.3436669707	1.2106430449
H	0	5.4530112217	-4.0238249784	0.1190508332
C	0	4.9649735573	-3.6715430182	2.2025660161
O	0	4.3642086352	-4.0591728410	3.2285962922
C	0	3.7800087452	-5.3290892310	0.6938065217
H	0	3.5811895440	-6.0211928188	1.5206467607
H	0	3.8959069158	-5.9262374632	-0.2146018690
C	0	2.6081200322	-4.4059964156	0.5319786421
N	0	2.2783145081	-3.5287649308	1.5560235255
H	0	2.7581607167	-3.5173527546	2.4565893311
C	0	1.7175264626	-4.1217091884	-0.4751599260

H	0	1.6015675560	-4.5661070406	-1.4508070275
C	0	1.2882890575	-2.7309347486	1.1530824761
H	0	0.9290030836	-1.8821806417	1.6985228638
N	0	0.8957876152	-3.0752952605	-0.0688144258
N	0	5.3820256940	-2.4080138660	2.0382571715
H	0	5.9709178653	-2.1989128610	1.2248144780
C	-1	5.0523839787	-1.3312791033	2.9657600162
H	0	5.9200508663	-0.6612303459	3.0112942834
H	0	4.9117115647	-1.7667221695	3.9578744950
C	0	3.8051934965	-0.5398152439	2.5396275658
H	0	3.6262051428	0.2558349273	3.2741043257
H	0	2.9322879654	-1.1931348202	2.5780214338
C	0	3.9603682488	0.0537359893	1.1413950771
H	0	4.3972883904	-0.6878340176	0.4608819646
H	0	4.6512863104	0.9043766953	1.1544613986
C	0	2.7070742564	0.5331862623	0.4241885154
O	0	2.8764711386	1.1295667161	-0.6464094122
O	0	1.5553028247	0.2451739618	0.9536472775
C	-1	-5.3949420843	-4.0724638634	2.2352380162
H	0	-5.2428332243	-3.3159968024	3.0123965117
H	0	-5.8988019533	-4.9265206413	2.7047974276
C	0	-4.0574364734	-4.5257962129	1.6523561125
H	0	-4.2146644085	-5.2703539646	0.8664480679
H	0	-3.4629077728	-5.0194791043	2.4306106158
C	0	-3.1881496868	-3.4244425141	1.0465396739
O	0	-3.5677118149	-2.2185714804	1.1860103301
O	0	-2.1206277446	-3.7950635218	0.4790600827
C	0	-6.3188974353	-3.5181522624	1.1534954527
O	0	-6.1474991631	-3.7461026372	-0.0527940306
N	0	-7.3866839831	-2.8176580373	1.6009103387
H	0	-7.4326432303	-2.5655504423	2.5788299232
C	-1	-8.3906410426	-2.2567197945	0.7033660162
H	0	-9.3307345121	-2.1562695884	1.2470315875
H	0	-8.5243920601	-2.9492350991	-0.1316830794
C	0	-7.9867010021	-0.8576796629	0.2017481259
O	0	-8.4577321791	0.1624762123	0.7050923382
N	0	-7.0861432509	-0.8622526366	-0.8128431039
H	0	-6.6642539238	-1.7417760670	-1.0896754714
C	0	-6.4934310398	0.3477535731	-1.3413428456
H	0	-6.7010639296	0.4519196891	-2.4101586116
H	0	-6.9483330823	1.1940987498	-0.8173812958
C	0	-4.9729707207	0.4090441171	-1.1590587159
O	0	-4.2870452474	0.9161104038	-2.0609627055
O	0	-4.5369798539	-0.0731537270	-0.0442236724
C	-1	-3.4554389093	3.5468550921	5.0751830162
H	-1	-3.4812039163	3.2409420927	6.1106320162
H	-1	-4.2795898946	4.1850541110	4.7926040162
H	0	-2.5521332783	4.1647820532	4.9670536609
C	0	-3.4221469334	2.4394392590	4.0154443760
H	0	-3.5215166427	2.9242477747	3.0354120922
H	0	-4.2837204366	1.7688545421	4.1089368917
C	0	-2.1236155544	1.6241051072	4.0225473407
H	0	-2.1837848454	0.8597903400	4.8058501171
H	0	-1.2638446323	2.2629434089	4.2435858479
C	0	-1.8636763098	0.9642592183	2.6782306167
O	0	-0.7358882251	1.1743530200	2.1472116715
O	0	-2.7982889015	0.2468710285	2.1834082241
C	-1	-5.5984797848	8.9647531413	2.1475400162
H	-1	-5.4557407944	8.5467731380	3.1330970162
H	-1	-6.6366767796	9.1925201652	1.9561660162

H	0	-5.0615080541	9.9215580505	2.1229158802
C	0	-5.0183192713	8.0074665761	1.1023110588
H	0	-3.9270499293	7.9864904944	1.2326217370
H	0	-5.1960020075	8.3867797440	0.0873027630
C	0	-5.5961711073	6.5925650874	1.2299697517
H	0	-6.6723368601	6.6174803095	1.0171812254
H	0	-5.4844363725	6.2370835999	2.2634945388
C	0	-4.9527166141	5.5701170973	0.2924090102
H	0	-5.0617161170	5.8902627435	-0.7539869815
H	0	-5.4534448044	4.6032783133	0.4014455493
N	0	-3.5407388811	5.3785454881	0.6247207649
H	0	-3.0074926499	6.1912105128	0.9007411427
C	0	-2.8318439871	4.2720656519	0.3262123213
N	0	-3.3983323371	3.2815512845	-0.3740737367
H	0	-2.9029110905	2.3786784834	-0.4266055080
H	0	-4.1106504800	3.4657330291	-1.0647451106
N	0	-1.5888797457	4.1230425393	0.7763744392
H	0	-1.1933771534	4.6878877598	1.5170926489
H	0	-0.9367822164	3.4277800602	0.3556465434
C	-1	-0.9487270232	-1.4140789655	7.5620570162
H	-1	0.0349459862	-1.0043369881	7.3862260162
H	-1	-1.1229980283	-1.6330049615	8.6051620162
H	0	-1.7058536561	-0.7016561009	7.2181606975
C	0	-1.0865167937	-2.7791620689	6.8552579648
H	0	-2.0468314711	-3.2345724015	7.1336517446
H	0	-0.3108929125	-3.4569172038	7.2356499245
C	0	-1.0113065402	-2.7550896829	5.3623230450
N	0	-1.0258621300	-3.9229619966	4.6063835359
C	0	-0.9888463331	-1.7390074976	4.4470247580
H	0	-0.9320359570	-0.6772524077	4.5946744584
C	0	-1.0241324335	-3.6282576202	3.2995178358
H	0	-1.0354658694	-4.3246967855	2.4763980271
N	0	-1.0163215686	-2.3031275058	3.1860570674
H	0	-1.0453352065	-1.7961401293	2.2647059210
C	-1	3.7012831523	6.2264789277	2.4539080162
H	-1	4.5629931639	6.7343869079	2.0465990162
H	-1	3.2301671639	6.7311149385	3.2844460162
H	0	2.9437493079	6.1970092299	1.6621172346
C	0	4.0743436911	4.7640147601	2.8023671976
H	0	5.0328037736	4.7061705272	3.3291035621
H	0	3.2966425057	4.3367402230	3.4467115499
C	0	4.0999766310	3.9137080105	1.5247916307
O	0	3.0169364864	3.8456747004	0.8942714083
O	0	5.1890534072	3.3577942683	1.1556048463
C	-1	12.1429119573	-2.2606622662	-0.6401669838
H	-1	13.1860409636	-1.9855922902	-0.6913149838
H	-1	11.9282219370	-3.1474292613	-1.2180499838
H	0	11.9380893053	-2.5370655138	0.4038110349
C	0	11.2300798995	-1.0801070636	-1.0471748964
H	0	11.6950986336	-0.5210238951	-1.8721985887
H	0	10.2760203442	-1.4651386941	-1.4242103832
C	0	10.9412627599	-0.1325787279	0.1322907121
H	0	10.2100865860	-0.6192895016	0.7922894967
H	0	11.8567697138	-0.0021282821	0.7265958989
C	0	10.4520690995	1.2735197701	-0.2552903186
H	0	10.3359256233	1.8850001847	0.6502776236
H	0	11.2276126542	1.7633060752	-0.8596922616
C	0	9.1569211351	1.3614603382	-1.0641627238
H	0	8.9922119987	2.3931486605	-1.3877895945
H	0	9.1913417395	0.7306403231	-1.9560975611

