

Supporting Information to:

***On the Effect of Varying Constraints in the QM-Only Modeling of
Enzymatic Reactions: the Case of Acetylene Hydratase***

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Table S1. Resolution and DPI values for 109 published protein structures.

Protein name	Resolution (Å)	DPI (Å)	Reference
Lysozyme	0.65	0.005	1
Crambin	0.83	0.021	2
Concanavalin A	0.94	0.034	2
Rubredoxin	1.00	0.049	2
Cytochrome c6	1.10	0.066	2
Ribonuclease MGMP	1.15	0.047	2
Ribonuclease MSA	1.20	0.045	2
Trypsin	1.20	0.027	1
Subtilisin Carlsberg	1.26	0.033	1
cMyBP-C	1.30	0.063	1
Plastocyanin, 295K	1.33	0.11	2
HEW lysozyme (ground-grown)	1.33	0.11	2
HEW lysozyme (space-grown)	1.40	0.12	2
γB-crystallin	1.49	0.14	2
Plastocyanin, 173K, Sydney	1.60	0.21	2
Immunoglobulin	1.70	0.22	2
β-purothionin	1.70	0.22	2
TGF-β2, 1TGI	1.80	0.16	2
Cd-azurin	1.80	0.21	2
EM lysozyme	1.90	0.28	2
Azurin II	1.90	0.23	2
TGF-β2, 1TFG	1.95	0.24	2
βB2-crystallin	2.10	0.22	2
Lactoferrin	2.20	0.43	2
α ₁ -purothionin	2.50	0.68	2
Ribonuclease A with RI	2.50	0.69	2
Rhodopsin kinase	2.50	0.30	3
Fab HyHEL-5 with HEWL	2.65	0.69	2
Turkey egg lysozyme	1.12	0.031	4
Human lysozyme	1.15	0.034	4
Dethiobiotin synthetase	0.97	0.022	5
Hen egg-white lysozyme	0.94	0.024	6
Human α-lactalbumin	1.15	0.038	7
Tyrosine phenol-lyase	2.04	0.15	8
Tyrosine phenol-lyase	2.00	0.12	8
Tyrosine phenol-lyase	2.25	0.16	8
Photosystem II	1.9	0.11	9
Azurin	1.35	0.06	10
Geranylgeranyl reductase	1.6	0.07	11
MenD	2.35	0.23	12
Glutamine synthetase adenylyl transferase	2.4	0.24	13

Subtilisin	2.3	0.39	14
SsgB	2.6	0.31	15
Trypanosomatid mitochondrial cytochrome c	1.55	0.09	16
MenD	2.5	0.34	17
MenD	2.8	0.35	17
S-adenosyl-l-homocysteine hydrolase	1.60	0.10	18
S-adenosyl-l-homocysteine hydrolase	2.00	0.22	18
S-adenosyl-l-homocysteine hydrolase	2.01	0.23	18
S-adenosyl-l-homocysteine hydrolase	2.20	0.27	18
S-adenosyl-l-homocysteine hydrolase	2.42	0.35	18
EsxA	1.4	0.07	19
EsxA	1.9	0.20	19
IspE	2.1	0.2	20
IspE	2.25	0.23	20
IspE	2.3	0.25	20
HpcH	1.6	0.08	21
HpcH	2.2	0.12	21
Oxalate decarboxylase	2.0	0.103	22
Oxalate decarboxylase	2.1	0.130	22
Oxalate decarboxylase	2.8	0.297	22
Oxalate decarboxylase	3.1	0.383	22
5-methylthioribose kinase	2.0	0.18	23
5-methylthioribose kinase	2.1	0.19	23
5-methylthioribose kinase	2.2	0.21	23
5-methylthioribose kinase	2.3	0.24	23
5-methylthioribose kinase	2.6	0.35	23
Thioredoxin ResA	1.95	0.1501	24
Thioredoxin ResA	2.0	0.1750	24
Thioredoxin ResA	2.4	0.2691	24
Thioredoxin ResA	2.6	0.3633	24
Thioredoxin ResA	3.1	0.5338	24
Uroporphyrinogen-III decarboxylase	2.3	0.35	25
Stellacyanin	1.8	0.17	26
Stellacyanin	1.9	0.21	26
Copper amine oxidase	2.43	0.32	27
rRNA methyltransferase	1.6	0.088	28
rRNA methyltransferase	1.8	0.127	28
rRNA methyltransferase	1.9	0.149	28
rRNA methyltransferase	2.2	0.27	28
Ketosteroid isomerase	1.1	0.03	29
Ketosteroid isomerase	1.3	0.05	29
glycerophosphodiesterase	1.9	0.12	30
ferredoxin	1.5	0.1	31
DHC2 diheme cytochrome c	1.5	0.107	32

Aminopeptidase P	1.9	0.09	33
Aminopeptidase P	2.1	0.12	33
Aminopeptidase P	2.0	0.1	33
Aminopeptidase P	2.4	0.21	33
Aminopeptidase P	2.4	0.16	33
Aminopeptidase P	2.4	0.16	33
Aminopeptidase P	2.5	0.18	33
Aminopeptidase P	2.4	0.15	33
Aminopeptidase P	2.4	0.16	33
Aminopeptidase P	2.4	0.15	33
Aminopeptidase P	2.3	0.17	33
Aminopeptidase P	2.0	0.10	33
Aminopeptidase P	1.7	0.06	34
Aminopeptidase P	1.7	0.06	34
Aminopeptidase P	1.75	0.07	34
Aminopeptidase P	2.2	0.12	34
Aminopeptidase P	2.4	0.17	34
Aminopeptidase P	2.6	0.21	34
Aminopeptidase P	2.9	0.36	34
Nitrite reductase	1.85	0.150	35
Nitrite reductase	1.90	0.182	35
Alcohol dehydrogenase	1.0	0.07	36
Alcohol dehydrogenase	1.2	0.03	36
Nitrogenase	1.16	0.027	37

Table S2. Resolution and coordinate error of main chain and of all atoms for 8 protein structures.

Protein name	Resolution (Å)	Coordinate error (Å) of main chain	Coordinate error (Å) of all atoms	References
Crambin	0.83	0.0096	0.021	38
βB2-crystallin	2.10	0.08	0.15	39
γB-crystallin	1.49	0.05	0.10	39
Turkey egg lysozyme	1.12	0.014	0.031	4
Human lysozyme	1.15	0.015	0.034	4
Dethiobiotin synthetase	0.97	0.017	0.022	5
Hen egg-white lysozyme	0.94	0.013	0.024	6
Human α-lactalbumin	1.15	0.017	0.038	7

References

1. Fisher, S. J.; Blakeley, M. P.; Cianci, M.; McSweeney, S.; Helliwell, J. R. Protonation-state Determination in Proteins Using High-resolution X-ray Crystallography: Effects of Resolution and Completeness. *Acta Crystallogr., Sect. D: Biol. Crystallogr.* **2012**, *D68*, 800-809.
2. Cruickshank, D. W. Remarks about Protein Structure Precision. *Acta Crystallogr.* **1999**, *D55*, 583-601.
3. Tesmer, J. J. G.; Nance, M. R.; Singh, P.; Lee, H. Structure of a Monomeric Variant of Rhodopsin Kinase at 2.5 Å Resolution. *Acta Crystallogr., Sect. F: Struct. Biol. Cryst. Commun.* **2012**, *F68*, 622-625.
4. Harata, K.; Abe, Y.; Muraki, M. Full-matrix Least-squares Refinement of Lysozymes and Analysis of Anisotropic Thermal Motion. *Proteins Struct. Funct. Genet.* **1998**, *30*, 232-243.
5. Sandalova, T.; Schneider, G.; Käck, H.; Lindqvist, Y. Structure of Dethiobiotin Synthetase at 0.97 Å Resolution. *Acta Crystallogr., Sect. D: Biol. Crystallogr.* **1999**, *D55*, 610-624.
6. Sauter, C.; Otálora, F.; Gavira, J.-A.; Vidal, O.; Giegé, R.; Garcia-Ruiz, J. M. Structure of Tetragonal Hen Egg-white Lysozyme at 0.94 Å from Crystals Grown by the Counter-diffusion Method. *Acta Crystallogr., Sect. D: Biol. Crystallogr.* **2001**, *D57*, 1119-1126.
7. Harata, K.; Abe, Y.; Muraki, M. Crystallographic Evaluation of Internal Motion of Human α -lactalbumin Refined by Full-matrix Least-squares Method. *J. Mol. Biol.* **1999**, *287*, 347-358.
8. Milić, D.; Demidkina, T. V.; Faleev, N. G.; Phillips, R. S.; Matković-Čalogović, D.; Antson, A. A. Crystallographic Snapshots of Tyrosine Phenol-lyase Show That Substrate Strain Plays a Role in C–C Bond Cleavage. *J. Am. Chem. Soc.* **2011**, *133*, 16468-16476.
9. Umena, Y.; Kawakami, K.; Shen, J.-R.; Kamiya, N. Crystal Structure of Oxygen-evolving Photosystem II at a Resolution of 1.9 Å. *Nature* **2011**, *473*,

55-61.