N	0	7.9393195203	0.9573904868	-0.2929052639
H	0	7.0885632971	1.3274038072	-0.7743623004
H	0	7.8611105275	-0.0854784401	-0.2134643713
H	0	7.8970306726	1.3822048165	0.6638546464
O	0	1.9345581697	1.4709775270	-3.4484746508
H	0	2.6886914230	2.0424541644	-3.7163516733
O	0	0.2941744696	2.4102925392	-0.1192600793
O	0	0.7552849287	3.7148830241	2.5634448338
H	0	0.3646235077	2.8531032958	2.3314734474
H	0	1.4730767930	3.8119566671	1.8970302864
O	0	-3.4117985971	-0.8150630435	-4.1787709210
H	0	-4.1377808406	-1.1431321122	-3.6158582157
H	0	-2.8568466536	-1.6117888163	-4.3280596945
O	0	-4.6488282784	-2.6131687714	-2.1998311448
H	0	-3.8230298741	-2.2493205678	-1.7955099189
H	0	-5.0665286652	-3.1147242427	-1.4738461722
O	0	2.1891162247	3.7208320054	-1.7323239726
H	0	2.5721539833	3.7088923567	-0.8235951665
O	0	5.8397800995	2.5055126801	-1.3069203237
H	0	5.3750395657	2.7414113225	-0.4507634769
H	0	6.2988948885	3.3300879219	-1.5380033874
O	0	4.1191539680	3.2527622918	-3.4981515033
H	0	4.6826821012	2.7318315150	-2.8910287032
O	0	7.4001850853	2.2360946094	2.1516846817
H	0	6.5843936424	2.7448380872	1.8845749423
H	0	7.0810955929	1.5928279165	2.8031272492
O	0	2.2275925336	-1.0978661464	-2.6518375695
H	0	1.5116571806	-0.8449512669	-2.0267885411
H	0	-1.0327807285	-4.8641618508	4.9805540378
H	0	3.4269653461	3.5872728853	-2.8559610990
Cl	0	7.6835841253	-2.1577033602	-0.2025835307
H	0	2.3901236175	-0.1863868403	-3.0197270133
O	0	-0.3061856582	0.4599061889	-4.5604174065
H	0	0.1467739111	-2.3643496779	-4.6292630647
O	0	0.9775028442	-1.9406711219	-4.9153949963
H	0	0.0971149005	-0.4102906325	-4.8084106747
H	0	1.4547481847	-1.7362180091	-4.0651833996
H	0	0.4966039131	0.9773058584	-4.2712910540

L_S3aa-fixed
E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.906578 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.342743 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.583685 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.751322 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.676647 au

Mn	0	-1.3709454277	2.0489964630	1.9464825817
Mn	0	1.0672856296	-2.5484426744	0.4416751042
Mn	0	0.0400603300	0.7268626818	-0.0422835823
Mn	0	2.6502870565	-0.4114890600	-0.3818958077
O	0	-0.2785301686	0.3584734027	1.6573064748
O	0	1.8753855834	0.9932141689	0.3703905404
O	0	2.4814281889	-1.4645649411	1.1015322202
O	0	0.9664046550	-1.1011267938	-0.7851495239
Ca	0	1.9392645665	0.3176164726	2.7857994856
C	-1	-0.6310045088	4.5528992406	5.4988066275
H	-1	-0.7213640811	5.4873704622	4.9648338374
H	-1	-0.8160569305	4.6199614712	6.5604772984
H	0	-1.4058675893	3.8936937244	5.0939847563
C	0	0.7390280253	3.8823109822	5.2694896014
H	0	0.8872530874	3.0928971310	6.0133372546

H	0	1.5645646769	4.5945030595	5.4118086037
C	0	0.9340548222	3.2059516390	3.9011814796
O	0	1.9341305058	2.4244220026	3.7811308399
O	0	0.1051736632	3.4382137630	2.9822152036
C	-1	3.1027695970	-6.6166082296	5.1696118649
H	-1	2.1547769474	-7.1038632194	5.3436675426
H	-1	3.8423790065	-6.7441960539	5.9462042054
H	0	3.5275176351	-7.1262916275	4.2907847468
C	0	2.8060852323	-5.1616874972	4.7814524702
H	0	3.7157258522	-4.6464796648	4.4488841805
H	0	2.4105737414	-4.5995773495	5.6351280808
C	0	1.7768713187	-5.1777430177	3.6419934658
H	0	0.8230913198	-5.5855691315	4.0102641709
H	0	2.1046485523	-5.8488558732	2.8410153039
C	0	1.4636955144	-3.8345969183	3.0160627764
O	0	1.5132286033	-2.7779552642	3.6757485442
O	0	1.1110949574	-3.8988260976	1.7775442474
C	-1	-4.9720255244	-4.7320920809	-1.1034355872
H	0	-5.6862079440	-5.5317565129	-1.3305391623
H	0	-5.3405633069	-4.1959786525	-0.2251469675
C	0	-4.8671836151	-3.7944321112	-2.3046266994
O	0	-4.2364610147	-4.1404416973	-3.3278452634
C	0	-3.5884844754	-5.3991158207	-0.8176910117
H	0	-3.3720474654	-6.0825169694	-1.6476248652
H	0	-3.6665382763	-6.0046547220	0.0894345042
C	0	-2.4289482181	-4.4480488813	-0.6692963224
N	0	-2.1874153091	-3.4884102471	-1.6415771119
H	0	-2.7116347495	-3.4343931035	-2.5150505775
C	0	-1.4314690581	-4.2578964901	0.2588153917
H	0	-1.2220735788	-4.7872576698	1.1743445605
C	0	-1.1462464328	-2.7380370680	-1.2842417648
H	0	-0.8362063302	-1.8493057702	-1.7967863291
N	0	-0.6233884879	-3.1888979488	-0.1426525120
N	0	-5.3456526774	-2.5541241217	-2.1328952304
H	0	-5.9247291520	-2.3685630158	-1.3064391420
C	-1	-5.0337529307	-1.4484934158	-3.0345342683
H	0	-5.9316721534	-0.8236008201	-3.1148283062
H	0	-4.8218622750	-1.8637690805	-4.0220485976
C	0	-3.8463620246	-0.5993087815	-2.5362894034
H	0	-3.6753829046	0.2133511611	-3.2536929601
H	0	-2.9412290015	-1.2071633926	-2.5510679188
C	0	-4.0631279431	-0.0277028068	-1.1311768578
H	0	-4.5859406617	-0.7530700441	-0.4964149369
H	0	-4.7052621937	0.8605156894	-1.1673839307
C	0	-2.8274614798	0.3742796370	-0.3224041057
O	0	-3.0268850477	0.8605508750	0.7990199516
O	0	-1.6625572821	0.1486952375	-0.8492003611
C	-1	5.5066280654	-3.8338651650	-2.3983540003
H	0	5.3507022421	-3.0778194332	-3.1748200480
H	0	6.0096138882	-4.6865217230	-2.8716972330
C	0	4.1684379224	-4.2982273752	-1.8222457124
H	0	4.3265672120	-5.0273859154	-1.0217262417
H	0	3.5858512303	-4.8111551876	-2.5975809772
C	0	3.2841788748	-3.1990292581	-1.2514620809
O	0	3.6282311251	-1.9935426611	-1.3868337580
O	0	2.2029176128	-3.5760138278	-0.6827963288
C	0	6.4390005952	-3.2890164091	-1.3221537226
O	0	6.3208219618	-3.5939810439	-0.1259177600
N	0	7.4512589975	-2.5073990731	-1.7596880360
H	0	7.4519167182	-2.1985396191	-2.7224440724

C	-1	8.4465835959	-1.9352948380	-0.8589179876
H	0	9.3710571716	-1.7712317144	-1.4135947573
H	0	8.6256804086	-2.6519253962	-0.0533590503
C	0	7.9930993635	-0.5743975087	-0.2939883025
O	0	8.4585362809	0.4804221026	-0.7263456926
N	0	7.0609076820	-0.6496653952	0.6881969547
H	0	6.6671920107	-1.5523093511	0.9299964873
C	0	6.4444417004	0.5211811745	1.2784918421
H	0	6.6652400280	0.5822708930	2.3481031538
H	0	6.8729188401	1.4003436364	0.7873549341
C	0	4.9188200168	0.5525476026	1.1194619773
O	0	4.2324814903	0.9784710667	2.0612647404
O	0	4.4800625196	0.1348546620	-0.0203721878
C	-1	3.2868066132	3.7500607509	-5.1255206891
H	-1	3.3169861549	3.4588811370	-6.1650901167
H	-1	4.0899776254	4.4127770545	-4.8389944907
H	0	2.3749752283	4.3546905226	-5.0128528029
C	0	3.2514919177	2.5967774683	-4.1035583495
H	0	3.6420283242	2.9687060302	-3.1481467169
H	0	3.9157874497	1.7765529697	-4.3985191444
C	0	1.8331359339	2.0784198842	-3.8563611224
H	0	1.4741496880	1.5005613729	-4.7199035336
H	0	1.1346390698	2.9153388151	-3.7568200276
C	0	1.6645892500	1.2376739306	-2.5965533570
O	0	0.5317069584	1.2865309806	-2.0449968296
O	0	2.6579105840	0.5372137484	-2.1952136556
C	-1	5.2579130547	9.2002556775	-2.1376370655
H	-1	5.1238805631	8.7905672566	-3.1278861100
H	-1	6.2887010940	9.4614718831	-1.9489688875
H	0	4.6886810626	10.1371579603	-2.0938051939
C	0	4.6975486879	8.1961591000	-1.1135170038
H	0	3.6009531103	8.2090314090	-1.1901996768
H	0	4.9348786342	8.5144089872	-0.0897163822
C	0	5.2173163309	6.7682164979	-1.3412786889
H	0	6.3092746062	6.7590031559	-1.2306154013
H	0	5.0021591005	6.4550850254	-2.3722673545
C	0	4.6508839230	5.7137102764	-0.3827994687
H	0	4.8420294978	6.0120153597	0.6587398734
H	0	5.1592418207	4.7596770947	-0.5556630383
N	0	3.2181890503	5.4948149219	-0.5988290526
H	0	2.6502664035	6.3034641195	-0.8130608145
C	0	2.5437648270	4.3969443477	-0.1838539686
N	0	3.1751996888	3.4230537569	0.4816531556
H	0	2.7122770835	2.5072218180	0.5837467039
H	0	3.9973141946	3.6001553895	1.0382077653
N	0	1.2509010817	4.2582671473	-0.4662162199
H	0	0.7952030558	4.7112237191	-1.2525446318
H	0	0.6818968228	3.4932510046	-0.0473188282
C	-1	0.9390246140	-1.2619402783	-7.6645721320
H	-1	-0.0572105614	-0.8890239501	-7.4778572995
H	-1	1.1145531561	-1.4609262885	-8.7114527992
H	0	1.6671491032	-0.5158302707	-7.3284178019
C	0	1.1578562136	-2.6186893058	-6.9701309123
H	0	2.1317456653	-3.0272187669	-7.2734762719
H	0	0.4058086130	-3.3316347069	-7.3319355400
C	0	1.1090754929	-2.5911827647	-5.4782320906
N	0	0.9708266727	-3.7523726176	-4.7277555476
C	0	1.2304686461	-1.5831001659	-4.5605892336
H	0	1.3579093289	-0.5257677041	-4.7015448115
C	0	1.0062384372	-3.4636944417	-3.4208236404

H	0	0.9292307940	-4.1635569800	-2.6053013276
N	0	1.1699270566	-2.1482490811	-3.3026764792
H	0	1.1805353741	-1.6416420951	-2.3779007690
C	-1	-3.9428357476	6.1443120860	-2.4292340743
H	-1	-4.8192096650	6.6165239536	-2.0104283531
H	-1	-3.4944986961	6.6759200507	-3.2555441270
H	0	-3.1814513803	6.1141334135	-1.6407431978
C	0	-4.2805528187	4.6862615805	-2.8304701672
H	0	-5.2153351542	4.6374191719	-3.3990050850
H	0	-3.4716994241	4.2898397262	-3.4554897087
C	0	-4.3564104464	3.7943723073	-1.5854485036
O	0	-3.2927042964	3.6571789596	-0.9350769065
O	0	-5.4765947004	3.2709190923	-1.2579957428
C	-1	-12.0660517177	-2.6714037815	0.5977266076
H	-1	-13.1177776804	-2.4334941239	0.6582995333
H	-1	-11.8172510702	-3.5576901161	1.1625195197
H	0	-11.8618404991	-2.9301917983	-0.4513170711
C	0	-11.2028653275	-1.4566553182	0.9969079541
H	0	-11.6376873184	-0.9668787065	1.8803955517
H	0	-10.1984642887	-1.7917887298	1.2803719529
C	0	-11.0772319837	-0.4456377728	-0.1579052362
H	0	-10.3700109903	-0.8495338410	-0.8956301180
H	0	-12.0429728955	-0.3635552278	-0.6764470029
C	0	-10.6632484635	0.9768448033	0.2522638467
H	0	-10.6187879003	1.6191042753	-0.6380851890
H	0	-11.4442512055	1.3995204395	0.8987219521
C	0	-9.3493740151	1.1189620636	1.0193089622
H	0	-9.2221083928	2.1546863214	1.3467758107
H	0	-9.3279676725	0.4812669764	1.9067694004
N	0	-8.1366765772	0.7780733664	0.2120430078
H	0	-7.3017192013	1.2143149243	0.6688689087
H	0	-7.9834010324	-0.2557949525	0.1462153057
H	0	-8.1430104283	1.1956198338	-0.7478243549
O	0	-2.1249409044	1.4891007268	3.5901331572
H	0	-2.9966117900	1.9354228684	3.6771311803
O	0	-0.5172133858	2.3417705259	0.2410308655
O	0	-0.9003207866	3.8235419979	-2.3750154171
H	0	-0.5302751118	2.9490448429	-2.1497312554
H	0	-1.6951392339	3.8651534206	-1.7914483249
O	0	3.6481632343	-1.0785897162	4.0156725956
H	0	4.3049335117	-1.4305855470	3.3821921829
H	0	3.0509776767	-1.8399885169	4.1587072149
O	0	4.7182732335	-2.6315864742	1.9615962943
H	0	3.9000607915	-2.2511847956	1.5465971464
H	0	5.1910692182	-3.0824130094	1.2358973047
O	0	-2.4832338719	3.5626011832	1.7496742620
H	0	-2.8382750673	3.4950110985	0.8361774072
O	0	-6.1492517414	2.4364005266	1.1771258247
H	0	-5.7133438090	2.7093608452	0.3132016340
H	0	-6.5817008105	3.2504984527	1.4823379139
O	0	-4.4741760484	3.0479563167	3.4032826236
H	0	-4.9969522924	2.5247113329	2.7642219719
O	0	-7.6730173302	2.0739177122	-2.2438638708
H	0	-6.8738865344	2.6074536994	-1.9827200492
H	0	-7.3299736188	1.4267918406	-2.8793171205
O	0	-1.0372776996	1.3717581230	5.9217861974
H	0	-1.5628782107	0.6416107041	6.2866428320
H	0	0.8558662361	-4.6849319054	-5.1058180843
H	0	-3.7510698159	3.3956343801	2.7967708413
Cl	0	-7.5390621745	-2.3065957864	0.2251946647

```
H   0   -1.4497969955    1.5119224472    4.9961663117
O   0    0.9913371120   -0.0720591510    4.9218686573
H   0    0.3149527730    0.5545392473    5.3001860696
H   0    0.9575719404   -2.8391327091    5.3381697072
O   0    0.5901482169   -2.5653795672    6.2098743408
H   0    0.8509585796   -0.9134170824    5.4053945235
H   0   -0.3666224685   -2.6966552605    6.1096852083
```