10. Alagaratnam, S.; Meeuwenoord, N. J.; Navarro, J. A. Hervás, M.; De la Rosa, M. A.; Hoffmann, M.; Einsle, O.; Ubbink, M.; Canters, G. W. Probing the Reactivity of Different Forms of Azurin by Flavin Photoreduction. *FEBS J.* **2011**, 278, 1506-1521.
11. Xu, Q.; Eguchi, T.; Mathews, I. I.; Rife, C. L.; Chiu, H.-J.; Farr, C. L.; Feuerhelm, J.; Jaroszewski, L.; Klock, H. E.; Knuth, M. W.; Miller, M. D.; Weekes, D.; Elsliger, M.-A.; Deacon, A. M.; Godzik, A.; Lesley, S. A.; Wilson, I. A. Insights into Substrate Specificity of Geranylgeranyl Reductases Revealed by the Structure of Digeranylgeranylglycerophospholipid Reductase, an Essential Enzyme in the Biosynthesis of Archaeal Membrane Lipids. *J. Mol. Biol.* **2010**, 404, 403-417.
12. Dawson, A.; Chen, M.; Fyfe, P. K.; Guo, Z.; Hunter, W. N. Structure and Reactivity of *Bacillus subtilis* MenD Catalyzing the First Committed Step in Menaquinone Biosynthesis. *J. Mol. Biol.* **2010**, 401, 253-264.
13. Xu, Y.; Carr, P. D.; Vasudevan, S. G.; Ollis, D. L. Structure of the Adenylylation Domain of *E. coli* Glutamine Synthetase Adenylyl Transferase: Evidence for Gene Duplication and Evolution of a New Active Site. *J. Mol. Biol.* **2010**, 396, 773-784.
14. Cianci, M.; Tomaszweski, B.; Helliwell, J. R.; Halling, P. J. Crystallographic Analysis of Counterion Effects on Subtilisin Enzymatic Action in Acetonitrile. *J. Am. Chem. Soc.* **2010**, 132, 2293-2300.
15. Xu, Q.; Traag, B. A.; Willemse, J.; McMullan, D.; Miller, M. D.; Elsliger, M.-A.; Abdubek, P.; Astakhova, T.; Axelrod, H. L.; Bakolitsa, C. et. Al. Structural and Functional Characterizations of SsgB, a Conserved Activator of Developmental Cell Division in Morphologically Complex Actinomycetes. *J. Biol. Chem.* **2009**, 284, 25268-25279.
16. Fülöp, V.; Sam, K. A.; Ferguson, S. J.; Ginger, M. L.; Allen, J. W. A. Structure of a Trypanosomatid Mitochondrial Cytochrome c with Heme Attached via Only One Thioether Bond and Implications for the Substrate Recognition Requirements of Heme Lyase. *FEBS J.* **2009**, 276, 2822-2832.
17. Dawson, A.; Fyfe, P. K.; Hunter, W. N. Specificity and Reactivity in Menaquinone

- Biosynthesis: The Structure of Escherichia coli MenD (2-Succinyl-5-Enolpyruvyl-6-Hydroxy-3-Cyclohexadiene-1-Carboxylate Synthase). *J. Mol. Biol.* **2008**, *384*, 1353-1368.
18. Reddy, M. C. M.; Kuppan, G.; Shetty, N. D.; Owen, J. L.; Ioerger, T. R. Sacchettini, J. C. Crystal Structures of Mycobacterium Tuberculosis S-adenosyl-L-homocysteine Hydrolase in Ternary Complex with Substrate and Inhibitors. *Protein Sci.* **2008**, *17*, 2134-2144.
19. Sundaramoorthy, R.; Fyfe, P. K.; Hunter, W. N. Structure of Staphylococcus aureus EsxA Suggests a Contribution to Virulence by Action as a Transport Chaperone and/or Adaptor Protein. *J. Mol. Biol.* **2008**, *383*, 603-614.
20. Sgraja, T.; Alphey, M. S.; Ghilagaber, S.; Marquez, R.; Robertson, M. N.; Hemmings, J. L.; Lauw, S.; Rohdich, F.; Bacher, A.; Eisenreich, W. et. Al. Characterization of Aquifex Aeolicus 4-Diphosphocytidyl-2C-methyl-d-erythritol Kinase - Ligand Recognition in a Template for Antimicrobial Drug Discovery. *FEBS J.* **2008**, *275*, 2779-2794.
21. Rea, D.; Fülop, V.; Bugg, T. D. H.; Roper, D. I. Structure and Mechanism of HpcH: A Metal Ion Dependent Class II Aldolase from the Homoprotocatechuate Degradation Pathway of Escherichia coli. *J. Mol. Biol.* **2007**, *373*, 866-876.
22. Just, V. J.; Burrell, M. R.; Bowater, L.; McRobbie, I.; Stevenson, C. E. M.; Lawson, D. M.; Bornemann, S. The Identity of the Active Site of Oxalate Decarboxylase and the Importance of the Stability of Active-site Lid Conformations. *Biochem. J.* **2007**, *407*, 397-406.
23. Ku, S.-Y.; Yip, P.; Cornell, K. A.; Riscoe, M. K.; Behr, J.-B.; Guillerm, G.; Howell, P. L. Structures of 5-Methylthioribose Kinase Reveal Substrate Specificity and Unusual Mode of Nucleotide Binding. *J. Biol. Chem.* **2007**, *282*, 22195-22206.
24. Lewin, A.; Crow, A.; Oubrie, A.; Le Brun, N. E. Molecular Basis for Specificity of the Extracytoplasmic Thioredoxin ResA. *J. Biol. Chem.* **2006**, *281*, 35467-35477.
25. Martins, B. M.; Grimm, B.; Mock, H.-P.; Huber, R.; Messerschmidt, A. Crystal Structure and Substrate Binding Modeling of the Uroporphyrinogen-III Decarboxylase from Nicotiana tabacum : Implications for the Catalytic

- Mechanism. *J. Biol. Chem.* **2001**, *276*, 44108-44116.
26. Koch, M.; Velarde, M.; Harrison, M. D.; Echt, S.; Fischer, M.; Messerschmidt, A.; Dennison, C. Crystal Structures of Oxidized and Reduced Stellacyanin from Horseradish Roots. *J. Am. Chem. Soc.* **2005**, *127*, 158-166.
27. McGrath, A. P.; Mithieux, S. M.; Collyer, C. A.; Bakhuis, J. G.; van den Berg, M.; Sein, A.; Heinz, A.; Schmelzer, C.; Weiss, A. S.; Guss, J. M. Structure and Activity of *Aspergillus nidulans* Copper Amine Oxidase. *Biochemistry* **2011**, *50*, 5718-5730.
28. O'Farrell, H. C.; Musayev, F. N.; Scarsdale, J. N.; Rife, J. P. Binding of Adenosine-Based Ligands to the MjDim1 rRNA Methyltransferase: Implications for Reaction Mechanism and Drug Design. *Biochemistry* **2010**, *49*, 2697-2704.
29. Sigala, P. A.; Caaveiro, J. M. M.; Ringe, D.; Petsko, G. A.; Herschlag, D. Hydrogen Bond Coupling in the Ketosteroid Isomerase Active Site. *Biochemistry* **2009**, *48*, 6932-6939.
30. Hadler, K. S.; Tanifum, E. A.; Yip, S. H.-C.; Mitić, N.; Guddat, L. W.; Jackson, C. J.; Gahan, L. R.; Nguyen, K.; Carr, P. D.; Ollis, D. L. et.al Substrate-Promoted Formation of a Catalytically Competent Binuclear Center and Regulation of Reactivity in a Glycerophosphodiesterase from *Enterobacter aerogenes*. *J. Am. Chem. Soc.* **2008**, *130*, 14129-14138.
31. Nielsen, M. S.; Harris, P.; Ooi, B. L.; Christensen, H. E. M. The 1.5 Å Resolution Crystal Structure of [Fe3S4]-Ferredoxin from the Hyperthermophilic Archaeon *Pyrococcus furiosus*. *Biochemistry* **2004**, *43*, 5188-5194.
32. Heitmann, D.; Einsle, O. Structural and Biochemical Characterization of DHC2, a Novel Diheme Cytochrome c from *Geobacter sulfurreducens*. *Biochemistry* **2005**, *44*, 12411-12419.
33. Graham, S. C.; Bond, C. S.; Freeman, H. C.; Guss, J. M. Structural and Functional Implications of Metal Ion Selection in Aminopeptidase P, a Metalloprotease with a Dinuclear Metal Center. *Biochemistry* **2005**, *44*, 13820-13836.
34. Graham, S. C.; Lilley, P. E.; Lee, M.; Schaeffer, P. M.; Kralicek, A. V.; Dixon, N. E.; Guss, J. M. Kinetic and Crystallographic Analysis of Mutant *Escherichia coli*

- Aminopeptidase P: Insights into Substrate Recognition and the Mechanism of Catalysis *Biochemistry* **2006**, *45*, 964-975.
35. Wijma, H. J.; MacPherson, I.; Farver, O.; Tocheva, E. I.; Pecht, I.; Verbeet, M. P.; Murphy, M. E. P.; Canters, G. W. Effect of the Methionine Ligand on the Reorganization Energy of the Type-1 Copper Site of Nitrite Reductase. *J. Am. Chem. Soc.* **2007**, *129*, 519-525.
36. Meijers, R.; Adoloh, H.-W.; Dauter, Z.; Wilson, K. S.; Lamzin, V. S.; Cedergren-Zeppezauer, E. S. Structural Evidence for a Ligand Coordination Switch in Liver Alcohol Dehydrogenase. *Biochemistry* **2007**, *46*, 5446-5454.
37. Einsle, O.; Tezcan, F. A.; Andrade, S. L. A.; Schmid, B.; Yoshida, M.; Howard, J. B.; Rees, D. C. Nitrogenase MoFe-Protein at 1.16 Å Resolution: A Central Ligand in the FeMo-Cofactor. *Science* **2002**, *297*, 1696-1700.
38. Stec, B.; Zhou, R.; Teeter, M. M. Full-matrix Refinement of the Protein Crambin at 0.83 Å and 130 K. *Acta Crystallogr., Sect. D: Biol. Crystallogr.* **1995**, *D51*, 663-681.
39. Tickle, I. J.; Laskowski, R. A.; Moss, D. S. Error Estimates of Protein Structure Coordinates and Deviations from Standard Geometry by Full-Matrix Refinement of γ B- and β B2-Crystallin. *Acta Crystallogr., Sect. D: Biol. Crystallogr.* **1998**, *D54*, 243-252.