L_S3aa

E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.928967 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.364362 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.609745 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.773669 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.698483 au

```
Mn   0   -1.3299190738    2.0169992309    1.9203883742
Mn   0    1.0039828441   -2.3783850166    0.6294522151
Mn   0    0.0882264942    0.7330595404   -0.0870345034
Mn   0    2.6854410808   -0.4343233250   -0.4099487205
O    0   -0.1994160959    0.3372594974    1.6148462894
O    0    1.9298130490    1.0091483792    0.2947634796
O    0    2.5037520208   -1.3988309009    1.1492011907
O    0    0.9755489908   -1.1028505501   -0.7551279400
Ca   0    2.0246239642    0.4579337809    2.7626816521
C   -1   -0.5842009880    4.6033110067    5.4433170335
H   -1   -0.6741619865    5.5316950069    4.8987640335
H   -1   -0.7655849879    4.6831970070    6.5047330335
H    0   -1.3543764870    3.9368533697    5.0435916190
C    0    0.7912885001    3.9423212465    5.2269942603
H    0    0.9312738373    3.1456524325    5.9659269205
H    0    1.6133519923    4.6537973939    5.3880400277
C    0    1.0083158826    3.2692868799    3.8627652085
O    0    2.0729485702    2.5803868026    3.7205357870
O    0    0.1295020665    3.3991089853    2.9709132461
C   -1    3.1225919941   -6.5780369992    5.2323720335
H   -1    2.1740539933   -7.0609939977    5.4152170335
H   -1    3.8644689939   -6.6982910004    6.0079710335
H    0    3.5416943796   -7.0839077257    4.3492894040
C    0    2.8327563126   -5.1173305905    4.8654230760
H    0    3.7439646612   -4.6021616232    4.5373431575
H    0    2.4488141854   -4.5659175792    5.7316517590
C    0    1.7990170303   -5.1001459872    3.7343237344
H    0    0.8469872505   -5.5248643097    4.0871442836
H    0    2.1242631672   -5.7393265193    2.9058746890
C    0    1.4857126540   -3.7363227464    3.1593727668
O    0    1.6369619043   -2.6919349113    3.8213484269
O    0    1.0241109428   -3.7657784734    1.9551963278
C   -1   -4.9685250030   -4.7478759862   -1.0357369665
H    0   -5.7253625782   -5.5168412942   -1.2321949133
H    0   -5.2904358529   -4.1885858241   -0.1536108744
C    0   -4.8705751096   -3.8271109053   -2.2516384459
O    0   -4.2719224341   -4.1967206946   -3.2854214321
C    0   -3.6107261200   -5.4608483566   -0.7808531553
H    0   -3.4174121051   -6.1378934511   -1.6211797838
H    0   -3.6898566122   -6.0716984875    0.1225316587
C    0   -2.4578917885   -4.5119558190   -0.6345700736
N    0   -2.1660564281   -3.6146111110   -1.6524982798
H    0   -2.6623285396   -3.6034502343   -2.5438958842
C    0   -1.5573461725   -4.2183801696    0.3611725576
H    0   -1.4117994719   -4.6766788101    1.3264632344
C    0   -1.1874501783   -2.7975424851   -1.2543579047
```

H	0	-0.8497902626	-1.9353476985	-1.7944491323
N	0	-0.7678844678	-3.1488297553	-0.0444862934
N	0	-5.3343783298	-2.5800065462	-2.0865770193
H	0	-5.8970039418	-2.3815991782	-1.2524297164
C	-1	-5.0290359978	-1.4869079861	-3.0048479665
H	0	-5.9200215379	-0.8499346390	-3.0705186746
H	0	-4.8442722399	-1.9135490249	-3.9930065421
C	0	-3.8195513231	-0.6537021831	-2.5364825076
H	0	-3.6337777333	0.1397285347	-3.2714968319
H	0	-2.9317722782	-1.2869734021	-2.5417241145
C	0	-4.0203762098	-0.0501933958	-1.1431510413
H	0	-4.5485221953	-0.7554864570	-0.4907715297
H	0	-4.6531831639	0.8442288767	-1.1945406920
C	0	-2.7791222416	0.3544007905	-0.3468904954
O	0	-2.9725468766	0.8336523554	0.7790850086
O	0	-1.6173084824	0.1426738263	-0.8843954725
C	-1	5.5078399984	-3.8894950031	-2.3754289665
H	0	5.3387884684	-3.1306356830	-3.1468171904
H	0	6.0192807961	-4.7323365407	-2.8579627510
C	0	4.1830877912	-4.3681877770	-1.7934740285
H	0	4.3558765958	-5.1017862862	-1.0003422499
H	0	3.6019037615	-4.8822494289	-2.5690416816
C	0	3.2799821247	-3.2886063283	-1.2040829608
O	0	3.6136645902	-2.0688478314	-1.3363565844
O	0	2.2218870810	-3.7035074129	-0.6485954059
C	0	6.4445039323	-3.3355192620	-1.3070144302
O	0	6.3295719921	-3.6239166832	-0.1065167147
N	0	7.4589619051	-2.5628632667	-1.7577256771
H	0	7.4590688406	-2.2688684294	-2.7251486031
C	-1	8.4572600014	-1.9800090078	-0.8679289665
H	0	9.3887072501	-1.8484691851	-1.4200390312
H	0	8.6184624390	-2.6750694954	-0.0402129611
C	0	8.0214133544	-0.5972523939	-0.3501848898
O	0	8.4898604832	0.4382309126	-0.8242465670
N	0	7.0971555245	-0.6305628232	0.6414859333
H	0	6.6921734118	-1.5193457039	0.9147363994
C	0	6.4890310996	0.5657782381	1.1844328677
H	0	6.7169427932	0.6742554528	2.2488024649
H	0	6.9148762641	1.4220158878	0.6522149163
C	0	4.9638564535	0.5910019254	1.0353793957
O	0	4.2877188135	1.0672015442	1.9602292406
O	0	4.5148415518	0.1122191520	-0.0768020329
C	-1	3.2965750105	3.6672830005	-5.1837029665
H	-1	3.3226420100	3.3639170004	-6.2198929665
H	-1	4.1022220116	4.3314059992	-4.9075739665
H	0	2.3855183809	4.2738827147	-5.0743524470
C	0	3.2666093658	2.5353436372	-4.1415270316
H	0	3.5924608995	2.9505004036	-3.1793786892
H	0	3.9832023894	1.7428126379	-4.3849434751
C	0	1.8655204715	1.9493918516	-3.9483306327
H	0	1.5961745130	1.3150405004	-4.8039540625
H	0	1.1170939961	2.7473446698	-3.9222362912
C	0	1.6903342915	1.1579520510	-2.6582273055
O	0	0.5710344874	1.2627234127	-2.0882479599
O	0	2.6706125057	0.4397602740	-2.2514981686
C	-1	5.2901690193	9.1473309973	-2.2661709665
H	-1	5.1519130186	8.7264269975	-3.2511219665
H	-1	6.3221770197	9.4083039956	-2.0839499665
H	0	4.7248231337	10.0872166360	-2.2337235147
C	0	4.7324290856	8.1619696270	-1.2261832356

H	0	3.6357532581	8.1737792612	-1.3011792645
H	0	4.9721143702	8.4960446474	-0.2079798856
C	0	5.2530200825	6.7327541637	-1.4351892773
H	0	6.3451432147	6.7248821091	-1.3262363791
H	0	5.0352435925	6.4052721527	-2.4611177511
C	0	4.6854020704	5.6960840996	-0.4608825990
H	0	4.8922082305	6.0011376314	0.5756947425
H	0	5.1778356858	4.7332849370	-0.6303447892
N	0	3.2477976614	5.4969684560	-0.6593190510
H	0	2.6860800038	6.3120942454	-0.8647808213
C	0	2.5700067341	4.4050770257	-0.2376647861
N	0	3.2039318883	3.4282652661	0.4186870034
H	0	2.7473223978	2.5083448296	0.5070089972
H	0	4.0293735374	3.5994710722	0.9719632188
N	0	1.2713816147	4.2766622945	-0.5008019038
H	0	0.8137212340	4.7135337271	-1.2954547410
H	0	0.7103873402	3.5092270286	-0.0775969653
C	-1	0.9288090024	-1.3684769957	-7.6563179665
H	-1	-0.0659369970	-0.9910619941	-7.4707049665
H	-1	1.1004120021	-1.5800829960	-8.7013729665
H	0	1.6600833709	-0.6216752885	-7.3285446161
C	0	1.1409789119	-2.7198395314	-6.9435292545
H	0	2.1125804474	-3.1363675688	-7.2433422252
H	0	0.3856420512	-3.4323067204	-7.2995793790
C	0	1.0945546097	-2.6870868587	-5.4491945951
N	0	0.9707317168	-3.8483451563	-4.6934922270
C	0	1.2131354952	-1.6773386942	-4.5337166708
H	0	1.3296296051	-0.6202396462	-4.6789664449
C	0	1.0135423725	-3.5576310919	-3.3867550397
H	0	0.9533044422	-4.2530908713	-2.5655160834
N	0	1.1666304349	-2.2407803238	-3.2734744954
H	0	1.1899164666	-1.7344333676	-2.3554655448
C	-1	-3.9185449856	6.1098570121	-2.4918649665
H	-1	-4.7924329848	6.5889880135	-2.0757309665
H	-1	-3.4717139847	6.6307260114	-3.3257949665
H	0	-3.1546350896	6.0938160510	-1.7052293878
C	0	-4.2490274028	4.6440782492	-2.8686836042
H	0	-5.1863561207	4.5791636045	-3.4312533750
H	0	-3.4406033067	4.2445817406	-3.4924709775
C	0	-4.3118470995	3.7677226417	-1.6115384332
O	0	-3.2473772783	3.6529341103	-0.9576635471
O	0	-5.4253727369	3.2324150760	-1.2802751440
C	-1	-12.0520939996	-2.6507769749	0.6645010335
H	-1	-13.1030599992	-2.4097009732	0.7257410335
H	-1	-11.8034800010	-3.5309929753	1.2387890335
H	0	-11.8550669701	-2.9258854568	-0.3818843086
C	0	-11.1811092926	-1.4337363439	1.0384842063
H	0	-11.6106746902	-0.9236507812	1.9129626019
H	0	-10.1780062398	-1.7692554202	1.3260406933
C	0	-11.0522585867	-0.4469948132	-0.1370121530
H	0	-10.3505169670	-0.8707339114	-0.8689073140
H	0	-12.0191619467	-0.3685750446	-0.6539057385
C	0	-10.6263903392	0.9804052133	0.2423142266
H	0	-10.5796948365	1.6036395442	-0.6613424558
H	0	-11.4021520726	1.4225296808	0.8820548598
C	0	-9.3094884518	1.1278692514	1.0027864176
H	0	-9.1722765140	2.1693650226	1.3071226707
H	0	-9.2919538478	0.5097398887	1.9040961918
N	0	-8.1010735697	0.7575776537	0.2021894545
H	0	-7.2624847596	1.1945112814	0.6515076716

H	0	-7.9571935351	-0.2792645909	0.1597788438
H	0	-8.1003768270	1.1525902748	-0.7667489899
O	0	-2.0874033224	1.4297206627	3.5516956038
H	0	-2.9675106398	1.8614469967	3.6338369500
O	0	-0.4786927198	2.3392067820	0.2159018031
O	0	-0.8603196167	3.8118583090	-2.4155513719
H	0	-0.4847110057	2.9392853977	-2.1939481632
H	0	-1.6520977741	3.8498794878	-1.8274219740
O	0	3.7303779478	-0.9339470689	3.9769479865
H	0	4.3826561164	-1.2969181517	3.3456040796
H	0	3.1437384609	-1.6985855389	4.1485396788
O	0	4.7697863515	-2.5692354041	1.9603174637
H	0	3.9362289034	-2.2148647863	1.5595572848
H	0	5.2209372902	-3.0450920056	1.2360367436
O	0	-2.4523275281	3.5230066035	1.7358267242
H	0	-2.8001124192	3.4654973979	0.8187058680
O	0	-6.1049567335	2.4118475468	1.1544624280
H	0	-5.6655949896	2.6804089178	0.2906821826
H	0	-6.5329495579	3.2291189645	1.4574598649
O	0	-4.4370070554	2.9798034226	3.3882211678
H	0	-4.9658737421	2.4744689234	2.7396000489
O	0	-7.5868859182	1.9830560574	-2.2813402877
H	0	-6.7993430457	2.5313140019	-2.0160055832
H	0	-7.2237092730	1.3228505597	-2.8916684504
O	0	-1.0050859270	1.4361138642	5.8839433275
H	0	-1.4939655981	0.6907766343	6.2685302963
H	0	0.8629948800	-4.7831426635	-5.0681018790
H	0	-3.7166631894	3.3388777436	2.7857919076
Cl	0	-7.5157451897	-2.3225510015	0.2908491826
H	0	-1.4214851724	1.5294134119	4.9530267955
O	0	1.0926236781	0.0900212321	4.9079883610
H	0	0.3783963795	0.6816938667	5.2756290194
H	0	1.1393373491	-2.6792104247	5.5074210907
O	0	0.7748662593	-2.3403228980	6.3562083677
H	0	1.0101898311	-0.7404080161	5.4227015401
H	0	-0.1822272036	-2.4767590855	6.2662144779

3L_S3d
E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.956975 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.39291 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.630948 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.78953 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.71523 au

Mn	0	1.09650800	2.19964800	-1.87625600
Mn	0	-0.88720900	-2.56381800	-0.75520100
Mn	0	-0.20725900	0.84326100	0.12162900
Mn	0	-2.83563900	-0.49092400	0.29314600
O	0	0.16607600	0.60466400	-1.60313900
O	0	-2.01931500	0.98551800	-0.35060900
O	0	-2.22035900	-1.58195700	-1.37347100
O	0	-0.78464000	-1.14198000	0.61253400
Ca	0	-2.02141200	0.45184300	-2.74560500
C	-1	0.52204300	4.65683000	-5.58396800
H	-1	0.58425100	5.58907400	-5.04188900
H	-1	0.71033900	4.73820200	-6.64415900
H	0	1.31832100	4.02179200	-5.17663700
C	0	-0.82563700	3.94797000	-5.35019800
H	0	-0.95793700	3.13347700	-6.07352300
H	0	-1.67282400	4.62775600	-5.51598800
C	0	-0.99949000	3.30866600	-3.96537700