Table S3. Relative energies in kcal/mol of various stationary points at different levels for the original structure and Structure1 with 0.1 Å random displacements at the fixed atoms.

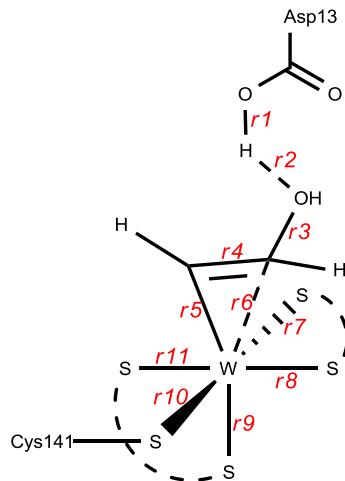
		Int1	TS1	Int2	TS2	Int3
B3LYP/BS1	<i>Original</i>	0	13.7	8.0	17.4	-18.4
	<i>Structure1</i>	0	15.1	9.2	19.3	-17.8
	Deviation	0	+1.4	+1.2	+1.9	+0.6
B3LYP/BS1-CPCM	<i>Original</i>	0	14.4	8.3	16.3	-17.5
	<i>Structure1</i>	0	16.5	10.2	18.7	-16.0
	Deviation	0	+2.1	+1.9	+2.4	+1.5
B3LYP/BS2	<i>Original</i>	0	19.4	16.4	24.8	-12.0
	<i>Structure1</i>	0	21.0	17.8	26.8	-11.2
	Deviation	0	+1.6	+1.4	+2.0	+0.8
ZPE	<i>Original</i>	0	0.4	1.5	-1.4	2.9
	<i>Structure1</i>	0	1.3	2.0	-0.5	3.8
	Deviation	0	+0.9	+0.5	+0.9	+1.1
B3LYP final ^a	<i>Original</i>	0	20.6	18.2	22.2	-8.3
	<i>Structure1</i>	0	23.7	20.8	25.7	-5.7
	Deviation	0	+3.1	+2.6	+3.5	+2.6

^a: with solvation, basis set, and ZPE corrections.

Table S4. Relative energies in kcal/mol of **Int2** at different levels for the original structure and Structure1 with 0.1 Å random displacements at the fixed atoms.

	B3LYP/BS1	B3LYP final
Original	8.0	18.2
Structure1	9.2	20.8
Structure2	8.2	18.4
Structure3	9.2	19.4
Structure4	8.7	19.9
Structure5	7.3	16.9
Structure6	8.9	20.1
Structure7	8.6	18.6
Structure8	7.1	17.2
Structure9	9.7	20.2
Structure10	8.0	17.7
Average	8.5	18.9
RMSD	0.9	1.5

Table S5. Selected bond distances ($r1$ to $r11$) of **Int2** for the original structure and 10 structures with 0.1 Å random displacements at the fixed atoms.



	$r1$	$r2$	$r3$	$r4$	$r5$	$r6$	$r7$	$r8$	$r9$	$r10$	$r11$
Original	1.059	1.395	1.479	1.403	1.933	2.167	2.517	2.568	2.562	2.510	2.387
Structure1	1.053	1.415	1.476	1.402	1.933	2.167	2.517	2.571	2.571	2.501	2.378
Structure2	1.059	1.394	1.479	1.403	1.933	2.166	2.516	2.564	2.562	2.509	2.390
Structure3	1.052	1.424	1.477	1.401	1.935	2.175	2.509	2.571	2.564	2.507	2.388
Structure4	1.054	1.415	1.477	1.402	1.933	2.174	2.514	2.570	2.561	2.509	2.386
Structure5	1.060	1.393	1.478	1.403	1.933	2.163	2.515	2.575	2.562	2.511	2.389
Structure6	1.059	1.400	1.479	1.401	1.934	2.174	2.517	2.566	2.564	2.505	2.385
Structure7	1.067	1.375	1.482	1.403	1.933	2.164	2.523	2.561	2.564	2.501	2.383
Structure8	1.058	1.400	1.478	1.403	1.933	2.168	2.516	2.588	2.550	2.528	2.396
Structure9	1.055	1.408	1.478	1.402	1.932	2.163	2.520	2.580	2.566	2.508	2.380
Structure10	1.060	1.392	1.479	1.402	1.934	2.171	2.519	2.566	2.559	2.513	2.389
Average	1.056	1.402	1.478	1.402	1.933	2.169	2.517	2.571	2.562	2.509	2.386
RMSD	0.004	0.015	0.002	0.001	0.001	0.005	0.004	0.008	0.005	0.007	0.005

Table S6. Selected bond distances of **Int2** for the original structure and 10 structures with 0.15 Å random displacements at the fixed atoms.

	r1	r2	r3	r4	r5	r6	r7	r8	r9	r10	r11
Original	1.059	1.395	1.479	1.403	1.933	2.167	2.517	2.568	2.562	2.510	2.387
Structure1	1.054	1.415	1.476	1.401	1.934	2.174	2.515	2.568	2.567	2.505	2.381
Structure2	1.060	1.394	1.481	1.402	1.933	2.160	2.519	2.559	2.571	2.496	2.377
Structure3	1.061	1.386	1.480	1.404	1.932	2.159	2.520	2.579	2.562	2.509	2.389
Structure4	1.054	1.414	1.479	1.403	1.931	2.162	2.520	2.598	2.557	2.517	2.384
Structure5	1.050	1.432	1.475	1.401	1.934	2.173	2.512	2.579	2.567	2.512	2.381
Structure6	1.068	1.375	1.481	1.402	1.933	2.168	2.523	2.572	2.557	2.504	2.388
Structure7	1.057	1.403	1.479	1.403	1.933	2.168	2.516	2.573	2.553	2.523	2.394
Structure8	1.060	1.393	1.482	1.403	1.932	2.161	2.516	2.569	2.571	2.503	2.394
Structure9	1.059	1.401	1.479	1.401	1.933	2.170	2.521	2.603	2.564	2.513	2.386
Structure10	1.050	1.433	1.478	1.402	1.931	2.162	2.523	2.589	2.573	2.498	2.373
Average	1.057	1.405	1.479	1.402	1.933	2.166	2.519	2.579	2.564	2.508	2.385
RMSD	0.006	0.020	0.002	0.001	0.001	0.005	0.004	0.017	0.007	0.008	0.007

Table S7. Selected bond distances of **Int2** for the original structure and 10 structures with 0.2 Å random displacements at the fixed atoms. Values for structures 6 and 7 refer to the conformers with standard dihedral angles.

	r1	r2	r3	r4	r5	r6	r7	r8	r9	r10	r11
Original	1.059	1.395	1.479	1.403	1.933	2.167	2.517	2.568	2.562	2.510	2.387
Structure1	1.063	1.390	1.482	1.402	1.932	2.159	2.520	2.580	2.560	2.510	2.378
Structure2	1.052	1.419	1.479	1.403	1.932	2.159	2.512	2.550	2.587	2.486	2.375
Structure3	1.054	1.417	1.478	1.403	1.933	2.168	2.513	2.577	2.568	2.519	2.386
Structure4	1.056	1.401	1.477	1.404	1.935	2.172	2.495	2.553	2.566	2.504	2.407
Structure5	1.046	1.445	1.476	1.403	1.932	2.164	2.519	2.605	2.538	2.552	2.390
Structure6	1.060	1.389	1.485	1.400	1.933	2.168	2.519	2.559	2.571	2.496	2.390
Structure7	1.052	1.426	1.477	1.402	1.933	2.169	2.509	2.566	2.559	2.512	2.398
Structure8	1.070	1.364	1.485	1.404	1.932	2.152	2.534	2.543	2.584	2.483	2.373
Structure9	1.053	1.433	1.477	1.400	1.935	2.185	2.511	2.576	2.569	2.502	2.384
Structure10	1.060	1.404	1.481	1.404	1.932	2.160	2.522	2.579	2.559	2.507	2.382
Average	1.057	1.409	1.480	1.403	1.933	2.166	2.515	2.569	2.566	2.507	2.386
RMSD	0.007	0.027	0.003	0.002	0.001	0.009	0.010	0.017	0.014	0.019	0.010

Table S8. Dihedral angle of C-C α -C β -S (in degree) of **Int1** for various structures.