O	0	-1.98459700	2.52388900	-3.80426300
O	0	-0.14790600	3.58303100	-3.07104200
C	-1	-2.90450500	-6.61323100	-5.36651200
H	-1	-1.94270200	-7.07276300	-5.53990300
H	-1	-3.63670600	-6.75445200	-6.14778400
H	0	-3.31449300	-7.14542400	-4.49435000
C	0	-2.62924200	-5.16580100	-4.95141800
H	0	-3.50783000	-4.70808500	-4.47990600
H	0	-2.35713800	-4.53907500	-5.80806200
C	0	-1.45977600	-5.20974200	-3.95315600
H	0	-0.53764100	-5.47764800	-4.48722400
H	0	-1.63802800	-5.98132100	-3.19809300
C	0	-1.20963600	-3.89751700	-3.25526800
O	0	-1.05667500	-2.84819800	-3.91255300
O	0	-1.17256800	-4.00451900	-1.96287100
C	-1	5.08552400	-4.56082400	0.96212400
H	0	5.97452600	-5.19432500	1.07726500
H	0	5.23620300	-3.96617300	0.05741300
C	0	4.98747900	-3.64658600	2.18430700
O	0	4.48679500	-4.05010000	3.25490200
C	0	3.84933100	-5.48637700	0.80468900
H	0	3.80971700	-6.16585600	1.66448200
H	0	3.97830100	-6.09811500	-0.09244300
C	0	2.56622300	-4.71815900	0.71186200
N	0	2.22472600	-3.87281600	1.75306500
H	0	2.76294400	-3.79859600	2.61593400
C	0	1.59174400	-4.51586300	-0.23882100
H	0	1.47347800	-4.95753700	-1.21629400
C	0	1.14265100	-3.16979200	1.40846800
H	0	0.73274900	-2.39900400	2.02522000
N	0	0.69883700	-3.55527700	0.22182100
N	0	5.38214000	-2.37564100	1.99805700
H	0	5.88500600	-2.15475900	1.13405800
C	-1	5.04772000	-1.29324900	2.92076700
H	0	5.90169000	-0.60553300	2.96326800
H	0	4.90978200	-1.72648300	3.91343200
C	0	3.77784200	-0.54584600	2.46995400
H	0	3.50343900	0.19320700	3.23323000
H	0	2.95018300	-1.25811300	2.40914500
C	0	3.96625600	0.13929600	1.11615700
H	0	4.45593700	-0.54205200	0.40770600
H	0	4.62810500	1.00964100	1.20064100
C	0	2.71582700	0.61845100	0.38760700
O	0	2.90642600	1.19124100	-0.71249900
O	0	1.57221000	0.36238200	0.90709100
C	-1	-5.42007500	-3.96187100	2.21238100
H	0	-5.26664300	-3.21320300	2.99608800
H	0	-5.92429100	-4.82123900	2.67142200
C	0	-4.08229400	-4.41270800	1.62377000
H	0	-4.24087700	-5.15830000	0.83870600
H	0	-3.47686300	-4.89620000	2.39691700
C	0	-3.24181400	-3.29889400	1.00851400
O	0	-3.68121600	-2.11322000	1.08507300
O	0	-2.14990800	-3.65046000	0.47059800
C	0	-6.33998300	-3.40190000	1.12875000
O	0	-6.19793300	-3.67517800	-0.07419600
N	0	-7.36753400	-2.64095900	1.56589300
H	0	-7.39271800	-2.35867900	2.53611600
C	-1	-8.40325200	-2.13141800	0.67411800
H	0	-9.29880200	-1.93079800	1.26303900

H	0	-8.62344700	-2.90402000	-0.06824400
C	0	-8.00351000	-0.81546000	-0.02391400
O	0	-8.44515900	0.26979000	0.35376600
N	0	-7.16773100	-0.97691700	-1.08105000
H	0	-6.73768800	-1.88839600	-1.19926800
C	0	-6.56668700	0.13846800	-1.78150700
H	0	-6.64262000	-0.00409600	-2.86276700
H	0	-7.12657800	1.03961400	-1.51375100
C	0	-5.08671600	0.35736500	-1.43494800
O	0	-4.34824500	0.85631100	-2.31328200
O	0	-4.72930900	0.01631900	-0.25723000
C	-1	-3.42268600	3.65677500	5.01358400
H	-1	-3.44943000	3.35634100	6.05058700
H	-1	-4.24211400	4.29985400	4.72863700
H	0	-2.51842000	4.27469100	4.90715400
C	0	-3.36887400	2.52949900	3.97892900
H	0	-3.48954600	2.98710100	2.98810300
H	0	-4.21123800	1.83852200	4.09424000
C	0	-2.04849600	1.74616900	3.99170000
H	0	-2.06155700	1.00748200	4.80153600
H	0	-1.20031200	2.41522500	4.16316500
C	0	-1.83174500	1.03346300	2.66818100
O	0	-0.71210400	1.22416800	2.09131800
O	0	-2.77689900	0.31927000	2.22330900
C	-1	-5.52859400	9.07589900	2.06148500
H	-1	-5.38794200	8.66189000	3.04896300
H	-1	-6.56516700	9.31058300	1.86987700
H	0	-4.97054600	10.01848500	2.01048800
C	0	-4.98547600	8.06747000	1.04079100
H	0	-3.89253000	8.02708800	1.15071500
H	0	-5.17308000	8.40672300	0.01369900
C	0	-5.59599900	6.67201900	1.24183800
H	0	-6.66683600	6.70514800	1.00673900
H	0	-5.51302300	6.37944100	2.29764100
C	0	-4.95622100	5.57571000	0.38850200
H	0	-5.01916900	5.83889100	-0.67785200
H	0	-5.49313200	4.63266300	0.53654700
N	0	-3.56283200	5.37174200	0.78646100
H	0	-3.05446900	6.18135500	1.11461000
C	0	-2.80333900	4.32674400	0.39427300
N	0	-3.30110700	3.37398800	-0.39458800
H	0	-2.81926100	2.45701100	-0.45156300
H	0	-4.15114200	3.50367100	-0.92090400
N	0	-1.54394200	4.22785400	0.81973400
H	0	-1.19281400	4.71515500	1.63340000
H	0	-0.88950500	3.54513700	0.39202000
C	-1	-0.94990400	-1.30996300	7.52229300
H	-1	0.03671100	-0.90832000	7.34393800
H	-1	-1.12466000	-1.52261000	8.56677000
H	0	-1.70228600	-0.59850600	7.16649100
C	0	-1.12492700	-2.69442200	6.87892700
H	0	-2.08158800	-3.12108900	7.21412400
H	0	-0.34753000	-3.36747300	7.26871000
C	0	-1.09189000	-2.70043800	5.39466700
N	0	-1.25155500	-3.86110600	4.66080400
C	0	-0.94943200	-1.70840200	4.45686900
H	0	-0.76894800	-0.65876500	4.62046500
C	0	-1.20288700	-3.53994900	3.34425500
H	0	-1.24905500	-4.26660500	2.54955600
N	0	-1.03085700	-2.23805500	3.18643400

H	0	-0.79329500	-1.43647200	1.56714800
C	-1	3.75107500	6.27156600	2.37339600
H	-1	4.61635700	6.77115300	1.96284800
H	-1	3.28474900	6.78372900	3.20188400
H	0	2.99123200	6.25987200	1.58283400
C	0	4.09268200	4.80083100	2.71476200
H	0	5.04492800	4.71774500	3.24847500
H	0	3.29866100	4.38222700	3.34413300
C	0	4.11760300	3.97152600	1.42831300
O	0	3.02798300	3.91805500	0.79708800
O	0	5.20008200	3.42245900	1.04312700
C	-1	12.12814500	-2.29178600	-0.68651900
H	-1	13.17323600	-2.02458300	-0.73985800
H	-1	11.90655400	-3.17977200	-1.25988300
H	0	11.92645500	-2.56468700	0.35928400
C	0	11.20977700	-1.11534200	-1.09258200
H	0	11.65547600	-0.57221100	-1.93856800
H	0	10.24615100	-1.50619200	-1.43989700
C	0	10.94749000	-0.14462900	0.07445200
H	0	10.23611200	-0.61660200	0.76629800
H	0	11.87657500	-0.00093600	0.64399800
C	0	10.44891300	1.25446400	-0.32839600
H	0	10.33603400	1.87686600	0.57002600
H	0	11.22112200	1.73822600	-0.94179000
C	0	9.15245600	1.33568500	-1.13682800
H	0	8.99531200	2.36388100	-1.47498400
H	0	9.18304000	0.69196200	-2.01964000
N	0	7.92949200	0.94982100	-0.36314500
H	0	7.08388200	1.32757300	-0.84362300
H	0	7.82704700	-0.09384300	-0.29865900
H	0	7.89254900	1.37100400	0.59483600
O	0	1.82753000	1.48602400	-3.52034600
H	0	3.31491700	2.38154000	-3.70564400
O	0	0.28482900	2.50706000	-0.17090600
O	0	0.79687200	3.68690400	2.55527500
H	0	0.39548300	2.82211600	2.34915100
H	0	1.46871500	3.79439600	1.84645100
O	0	-3.21249500	-1.13581500	-4.21328300
H	0	-3.91541500	-1.54855700	-3.67126300
H	0	-2.52950900	-1.83856300	-4.27928100
O	0	-4.44870100	-2.79032800	-2.23942800
H	0	-3.61046400	-2.43905500	-1.83719500
H	0	-4.94963700	-3.16368200	-1.49026800
O	0	2.33456000	3.84909900	-1.72215200
H	0	2.72436700	3.79413100	-0.79726800
O	0	5.81381900	2.51159700	-1.39535600
H	0	5.36993400	2.76848100	-0.53346600
H	0	6.30330900	3.31561900	-1.63798600
O	0	4.07695400	3.00434900	-3.55012200
H	0	4.62822400	2.56748000	-2.86382200
O	0	7.39539700	2.25619100	2.06740200
H	0	6.59137500	2.77647000	1.79700200
H	0	7.07469600	1.64752000	2.75048900
O	0	2.90255200	-0.93699400	-2.49685300
H	0	2.21753100	0.61446100	-3.26937200
H	0	-1.37484900	-4.78958400	5.04162100
H	0	3.07305800	3.70744700	-2.38357700
Cl	0	7.49441700	-2.12465200	-0.46700500
H	0	3.17083900	-0.25913900	-1.84599100
O	0	-0.32710200	0.07009300	-4.46261200

H	0	-0.02397700	-0.83433900	-4.64086200
O	0	0.44674400	-1.98957400	-1.81129500
H	0	2.05157200	-1.26511100	-2.12511800
H	0	0.01748400	-1.78661700	-2.66491400
H	0	0.47949900	0.60508100	-4.20078000

7L_S3d

E (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5854.953325 au
H (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.389478 au
G (IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.628796 au
E (IEFPCM/B3LYP-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5856.785923 au
E (IEFPCM/B3LYP*-D3/SDD,6-311+G(2d,p)//IEFPCM/B3LYP-D3/SDD,6-31G(d)) = -5853.711141 au

Mn	0	1.09158600	2.21377800	-1.86555400
Mn	0	-0.88377800	-2.56629400	-0.76109400
Mn	0	-0.20424200	0.83908600	0.12649600
Mn	0	-2.83163600	-0.49736800	0.29211100
O	0	0.16871600	0.60509100	-1.60997600
O	0	-2.01291400	0.98265200	-0.34452200
O	0	-2.21706600	-1.57984300	-1.37469000
O	0	-0.77796800	-1.15026400	0.61075700
Ca	0	-2.01183700	0.46749200	-2.74178500
C	-1	0.52216100	4.67005700	-5.57197000
H	-1	0.58378100	5.60094100	-5.02749300
H	-1	0.71063800	4.75423700	-6.63191000
H	0	1.31826700	4.03337700	-5.16617100
C	0	-0.82592700	3.96106200	-5.34060800
H	0	-0.95403800	3.14257700	-6.06012200
H	0	-1.67243000	4.63977300	-5.51464800
C	0	-1.00644600	3.32981600	-3.95247000
O	0	-1.99028100	2.54141600	-3.79424200
O	0	-0.16439700	3.61282200	-3.05275300
C	-1	-2.89872300	-6.60225700	-5.38408600
H	-1	-1.93665100	-7.06085700	-5.55844900
H	-1	-3.63068800	-6.74184800	-6.16587200
H	0	-3.30848600	-7.13643200	-4.51306700
C	0	-2.62455000	-5.15534600	-4.96623000
H	0	-3.50288200	-4.69994900	-4.49202500
H	0	-2.35494200	-4.52634800	-5.82199900
C	0	-1.45303400	-5.20012800	-3.97027500
H	0	-0.53128600	-5.46343300	-4.50721300
H	0	-1.62811400	-5.97514600	-3.21804200
C	0	-1.20507100	-3.89041800	-3.26721400
O	0	-1.04881700	-2.83883900	-3.92037700
O	0	-1.17262400	-4.00166700	-1.97491700
C	-1	5.08893000	-4.56201100	0.95147800
H	0	5.97960800	-5.19329000	1.06617300
H	0	5.23968700	-3.96448700	0.04865500
C	0	4.98708000	-3.65101700	2.17588200
O	0	4.48162300	-4.05660300	3.24337000
C	0	3.85568800	-5.49030300	0.78941700
H	0	3.81697200	-6.17278000	1.64687300
H	0	3.98693300	-6.09865600	-0.10968200
C	0	2.57112900	-4.72448800	0.69878700
N	0	2.22863800	-3.88340700	1.74301700
H	0	2.76784700	-3.81056600	2.60539800
C	0	1.59676300	-4.51964800	-0.25153700
H	0	1.47977000	-4.95750700	-1.23089100
C	0	1.14527000	-3.18098800	1.40105200
H	0	0.73384700	-2.41342500	2.02078200
N	0	0.70215900	-3.56256800	0.21292400

N	0	5.38563900	-2.38044500	1.99482200
H	0	5.89000300	-2.15773600	1.13216600
C	-1	5.04905700	-1.29947900	2.91846900
H	0	5.90296800	-0.61195200	2.96448300
H	0	4.90841900	-1.73446000	3.90998200
C	0	3.77986100	-0.55165800	2.46558200
H	0	3.50356000	0.18633500	3.22919100
H	0	2.95269900	-1.26435800	2.40240700
C	0	3.96902400	0.13587600	1.11274900
H	0	4.45604400	-0.54547700	0.40248100
H	0	4.63313800	1.00437900	1.19835500
C	0	2.71839200	0.61883000	0.38708200
O	0	2.90571300	1.20205200	-0.70794800
O	0	1.57485200	0.35471400	0.90348900
C	-1	-5.41723500	-3.97157700	2.20103400
H	0	-5.26418200	-3.22453000	2.98638600
H	0	-5.92117800	-4.83208000	2.65825200
C	0	-4.07926600	-4.42068000	1.61179900
H	0	-4.23713100	-5.16425500	0.82469100
H	0	-3.47435200	-4.90605000	2.38416100
C	0	-3.23799900	-3.30564300	0.99995900
O	0	-3.67624800	-2.11963500	1.08030100
O	0	-2.14626000	-3.65606500	0.46140000
C	0	-6.33730400	-3.40969900	1.11861000
O	0	-6.19516100	-3.68064300	-0.08483000
N	0	-7.36531000	-2.65034500	1.55752300
H	0	-7.39075700	-2.37059500	2.52846700
C	-1	-8.40101400	-2.13870300	0.66682700
H	0	-9.29674500	-1.93995800	1.25609000
H	0	-8.62074900	-2.90928800	-0.07776000
C	0	-8.00115400	-0.82056500	-0.02706400
O	0	-8.44390200	0.26332500	0.35322200
N	0	-7.16327400	-0.97839900	-1.08308700
H	0	-6.73252000	-1.88926600	-1.20333900
C	0	-6.56169100	0.13948000	-1.77917800
H	0	-6.63574100	-0.00004900	-2.86095300
H	0	-7.12269100	1.03943100	-1.50975100
C	0	-5.08233700	0.35866300	-1.42974800
O	0	-4.34326900	0.86111300	-2.30532200
O	0	-4.72611000	0.01470400	-0.25235900
C	-1	-3.42429700	3.64088400	5.02215000
H	-1	-3.45110700	3.33778400	6.05837500
H	-1	-4.24399000	4.28427600	4.73867600
H	0	-2.52034700	4.25953700	4.91737800
C	0	-3.36936100	2.51550300	3.98526000
H	0	-3.49080700	2.97431300	2.99518200
H	0	-4.21064400	1.82308700	4.09977100
C	0	-2.04770900	1.73428900	3.99608000
H	0	-2.05817400	0.99533000	4.80577600
H	0	-1.20048800	2.40469900	4.16686300
C	0	-1.82973500	1.02226800	2.67222600
O	0	-0.70736600	1.21017500	2.09922600
O	0	-2.77527900	0.31093700	2.22370900
C	-1	-5.53232800	9.06648000	2.08348300
H	-1	-5.39167400	8.65001600	3.06992800
H	-1	-6.56897800	9.30112900	1.89225700
H	0	-4.97527400	10.00990600	2.03609200
C	0	-4.98787500	8.06335900	1.05855600
H	0	-3.89532400	8.02097400	1.17164000
H	0	-5.17194700	8.40956100	0.03312200