	0.1 Å	0.15 Å	0.2 Å
Original		91.3	
Structure 1	81.5	98.0	83.7
Structure 2	82.4	84.7	76.9
Structure 3	70.7	82.4	76.2
Structure 4	75.2	89.2	93.3
Structure 5	91.5	101.9	84.3
Structure 6	72.0	92.9	98.6(161.7) ^a
Structure 7	87.6	89.6	76.1(166.3) ^a
Structure 8	93.3	72.0	84.2
Structure 9	86.5	95.3	71.5
Structure 10	97.6	80.2	82.2
Average	83.8	88.6	86.3(98.0)
RMSD	11.5	9.0	11.8(34.1)

^a: there are two different local minima, see text in the main paper.

Table S9. Dihedral angle of C-C α -C β -S (in degree) of **Int2** for various structures.

	0.1 Å	0.15 Å	0.2 Å
Original		110.4	
Structure 1	110.5	123.4	98.9
Structure 2	110.6	106.1	99.8
Structure 3	121.4	98.0	106.2
Structure 4	116.7	106.4	110.6
Structure 5	104.3	119.4	95.6
Structure 6	121.7	112.8	96.4(166.9) ^a
Structure 7	108.2	109.8	89.4(166.9) ^a
Structure 8	109.6	92.7	104.1
Structure 9	108.4	120.9	131.9
Structure 10	117.5	97.4	96.2
Average	112.9	108.7	102.9(117.7)
RMSD	6.2	10.2	13.5(37.4)

^a: there are two different local minima, see text in the main paper.

Preparation of Structures with Displacements

Random displacements at **Int2** of the QM-only model were performed for the ten atoms (number 1, 5, 10, 13, 22, 23, 29, 38, 57, and 58) that were fixed during the geometry optimization. A python code (main text shown below) was written to perform the displacements.

```
for i in range(0,l):
    dx=random.uniform(-s,s)
    a=math.sqrt(s**2-(dx)**2)
    dy=random.uniform(-a,a)
    b=math.sqrt(s**2-(dx)**2-(dy)**2)
    q=random.sample([-b,b],1)
    dz=q[0]
    x.append(X[i]+dx)
    y.append(Y[i]+dy)
    z.append(Z[i]+dz)
print x
print y
print z
```

Note: s is the value (0.1, 0.15, and 0.2 Å) of the random displacement.

Ten distorted structures of **Int2** were generated in this manner and then subjected to geometry optimization. The resulting optimized geometries of **Int2** served as starting points for subsequent geometry optimizations of the other stationary points. These optimizations were done first for **TS1** and **TS2**, and then for **Int1** and **Int3**, in the case of 0.1 Å displacements, and directly for **Int1** in the case of larger displacements.

Cartesian Coordinates for Selected Structures

Int1-Original

C	6.49700000	0.88000000	4.91400000
C	6.07100000	-0.56200000	5.16800000
O	6.06700000	-1.05200000	6.29600000
N	5.68900000	-1.20700000	4.03600000
C	4.85900000	-2.40300000	4.05500000
C	3.45000000	-2.07800000	3.53900000
C	3.47200000	-1.53600000	2.09700000
O	4.25900000	-0.55600000	1.85400000
O	2.73200000	-2.09900000	1.26100000
C	-5.18700000	-2.44300000	-0.89000000
C	-4.04200000	-1.75900000	-0.14200000
S	-2.52200000	-1.71800000	-1.17400000
C	8.50100000	-0.45000000	-2.99700000
C	7.32400000	-0.79800000	-2.14700000
C	6.98000000	-0.27000000	-0.92100000
C	6.30400000	-1.75700000	-2.47100000
N	5.80700000	-0.82900000	-0.46500000
C	5.37000000	-1.73700000	-1.40100000
C	6.07800000	-2.63200000	-3.55200000
C	4.21900000	-2.52900000	-1.38700000
C	4.94800000	-3.44000000	-3.53400000
C	4.02900000	-3.38100000	-2.46100000
C	2.46200000	5.59300000	-2.71900000
C	1.51300000	5.64000000	-1.52000000
N	0.61100000	4.48800000	-1.53400000
C	-0.71900000	4.50600000	-1.56200000
N	-1.39400000	5.64500000	-1.22700000
N	-1.40900000	3.45300000	-1.99300000
C	-2.60200000	2.31000000	4.55100000
C	-3.75800000	1.78500000	3.70500000
O	-4.69300000	2.86100000	3.59100000
C	-3.25900000	1.30900000	2.35200000
S	-2.03900000	0.05500000	2.36700000
C	-3.72200000	1.82900000	1.18300000
S	-3.03300000	1.35900000	-0.33900000
C	-4.90400000	2.77700000	1.18700000
C	-5.62100000	2.69100000	2.53300000
C	1.54000000	2.10500000	-4.14700000
C	2.26000000	1.48000000	-2.95100000
O	3.30000000	2.39400000	-2.58900000
C	1.33300000	1.22200000	-1.76900000
S	-0.19600000	0.39600000	-2.09800000
C	1.67000000	1.62600000	-0.52000000
S	0.51100000	1.52900000	0.81800000
C	3.05300000	2.13800000	-0.18000000
C	3.97000000	1.98300000	-1.39400000
W	-1.08600000	-0.21200000	0.23100000
O	1.99100000	-4.54100000	0.21700000
C	-0.20600000	-1.66900000	1.35400000
C	0.12700000	-1.84600000	0.10800000
C	-5.27800000	-3.96500000	-0.63500000
O	-6.17700000	-4.43800000	0.06800000
N	-4.36600000	-4.75900000	-1.23700000
N	-6.49100000	-1.92900000	-0.46300000
C	-7.32700000	-1.25600000	-1.31100000
O	-6.96900000	-0.73500000	-2.36200000
C	-4.44300000	-6.19700000	-1.02800000
C	-8.78500000	-1.22000000	-0.85100000
H	5.63100000	1.53700000	5.05100000
H	3.00000000	-1.32200000	4.19500000
H	2.82100000	-2.97200000	3.56700000
H	4.83300000	-2.77400000	5.08300000
H	5.49200000	-0.64800000	3.20100000
H	8.19600000	-0.06600000	-3.98000000
H	9.14600000	-1.31900000	-3.18600000
H	7.49700000	0.47900000	-0.33400000
H	5.28400000	-0.63100000	0.40500000
H	6.77500000	-2.67500000	-4.38600000
H	4.76000000	-4.12200000	-4.36000000
H	3.51200000	-2.45100000	-0.56900000
H	3.13800000	-4.00600000	-2.48400000
H	3.00000000	4.64300000	-2.75100000
H	1.90400000	5.70400000	-3.65400000

H	2.07800000	5.63500000	-0.58000000
H	0.91200000	6.55200000	-1.54100000
H	1.03900000	3.55600000	-1.55000000
H	-2.40100000	5.59900000	-1.26800000
H	-1.01500000	6.21200000	-0.48400000
H	-2.29700000	3.22700000	-1.54000000
H	-0.91200000	2.57700000	-2.22500000
H	-3.83200000	-2.25900000	0.81000000
H	-4.35800000	-0.74000000	0.06900000
H	-2.07400000	3.10000000	4.01000000
H	-1.89400000	1.51100000	4.77900000
H	-4.24900000	0.94700000	4.23400000
H	-5.58600000	2.52100000	0.36700000
H	-6.14000000	1.72200000	2.62300000
H	1.03600000	3.03500000	-3.87000000
H	0.79700000	1.41600000	-4.55200000
H	2.71800000	0.52700000	-3.26600000
H	3.45000000	1.54600000	0.65400000
H	4.29100000	0.94000000	-1.49300000
H	2.19300000	-3.74200000	0.74700000
H	-2.98600000	2.72200000	5.49000000
H	-4.57000000	3.81100000	1.01800000
H	-6.36500000	3.48700000	2.64300000
H	2.27300000	2.33500000	-4.92700000
H	3.18600000	6.41300000	-2.65100000
H	4.86400000	2.60800000	-1.31000000
H	3.01600000	3.18700000	0.15600000
H	7.25600000	1.16800000	5.64500000
H	6.88300000	1.03400000	3.90300000
H	9.12200000	0.31900000	-2.52500000
H	5.31400000	-3.18300000	3.42900000
H	-5.09000000	-2.23600000	-1.96000000
H	2.83500000	-4.73600000	-0.20800000
H	-0.08100000	-2.06900000	2.35000000
H	-9.31900000	-2.06600000	-1.29700000
H	-8.88700000	-1.28400000	0.23600000
H	-9.24800000	-0.29900000	-1.21000000
H	0.66600000	-2.51900000	-0.54300000
H	-3.53900000	-4.33800000	-1.64600000
H	-6.92900000	-2.54500000	0.21700000
H	-5.45700000	-6.54300000	-1.24300000
H	-3.73900000	-6.69100000	-1.70200000
H	-4.20400000	-6.47500000	0.00400000