C	0	-5.60093800	6.66759100	1.24853400
H	0	-6.67118800	6.70422800	1.01116100
H	0	-5.52063400	6.36741800	2.30238100
C	0	-4.96057900	5.57654500	0.38867900
H	0	-5.02231100	5.84625200	-0.67610100
H	0	-5.49769300	4.63266600	0.52997900
N	0	-3.56813300	5.36911700	0.78715200
H	0	-3.05623400	6.17784500	1.11174500
C	0	-2.81412000	4.31537200	0.40831200
N	0	-3.31521700	3.35964700	-0.37491900
H	0	-2.82796300	2.44649700	-0.43722700
H	0	-4.14984700	3.49836200	-0.92323300
N	0	-1.56013300	4.20704900	0.84642700
H	0	-1.20786900	4.71074000	1.64929200
H	0	-0.89985300	3.52976000	0.41653600
C	-1	-0.94952800	-1.33100600	7.51866500
H	-1	0.03692100	-0.92840900	7.34154700
H	-1	-1.12439700	-1.54641400	8.56255600
H	0	-1.70224500	-0.61909300	7.16448900
C	0	-1.12474800	-2.71442200	6.87315500
H	0	-2.08132100	-3.14128600	7.20836000
H	0	-0.34729500	-3.38823500	7.26153400
C	0	-1.09255200	-2.71819500	5.38908200
N	0	-1.25346700	-3.87741100	4.65342200
C	0	-0.94852600	-1.72469900	4.45305900
H	0	-0.76693200	-0.67557500	4.61854600
C	0	-1.20387400	-3.55415700	3.33744300
H	0	-1.25013500	-4.27965800	2.54171100
N	0	-1.03007800	-2.25223000	3.18178600
H	0	-0.78656900	-1.44732800	1.56462100
C	-1	3.74869500	6.26605400	2.39018600
H	-1	4.61381100	6.76712900	1.98110100
H	-1	3.28193500	6.77585900	3.21988200
H	0	2.98884500	6.25863700	1.59959500
C	0	4.08966400	4.79331700	2.72251600
H	0	5.04271200	4.70554500	3.25405000
H	0	3.29626600	4.37098500	3.35017200
C	0	4.11170100	3.97309300	1.42995700
O	0	3.02302600	3.93383600	0.79612900
O	0	5.19047500	3.41822800	1.04302400
C	-1	12.13074800	-2.28519700	-0.68985800
H	-1	13.17571500	-2.01732900	-0.74229100
H	-1	11.90972700	-3.17182500	-1.26554000
H	0	11.92894400	-2.56097900	0.35513400
C	0	11.21166200	-1.10803300	-1.09338200
H	0	11.66099100	-0.55814800	-1.93305100
H	0	10.25111500	-1.49877900	-1.44916800
C	0	10.93992000	-0.14568100	0.07855100
H	0	10.22527100	-0.62389200	0.76266200
H	0	11.86524800	-0.00397400	0.65466100
C	0	10.44130000	1.25534900	-0.31775600
H	0	10.32387400	1.87201200	0.58403900
H	0	11.21579800	1.74375200	-0.92454600
C	0	9.14819700	1.34088200	-1.13135100
H	0	8.99316100	2.37067800	-1.46556300
H	0	9.18191200	0.70098600	-2.01682600
N	0	7.92182500	0.95258600	-0.36412100
H	0	7.07789000	1.33082400	-0.84687100
H	0	7.81975600	-0.09133200	-0.30326100
H	0	7.88111800	1.37073300	0.59510700

```
O      0    1.81759900    1.52239600   -3.51322700
H      0    3.30683000    2.41252000   -3.70420400
O      0    0.28807200    2.51470100   -0.14703100
O      0    0.79898300    3.68310100    2.56564000
H      0    0.39626800    2.82083600    2.35229500
H      0    1.46363000    3.79754400    1.85137200
O      0   -3.20299700   -1.11970800   -4.20983100
H      0   -3.90842200   -1.53278900   -3.67154700
H      0   -2.52187500   -1.82393900   -4.27729200
O      0   -4.44301600   -2.78843700   -2.24825200
H      0   -3.60499900   -2.43742900   -1.84552400
H      0   -4.94443400   -3.16089600   -1.49895300
O      0    2.32010100    3.85607100   -1.71423000
H      0    2.71312500    3.80264900   -0.78950400
O      0    5.80660000    2.51832600   -1.39998000
H      0    5.36124400    2.77012800   -0.53749900
H      0    6.30031400    3.32233300   -1.63411100
O      0    4.06624600    3.03744500   -3.54501000
H      0    4.62189500    2.59682600   -2.86440100
O      0    7.38194500    2.24996800    2.06954600
H      0    6.57910500    2.77206700    1.79852400
H      0    7.05932600    1.64092900    2.75139600
O      0    2.88517300   -0.90516300   -2.51689300
H      0    2.20546000    0.64631100   -3.27066600
H      0   -1.37786300   -4.80637400    5.03268800
H      0    3.05830000    3.72215900   -2.37861300
Cl     0    7.50258600   -2.12444500   -0.46570000
H      0    3.16261000   -0.23840600   -1.85835800
O      0   -0.32779600    0.09950400   -4.47291700
H      0   -0.01671200   -0.80355700   -4.64449300
O      0    0.44786600   -1.98931100   -1.81692100
H      0    2.03596800   -1.23513400   -2.14157100
H      0    0.01630900   -1.79393400   -2.67162600
H      0    0.47345900    0.63928000   -4.20678100
```

Additional references

1) M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman,

G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J.

Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov,

J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A.

Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W.

Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y.

Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery Jr., J. E. Peralta, F.

Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith,

R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J.

Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, D. J. Fox, *Gaussian 16*, Revision B.01, Gaussian, Inc., Wallingford CT **2016**.

2) a) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785–789; b) A. D. Becke, *J. Chem. Phys.* **1992**, *96*, 2155–2160; c) A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648–5652.

3) a) M. Cossi, V. Barone, B. Mennucci, J. Tomasi, *Chem. Phys. Lett.* **1998**, *286*, 253−260; b) E. Cances, B. Mennucci, J. Tomasi, *J. Chem. Phys.* **1997**, *107*, 3032−3041; c) B. Mennucci, J. Tomasi, *J. Chem. Phys.* **1997**, *106*, 5151−5158.

4) S. Grimme, *J. Comput. Chem.* **2006**, *27*, 1787–1799.

5) a) A. Bergner, M. Dolg, W. Küchle, H. Stoll, H. Preuß, *Mol. Phys.* **1993**, *80*, 1431−1441; b) M. Dolg, U. Wedig, H. Stoll, H. Preuss, *J. Chem. Phys.* **1987**, *86*, 866−872.

6) K. Fukui, *Acc. Chem. Res.* **1981**, *14*, 363–368.

7) M. Amin, D. Kaur, M. R. Gunner, G. Brudvig, *Inorg. Chem. Commun.* **2021**, *133*, 108890.

8) a) M. Reiher, O. Salomon and B. Artur Hess, *Theor. Chem. Acc.* **2001**, *107*, 48-55; b) O. Salomon, M. Reiher and B. A. Hess, *J. Chem. Phys.* **2002**, *117*, 4729-4737; c) P. E. M. Siegbahn, *J. Biol. Inorg. Chem.* **2006**, *11*, 695–701.

9) P. E. M. Siegbahn and M. R. A. Blomberg, *J. Chem. Theory Comput.* **2014**, *10*, 268-272.

10) a) L. Noodleman, T. Lovell, W.-G. Han, J. Li, F. Himo, *Chem. Rev.* **2004**, *104*, 459–508; b) L. Noodleman, *J. Chem. Phys.* **1981**, *74*, 5737–5743; c) L. Noodleman, D. A. Case, *Adv. Inorg. Chem.* **1992**, *38*, 423–470.

11) Y.-T. Song, X.-C. Li, P. E. M. Siegbahn, *J. Phys. Chem. B* **2023**, *127*, 6643–6647.

12) Y. Umena, K. Kawakami, J.-R. Shen, N. Kamiya, *Nature* **2011**, *473*, 55−60.