New coordinates after applying displacements of 0.1 Å (atoms 1, 5, 10, 13, 22, 23, 29, 38, 57, 58)

C	6.547	0.803	4.955	Structure1-010
C	4.946	-2.427	4.098	Structure1-010
C	-5.092	-2.442	-0.920	Structure1-010
C	8.503	-0.370	-3.057	Structure1-010
C	3.954	-3.334	-2.415	Structure1-010
C	2.430	5.680	-2.758	Structure1-010
C	-2.544	2.336	4.474	Structure1-010
C	1.543	2.098	-4.247	Structure1-010
C	-4.454	-6.288	-1.068	Structure1-010
C	-8.723	-1.210	-0.929	Structure1-010
C	6.430	0.901	4.985	Structure2-010
C	4.836	-2.403	4.152	Structure2-010
C	-5.167	-2.391	-0.972	Structure2-010
C	8.545	-0.507	-2.928	Structure2-010
C	4.116	-3.337	-2.481	Structure2-010
C	2.480	5.670	-2.657	Structure2-010
C	-2.701	2.326	4.543	Structure2-010
C	1.548	2.170	-4.071	Structure2-010
C	-4.478	-6.283	-1.066	Structure2-010
C	-8.768	-1.292	-0.918	Structure2-010
C	6.419	0.841	4.867	Structure3-010
C	4.909	-2.359	3.981	Structure3-010
C	-5.214	-2.479	-0.979	Structure3-010
C	8.531	-0.456	-2.902	Structure3-010
C	3.955	-3.401	-2.397	Structure3-010
C	2.518	5.560	-2.795	Structure3-010
C	-2.569	2.356	4.633	Structure3-010
C	1.555	2.020	-4.096	Structure3-010
C	-4.417	-6.150	-0.944	Structure3-010
C	-8.824	-1.171	-0.773	Structure3-010

C	6.408	0.881	4.960	Structure4-010
C	4.887	-2.332	3.991	Structure4-010
C	-5.170	-2.535	-0.926	Structure4-010
C	8.521	-0.440	-2.900	Structure4-010
C	3.956	-3.402	-2.527	Structure4-010
C	2.500	5.559	-2.633	Structure4-010
C	-2.700	2.322	4.535	Structure4-010
C	1.492	2.075	-4.229	Structure4-010
C	-4.419	-6.160	-1.118	Structure4-010
C	-8.822	-1.184	-0.765	Structure4-010
C	6.422	0.911	4.856	Structure5-010
C	4.913	-2.473	4.102	Structure5-010
C	-5.206	-2.363	-0.832	Structure5-010
C	8.551	-0.508	-2.933	Structure5-010
C	3.973	-3.339	-2.390	Structure5-010
C	2.544	5.590	-2.662	Structure5-010
C	-2.509	2.327	4.583	Structure5-010
C	1.607	2.069	-4.081	Structure5-010
C	-4.385	-6.190	-0.947	Structure5-010
C	-8.744	-1.286	-0.913	Structure5-010
C	6.523	0.857	4.820	Structure6-010
C	4.879	-2.372	3.962	Structure6-010
C	-5.155	-2.410	-0.978	Structure6-010
C	8.531	-0.450	-2.902	Structure6-010
C	4.065	-3.416	-2.548	Structure6-010
C	2.381	5.602	-2.662	Structure6-010
C	-2.582	2.280	4.644	Structure6-010
C	1.606	2.133	-4.077	Structure6-010
C	-4.459	-6.111	-1.077	Structure6-010
C	-8.822	-1.249	-0.762	Structure6-010
C	6.538	0.869	5.005	Structure7-010
C	4.917	-2.463	3.999	Structure7-010
C	-5.156	-2.402	-0.804	Structure7-010
C	8.427	-0.404	-3.046	Structure7-010
C	4.081	-3.401	-2.544	Structure7-010
C	2.473	5.502	-2.758	Structure7-010
C	-2.605	2.265	4.640	Structure7-010
C	1.442	2.115	-4.130	Structure7-010
C	-4.487	-6.238	-1.108	Structure7-010
C	-8.738	-1.147	-0.800	Structure7-010
C	6.506	0.957	4.977	Structure8-010
C	4.951	-2.408	4.015	Structure8-010
C	-5.283	-2.433	-0.918	Structure8-010
C	8.571	-0.440	-3.068	Structure8-010
C	4.061	-3.382	-2.367	Structure8-010
C	2.493	5.659	-2.651	Structure8-010
C	-2.555	2.381	4.604	Structure8-010
C	1.636	2.120	-4.120	Structure8-010
C	-4.398	-6.129	-0.971	Structure8-010
C	-8.733	-1.269	-0.780	Structure8-010
C	6.542	0.796	4.883	Structure9-010
C	4.870	-2.345	3.974	Structure9-010
C	-5.221	-2.358	-0.929	Structure9-010
C	8.564	-0.493	-2.932	Structure9-010
C	3.963	-3.401	-2.534	Structure9-010
C	2.446	5.684	-2.757	Structure9-010
C	-2.586	2.230	4.493	Structure9-010
C	1.581	2.168	-4.212	Structure9-010
C	-4.527	-6.213	-1.080	Structure9-010
C	-8.728	-1.170	-0.916	Structure9-010
C	6.500	0.863	5.013	Structure10-010
C	4.839	-2.426	3.959	Structure10-010
C	-5.208	-2.451	-0.987	Structure10-010
C	8.518	-0.385	-3.071	Structure10-010
C	4.110	-3.370	-2.404	Structure10-010
C	2.415	5.661	-2.663	Structure10-010
C	-2.694	2.294	4.589	Structure10-010
C	1.536	2.198	-4.110	Structure10-010
C	-4.384	-6.173	-0.951	Structure10-010
C	-8.753	-1.168	-0.930	Structure10-010

New coordinates after applying displacements of 0.15 Å (atoms 1, 5, 10, 13, 22, 23, 29, 38, 57, 58)

C	6.482	0.808	5.045	Structure1-015
C	4.807	-2.399	4.195	Structure1-015
C	-5.121	-2.510	-1.006	Structure1-015
C	8.390	-0.456	-2.897	Structure1-015
C	4.056	-3.355	-2.316	Structure1-015
C	2.501	5.498	-2.610	Structure1-015
C	-2.712	2.229	4.488	Structure1-015
C	1.671	2.037	-4.116	Structure1-015
C	-4.567	-6.117	-1.001	Structure1-015
C	-8.759	-1.177	-0.992	Structure1-015
 C	 6.571	 0.995	 4.976	 Structure2-015
C	4.957	-2.479	4.140	Structure2-015
C	-5.088	-2.425	-0.779	Structure2-015
C	8.521	-0.306	-3.036	Structure2-015
C	3.975	-3.292	-2.569	Structure2-015
C	2.327	5.657	-2.734	Structure2-015
C	-2.477	2.257	4.487	Structure2-015
C	1.512	1.967	-4.197	Structure2-015
C	-4.583	-6.150	-1.003	Structure2-015
C	-8.755	-1.298	-0.975	Structure2-015
 C	 6.367	 0.954	 4.925	 Structure3-015
C	5.007	-2.414	4.031	Structure3-015
C	-5.274	-2.423	-0.769	Structure3-015
C	8.484	-0.401	-3.138	Structure3-015
C	3.975	-3.380	-2.321	Structure3-015
C	2.546	5.537	-2.830	Structure3-015
C	-2.654	2.448	4.578	Structure3-015
C	1.466	2.128	-4.019	Structure3-015
C	-4.300	-6.169	-1.062	Structure3-015
C	-8.788	-1.156	-0.986	Structure3-015
 C	 6.373	 0.798	 4.903	 Structure4-015
C	4.997	-2.433	4.002	Structure4-015
C	-5.232	-2.345	-0.785	Structure4-015
C	8.405	-0.409	-3.105	Structure4-015
C	4.150	-3.315	-2.519	Structure4-015
C	2.351	5.594	-2.819	Structure4-015
C	-2.505	2.417	4.513	Structure4-015
C	1.622	2.133	-4.269	Structure4-015
C	-4.567	-6.239	-0.955	Structure4-015
C	-8.697	-1.227	-0.729	Structure4-015
 C	 6.545	 0.758	 4.988	 Structure5-015
C	4.754	-2.425	4.159	Structure5-015
C	-5.181	-2.477	-1.035	Structure5-015
C	8.477	-0.541	-2.881	Structure5-015
C	3.956	-3.453	-2.352	Structure5-015
C	2.334	5.659	-2.762	Structure5-015
C	-2.559	2.228	4.433	Structure5-015
C	1.602	2.111	-4.283	Structure5-015
C	-4.497	-6.213	-0.889	Structure5-015
C	-8.834	-1.290	-0.727	Structure5-015
 C	 6.362	 0.914	 4.860	 Structure6-015
C	4.900	-2.413	3.911	Structure6-015
C	-5.130	-2.463	-0.752	Structure6-015
C	8.460	-0.384	-3.126	Structure6-015
C	4.089	-3.453	-2.578	Structure6-015
C	2.367	5.488	-2.768	Structure6-015
C	-2.596	2.277	4.697	Structure6-015
C	1.440	2.193	-4.216	Structure6-015
C	-4.465	-6.271	-1.157	Structure6-015
C	-8.661	-1.165	-0.786	Structure6-015
 C	 6.402	 0.915	 4.804	 Structure7-015
C	4.819	-2.303	3.951	Structure7-015
C	-5.278	-2.405	-1.003	Structure7-015
C	8.561	-0.323	-3.049	Structure7-015
C	4.147	-3.413	-2.547	Structure7-015
C	2.492	5.489	-2.616	Structure7-015
C	-2.521	2.305	4.425	Structure7-015
C	1.496	2.228	-4.221	Structure7-015
C	-4.428	-6.191	-0.879	Structure7-015
C	-8.702	-1.343	-0.872	Structure7-015
 C	 6.430	 1.013	 4.932	 Structure8-015

C	4.996	-2.434	4.108	Structure8-015
C	-5.049	-2.432	-0.947	Structure8-015
C	8.567	-0.322	-3.040	Structure8-015
C	4.006	-3.303	-2.587	Structure8-015
C	2.500	5.696	-2.821	Structure8-015
C	-2.567	2.364	4.686	Structure8-015
C	1.591	2.078	-4.008	Structure8-015
C	-4.333	-6.190	-0.927	Structure8-015
C	-8.926	-1.177	-0.876	Structure8-015
C	6.542	0.821	4.784	Structure9-015
C	4.825	-2.372	3.912	Structure9-015
C	-5.288	-2.528	-0.817	Structure9-015
C	8.563	-0.512	-2.875	Structure9-015
C	3.994	-3.509	-2.532	Structure9-015
C	2.471	5.731	-2.659	Structure9-015
C	-2.488	2.281	4.644	Structure9-015
C	1.686	2.139	-4.145	Structure9-015
C	-4.538	-6.282	-0.948	Structure9-015
C	-8.719	-1.126	-0.753	Structure9-015
C	6.463	0.786	4.803	Structure10-015
C	4.982	-2.342	4.116	Structure10-015
C	-5.214	-2.314	-0.818	Structure10-015
C	8.369	-0.439	-3.068	Structure10-015
C	4.012	-3.461	-2.335	Structure10-015
C	2.567	5.545	-2.814	Structure10-015
C	-2.520	2.335	4.674	Structure10-015
C	1.412	2.082	-4.221	Structure10-015
C	-4.343	-6.221	-1.137	Structure10-015
C	-8.903	-1.193	-0.940	Structure10-015

New coordinates after applying displacements of 0.2 Å (atoms 1, 5, 10, 13, 22, 23, 29, 38, 57, 58)

C	6.421	0.753	5.048	Structure1-020
C	4.824	-2.522	3.897	Structure1-020
C	-5.308	-2.298	-0.956	Structure1-020
C	8.334	-0.462	-2.888	Structure1-020
C	4.220	-3.376	-2.517	Structure1-020
C	2.306	5.708	-2.670	Structure1-020
C	-2.660	2.121	4.519	Structure1-020
C	1.613	1.994	-4.297	Structure1-020
C	-4.441	-6.167	-1.226	Structure1-020
C	-8.930	-1.272	-0.724	Structure1-020
C	6.394	0.747	5.022	Structure2-020
C	5.055	-2.447	4.064	Structure2-020
C	-5.070	-2.370	-1.034	Structure2-020
C	8.303	-0.451	-2.966	Structure2-020
C	4.136	-3.416	-2.296	Structure2-020
C	2.610	5.658	-2.838	Structure2-020
C	-2.607	2.435	4.395	Structure2-020
C	1.368	2.051	-4.060	Structure2-020
C	-4.335	-6.252	-1.187	Structure2-020
C	-8.871	-1.074	-0.958	Structure2-020
C	6.337	0.839	4.802	Structure3-020
C	4.932	-2.534	4.188	Structure3-020
C	-5.216	-2.584	-0.751	Structure3-020
C	8.571	-0.330	-2.853	Structure3-020
C	3.876	-3.341	-2.584	Structure3-020
C	2.560	5.636	-2.888	Structure3-020
C	-2.792	2.334	4.493	Structure3-020
C	1.504	1.929	-4.235	Structure3-020
C	-4.633	-6.169	-1.084	Structure3-020
C	-8.930	-1.211	-0.713	Structure3-020
C	6.666	0.863	4.808	Structure4-020
C	4.815	-2.442	4.246	Structure4-020
C	-5.130	-2.343	-1.053	Structure4-020
C	8.323	-0.479	-2.912	Structure4-020
C	3.923	-3.325	-2.622	Structure4-020
C	2.622	5.620	-2.601	Structure4-020
C	-2.550	2.140	4.643	Structure4-020
C	1.392	2.103	-4.013	Structure4-020
C	-4.546	-6.354	-1.098	Structure4-020
C	-8.656	-1.370	-0.819	Structure4-020
C	6.506	0.697	4.993	Structure5-020

C	4.775	-2.291	4.197	Structure5-020
C	-5.371	-2.506	-0.842	Structure5-020
C	8.397	-0.437	-3.167	Structure5-020
C	3.969	-3.485	-2.301	Structure5-020
C	2.474	5.614	-2.520	Structure5-020
C	-2.778	2.285	4.458	Structure5-020
C	1.414	2.104	-4.302	Structure5-020
C	-4.611	-6.142	-0.935	Structure5-020
C	-8.586	-1.211	-0.870	Structure5-020
 C	 6.592	 0.758	 5.042	Structure6-020
C	4.845	-2.365	3.859	Structure6-020
C	-5.132	-2.484	-1.077	Structure6-020
C	8.580	-0.527	-2.831	Structure6-020
C	3.994	-3.428	-2.652	Structure6-020
C	2.374	5.689	-2.566	Structure6-020
C	-2.539	2.405	4.715	Structure6-020
C	1.455	1.939	-4.075	Structure6-020
C	-4.360	-6.292	-1.184	Structure6-020
C	-8.750	-1.335	-1.011	Structure6-020
 C	 6.608	 1.029	 4.990	Structure7-020
C	4.988	-2.287	3.955	Structure7-020
C	-5.145	-2.572	-1.036	Structure7-020
C	8.513	-0.480	-2.800	Structure7-020
C	3.894	-3.428	-2.321	Structure7-020
C	2.405	5.526	-2.540	Structure7-020
C	-2.432	2.231	4.618	Structure7-020
C	1.341	2.116	-4.133	Structure7-020
C	-4.402	-6.050	-1.158	Structure7-020
C	-8.699	-1.056	-0.776	Structure7-020
 C	 6.496	 1.058	 4.822	Structure8-020
C	4.783	-2.473	3.884	Structure8-020
C	-5.142	-2.264	-0.813	Structure8-020
C	8.656	-0.438	-3.124	Structure8-020
C	4.190	-3.498	-2.445	Structure8-020
C	2.530	5.580	-2.531	Structure8-020
C	-2.625	2.383	4.366	Structure8-020
C	1.398	2.233	-4.089	Structure8-020
C	-4.547	-6.300	-0.892	Structure8-020
C	-8.859	-1.199	-1.035	Structure8-020
 C	 6.639	 1.009	 4.971	Structure9-020
C	4.997	-2.527	4.131	Structure9-020
C	-5.080	-2.504	-1.047	Structure9-020
C	8.548	-0.485	-2.806	Structure9-020
C	3.860	-3.340	-2.561	Structure9-020
C	2.275	5.654	-2.753	Structure9-020
C	-2.584	2.323	4.750	Structure9-020
C	1.491	2.282	-4.068	Structure9-020
C	-4.624	-6.254	-0.966	Structure9-020
C	-8.878	-1.283	-1.016	Structure9-020
 C	 6.430	 0.810	 4.740	Structure10-020
C	4.953	-2.545	4.161	Structure10-020
C	-5.252	-2.277	-0.800	Structure10-020
C	8.492	-0.587	-2.852	Structure10-020
C	4.128	-3.374	-2.634	Structure10-020
C	2.375	5.673	-2.557	Structure10-020
C	-2.745	2.174	4.584	Structure10-020
C	1.361	2.095	-4.235	Structure10-020
C	-4.559	-6.168	-1.189	Structure10-020
C	-8.901	-1.340	-0.742	Structure10-020

TS1-Original

C	6.49099500	0.98084700	4.91173500
C	6.13289000	-0.47572500	5.11086300
O	6.40094900	-1.07401000	6.15310700
N	5.48988300	-1.02110300	4.05431600
C	4.87554800	-2.32737200	4.10582100
C	3.40723200	-2.26505700	3.69545800
C	3.23893100	-1.85165600	2.23096200
O	3.97485200	-0.92831500	1.76881300
O	2.36027400	-2.49796600	1.59023700
C	-5.16496700	-2.51659100	-0.84754900
C	-3.97979500	-1.75326900	-0.26001600
S	-2.81356900	-1.30155800	-1.60380100
C	8.51240600	-0.46903200	-2.97405700
C	7.40652100	-0.90301900	-2.06279600
C	7.18495100	-0.52889800	-0.75553100
C	6.34901500	-1.81773900	-2.40390200
N	6.07008000	-1.17043400	-0.25256000
C	5.53568100	-1.95806600	-1.24700100
C	5.99317100	-2.51592000	-3.57291100
C	4.39959200	-2.77023400	-1.21883100
C	4.84780400	-3.30258000	-3.55916700
C	4.05853800	-3.42034400	-2.39353400
C	2.43377000	5.53819800	-2.80425900
C	1.63514500	5.59965300	-1.50126400
N	0.67249400	4.49974800	-1.43838900
C	-0.65611600	4.60216500	-1.37674600
N	-1.22545900	5.76037100	-0.92680700
N	-1.43556100	3.62602500	-1.82089200
C	-2.61765800	2.34444100	4.51468900
C	-3.82611400	1.90293400	3.70577600
O	-4.72276700	3.01805900	3.66801900
C	-3.38679200	1.46534800	2.32373000
S	-2.19229100	0.18243000	2.26294700
C	-3.88106700	2.03478900	1.19788000
S	-3.27154600	1.56305700	-0.36340800
C	-5.03658500	3.00977600	1.27094700
C	-5.69808200	2.91364800	2.64507600
C	1.53645800	2.02021900	-4.17418900
C	2.21853800	1.38769600	-2.97235500
O	3.30743900	2.24204100	-2.60190100
C	1.25807400	1.20381000	-1.81020900
S	-0.36179400	0.60733600	-2.19910500
C	1.62702000	1.50757900	-0.53946800
S	0.47774400	1.40993300	0.79649000
C	3.04570600	1.91956700	-0.19592300
C	3.95498300	1.76748100	-1.41870000
W	-1.35740200	-0.07944200	0.05246700
O	1.52003500	-1.77959600	-0.61569100
C	-0.71317800	-1.68587500	1.00800600
C	-0.32321200	-1.85462300	-0.27022500
C	-5.19947300	-3.99666400	-0.41890800
O	-5.90012800	-4.37607500	0.52035300
N	-4.43455900	-4.83571500	-1.16553600
N	-6.44787800	-1.94321600	-0.45933900
C	-7.38844000	-1.60954300	-1.39718100
O	-7.16410100	-1.53676300	-2.60014700
C	-4.39618600	-6.26726400	-0.92232900
C	-8.77039000	-1.31623000	-0.83309400
H	5.85318700	1.59570900	5.55607400
H	2.87975600	-1.53809600	4.32675100
H	2.92717700	-3.23662200	3.83719200
H	4.98962300	-2.69685200	5.12852100
H	5.19553200	-0.47193300	3.25068700
H	8.12544500	0.00579800	-3.88538300
H	9.13251400	-1.31563700	-3.29815600
H	7.75439700	0.15136400	-0.13565300
H	5.56751500	-0.99288100	0.61677000
H	6.59659700	-2.43183700	-4.47391800
H	4.54988600	-3.83579600	-4.45858500
H	3.79970500	-2.87087200	-0.32475100
H	3.16555700	-4.03798300	-2.41444500
H	2.94553000	4.57617500	-2.89407600
H	1.77374800	5.66612500	-3.66762500
H	2.30441300	5.53781700	-0.63542600
H	1.08630600	6.54232000	-1.42999000
H	1.03984600	3.54868300	-1.53095100
H	-2.23456200	5.77129500	-0.88965200
H	-0.76504900	6.23147000	-0.16162700

H	-2.31266000	3.41007400	-1.33457000
H	-1.00233000	2.74223100	-2.14788400
H	-3.45836100	-2.33804200	0.50449700
H	-4.35994800	-0.84525900	0.21057200
H	-2.07485200	3.12746200	3.97708000
H	-1.93757300	1.50786900	4.68368100
H	-4.33093600	1.06495700	4.22151600
H	-5.76212300	2.78612900	0.47846400
H	-6.24983100	1.96248500	2.73039500
H	1.05499600	2.96643900	-3.91083100
H	0.77667000	1.35118000	-4.58090300
H	2.62860200	0.40788500	-3.27090800
H	3.41436800	1.28055200	0.61599400
H	4.23763000	0.71443900	-1.55288900
H	1.94032900	-2.01801500	0.31258900
H	-2.93831700	2.74226500	5.48415100
H	-4.68932600	4.04026000	1.10401300
H	-6.40696000	3.73264300	2.80889700
H	2.28122300	2.22192000	-4.95126800
H	3.18228300	6.33779500	-2.82099100
H	4.87408600	2.35129400	-1.31249100
H	3.06114800	2.95502300	0.17901200
H	7.52422500	1.14586400	5.22948400
H	6.37228700	1.32217300	3.87974300
H	9.17511900	0.25284700	-2.48448100
H	5.41062700	-3.02580700	3.44608900
H	-5.14139200	-2.45288300	-1.93879100
H	1.70166500	-0.84084600	-0.77966800
H	-0.66407300	-2.17996000	1.97021200
H	-9.45465500	-2.11303700	-1.14226800
H	-8.78954200	-1.23741200	0.25739500
H	-9.13589500	-0.38289500	-1.26821300
H	-0.44117200	-2.59727500	-1.04337300
H	-3.83448400	-4.42939500	-1.87086300
H	-6.77986100	-2.26478400	0.44239100
H	-5.15725400	-6.48912400	-0.17378900
H	-4.61510600	-6.82205200	-1.84133000
H	-3.41960900	-6.58915400	-0.54160700

Int2-Original

C	6.49746000	0.88007800	4.91444100
C	6.13391500	-0.57685500	5.08068100
O	6.42479100	-1.21437100	6.09031900
N	5.45069500	-1.08739400	4.02596300
C	4.85948300	-2.40341900	4.05469800
C	3.36478500	-2.36374500	3.76684000
C	3.09755900	-1.92462400	2.34132300
O	3.82089700	-1.10113900	1.75820700
O	2.06746700	-2.51530800	1.81713600
C	-5.18722700	-2.44326200	-0.88955800
C	-3.97025900	-1.75166900	-0.28384300
S	-2.77599300	-1.32748800	-1.61217700
C	8.50106800	-0.44970500	-2.99701900
C	7.39021200	-0.88506700	-2.09147500
C	7.16305200	-0.50934100	-0.78752500
C	6.32731000	-1.79175800	-2.44032900
N	6.03114400	-1.13528100	-0.29814100
C	5.49414500	-1.91841600	-1.29577900
C	5.98860100	-2.49681600	-3.60968600
C	4.34376600	-2.71198500	-1.28896700
C	4.84284300	-3.28206000	-3.61035400
C	4.02852500	-3.38116900	-2.46122500
C	2.46219100	5.59347700	-2.71887800
C	1.67567600	5.60748900	-1.40588000
N	0.72101000	4.50080200	-1.36468800
C	-0.60921700	4.59533400	-1.28194600
N	-1.17222900	5.73334400	-0.77015000
N	-1.39103100	3.64061100	-1.75932100
C	-2.60245300	2.30979100	4.55097900
C	-3.80118500	1.86748200	3.72726600
O	-4.70973500	2.97487400	3.70918100
C	-3.35584700	1.45307900	2.33951600
S	-2.14767700	0.17783500	2.26468700
C	-3.85262500	2.03707100	1.22360900
S	-3.23987800	1.59032300	-0.34773400
C	-5.00978000	3.00898000	1.31003400
C	-5.67784300	2.88478600	2.67805300
C	1.54036800	2.10507000	-4.14692700
C	2.24275000	1.43522200	-2.97860500
O	3.34100800	2.28167000	-2.60837400
C	1.30042200	1.21365800	-1.80829400
S	-0.33237100	0.65055600	-2.20901900
C	1.68334600	1.48738300	-0.53342000
S	0.56952900	1.34439800	0.82550100
C	3.10028700	1.92504300	-0.21168000
C	3.99970600	1.79058200	-1.44199600
W	-1.34192800	-0.08855000	0.03373700
O	1.35994100	-1.81083800	-0.41557500
C	-0.77123600	-1.71968700	0.90013500
C	-0.11613000	-1.83711200	-0.33455800
C	-5.27600100	-3.93875100	-0.52173100
O	-6.06171500	-4.34888100	0.33384200
N	-4.45164900	-4.75834300	-1.22780500
N	-6.45168700	-1.83375600	-0.48985600
C	-7.40400800	-1.51372100	-1.42304800
O	-7.19381500	-1.45925500	-2.62943600
C	-4.44316900	-6.19709100	-1.02849100
C	-8.78467200	-1.21973400	-0.85069000
H	5.87454700	1.48178400	5.58492000
H	2.86533500	-1.65978100	4.44429200
H	2.90837500	-3.34458100	3.92255700
H	5.05588400	-2.81354100	5.04833900
H	5.16402400	-0.50648700	3.24886400
H	8.11725100	0.04102600	-3.90070300
H	9.11183700	-1.29843900	-3.33195100
H	7.73356200	0.16340800	-0.16098200
H	5.56534800	-0.98129600	0.58779800
H	6.60802900	-2.42053900	-4.50010000
H	4.56102500	-3.82436600	-4.50900200
H	3.70876100	-2.78606400	-0.41681400
H	3.13040900	-3.99073000	-2.49441700
H	2.97940600	4.63837500	-2.84420100
H	1.79238800	5.74290900	-3.57115100
H	2.35625500	5.52703200	-0.55000500
H	1.12052100	6.54327800	-1.30055300
H	1.08895600	3.55397600	-1.48959800
H	-2.18070600	5.72760300	-0.70822300
H	-0.70614600	6.14712600	0.02496300

H	-2.26460800	3.39853800	-1.27111100
H	-0.95968300	2.76627100	-2.12046800
H	-3.47409200	-2.37070400	0.47025700
H	-4.30881600	-0.83575400	0.20313300
H	-2.06898000	3.11062900	4.03030800
H	-1.91137400	1.47915800	4.70377200
H	-4.29870900	1.01648700	4.22928300
H	-5.73220900	2.79862200	0.51100200
H	-6.22524100	1.92926400	2.74224000
H	1.06357700	3.04171500	-3.84494700
H	0.77305900	1.44960700	-4.56054700
H	2.65122100	0.46706900	-3.31695100
H	3.49074100	1.30445900	0.60340800
H	4.28140500	0.73932800	-1.59505400
H	1.83154500	-2.14111700	0.85460700
H	-2.93284000	2.68420600	5.52677800
H	-4.66631900	4.04444900	1.16389600
H	-6.39227500	3.69695300	2.85404000
H	2.27165000	2.33285700	-4.93023300
H	3.20471000	6.39903700	-2.71804100
H	4.92042900	2.37321600	-1.33568400
H	3.10146600	2.96265100	0.15848500
H	7.53669800	1.02940700	5.21875700
H	6.36424000	1.25030500	3.89429400
H	9.17011300	0.25877300	-2.49730800
H	5.35499000	-3.06045800	3.32642400
H	-5.15891400	-2.34605300	-1.97824400
H	1.62991800	-0.93656400	-0.74152900
H	-0.77437500	-2.23993400	1.85350300
H	-9.43009400	-2.08896300	-1.01754200
H	-8.77006900	-0.99660900	0.21996200
H	-9.21579000	-0.37564000	-1.39290800
H	-0.47121800	-2.46753100	-1.14753100
H	-3.77369500	-4.32983200	-1.84539500
H	-6.78785200	-2.14920400	0.41235500
H	-5.27991500	-6.43761400	-0.37205600
H	-4.56472500	-6.72139100	-1.98291200
H	-3.51346200	-6.53870200	-0.55710500

TS2-Original

C	6.44927900	-0.49571900	4.86939200
C	6.14435200	-1.94419000	4.56478300
O	6.53082700	-2.85888500	5.28685800
N	5.39535700	-2.12690000	3.44165900
C	4.76420600	-3.39788000	3.15432500
C	3.25740200	-3.34694600	3.39978100
C	2.53746300	-2.35700300	2.48611800
O	3.15152700	-1.70171500	1.63084800
O	1.25520400	-2.31735600	2.70345800
C	-5.27958400	-1.94896200	-1.57923300
C	-4.10557700	-1.57481400	-0.66966700
S	-2.56218300	-1.29915100	-1.62822500
C	8.43726300	0.34949700	-3.11230500
C	7.34445000	-0.33719400	-2.35191800
C	7.15752200	-0.37528900	-0.99061400
C	6.25691700	-1.08395500	-2.93142500
N	6.02302400	-1.10819300	-0.68578000
C	5.44501700	-1.54552600	-1.86104300
C	5.88036900	-1.39196900	-4.25147100
C	4.27647500	-2.28284400	-2.06520000
C	4.71832300	-2.12340200	-4.46233500
C	3.92234800	-2.55372300	-3.37885200
C	2.48666600	6.17351200	-1.17925600
C	1.55220500	5.88226500	-0.00184300
N	0.66001700	4.76686000	-0.31081400
C	-0.67317800	4.76985200	-0.28408900
N	-1.33780100	5.75996800	0.38808700
N	-1.37073300	3.87335100	-0.96800900
C	-2.62872600	1.10721100	4.94033600
C	-3.78734400	0.79288300	4.00111300
O	-4.74133600	1.84594400	4.18457700
C	-3.29242700	0.68798900	2.57091900
S	-2.09699800	-0.56424300	2.25048000
C	-3.74095400	1.51359100	1.59344900
S	-3.04785700	1.46981400	-0.00664900
C	-4.91403300	2.43606800	1.84901300
C	-5.65137700	1.98098100	3.10654000
C	1.51497400	3.21874200	-3.49942900
C	2.23222700	2.24821100	-2.56023300
O	3.34448500	2.97233900	-2.00867900
C	1.32275500	1.70186400	-1.46641300
S	-0.21114100	1.01016100	-1.98915100
C	1.69178800	1.74469600	-0.16120700
S	0.59360300	1.23170600	1.13391600
C	3.08888200	2.15603500	0.25791900
C	3.99150600	2.23771300	-0.97221600
W	-1.13008300	-0.22138100	0.12173600
O	1.57171500	-1.64147300	-0.80513900
C	-0.37744900	-2.01269600	0.66791600
C	0.19241000	-1.85276800	-0.61169600
C	-5.43218200	-3.47178300	-1.79497400
O	-6.39472900	-4.09080100	-1.32997600
N	-4.48234800	-4.09727000	-2.52836700
N	-6.56240200	-1.52080700	-1.01405300
C	-7.41219000	-0.68511100	-1.69141900
O	-7.07395200	0.03512000	-2.62333600
C	-4.59006000	-5.53342600	-2.73696100
C	-8.85889500	-0.73154800	-1.19638700
H	5.77305000	-0.14765100	5.65804200
H	3.04026400	-3.08532600	4.44182500
H	2.80546800	-4.33190900	3.23117500
H	5.23734300	-4.13754500	3.80288600
H	4.98829000	-1.32945300	2.97153700
H	8.03602800	1.09728800	-3.80831600
H	9.02490200	-0.35857100	-3.71132600
H	7.75458600	0.06630300	-0.20396100
H	5.61668400	-1.24004600	0.22810700
H	6.48282900	-1.05358400	-5.09105700
H	4.40678900	-2.35880000	-5.47670700
H	3.63519500	-2.58395400	-1.24627600
H	3.00387200	-3.09923500	-3.57270900
H	3.02982700	5.27129700	-1.47370900
H	1.91726100	6.52739100	-2.04403100
H	2.13238400	5.63893100	0.89677400
H	0.94089100	6.75985400	0.22643600
H	1.08427400	3.87188400	-0.58274900
H	-2.34532600	5.68664300	0.38551400
H	-0.93936400	6.06037500	1.26604700

H	-2.23982600	3.49992300	-0.56635400
H	-0.88076900	3.10262500	-1.46073600
H	-3.93073400	-2.33721900	0.09764000
H	-4.37196400	-0.64539000	-0.16962000
H	-2.13171600	2.02719900	4.61863800
H	-1.89602200	0.29762400	4.93317800
H	-4.25540900	-0.16224900	4.30308700
H	-5.58716000	2.42689000	0.98228800
H	-6.17171000	1.02843200	2.91197500
H	1.07285500	4.05358700	-2.94918200
H	0.72079200	2.70328600	-4.04294700
H	2.62269300	1.40205000	-3.14933000
H	3.48398700	1.41321800	0.96234200
H	4.23620100	1.22666700	-1.32600500
H	0.64688500	-1.94806900	1.86820800
H	-2.99952100	1.24561000	5.96218900
H	-4.57590300	3.47461900	1.98242600
H	-6.39805800	2.71692900	3.42522300
H	2.23290700	3.62610700	-4.21885600
H	3.20784700	6.94905000	-0.89956400
H	4.92823000	2.76291200	-0.75754500
H	3.08401100	3.11710000	0.79835200
H	7.46892000	-0.41448100	5.25266100
H	6.33315300	0.16354300	4.00432900
H	9.13072800	0.86485000	-2.43932800
H	4.95680600	-3.67677100	2.11270700
H	-5.16604100	-1.43636600	-2.53971200
H	1.98210700	-1.41468600	0.04798700
H	-0.89579700	-2.86345700	1.10980200
H	-9.41097400	-1.47559100	-1.78158200
H	-8.93511100	-1.00217700	-0.13924600
H	-9.32081700	0.24327100	-1.36145000
H	-0.20788200	-2.32557100	-1.50734200
H	-3.61808700	-3.60537300	-2.72964500
H	-7.00817500	-2.26911300	-0.49238400
H	-5.58265600	-5.77440100	-3.12457200
H	-3.83260000	-5.84431100	-3.45997800
H	-4.44774400	-6.09516100	-1.80598100

Int3-Original

C	6.43149800	1.17297900	4.85613300
C	5.96282100	-0.22910600	5.23872100
O	5.83593400	-0.57612300	6.41148400
N	5.69063300	-1.01687600	4.16106000
C	4.79717300	-2.16779200	4.24645400
C	3.39062000	-1.79548500	3.77064500
C	3.39116800	-1.35866000	2.30121700
O	4.25617000	-0.49772600	1.93317000
O	2.54035200	-1.91827700	1.56576200
C	-5.22023700	-2.59487200	-0.73879800
C	-4.32119000	-1.47085800	-0.27939400
S	-2.71923300	-1.65105100	-1.12880400
C	8.48111700	-0.77213600	-2.91493900
C	7.33567700	-1.10228900	-2.01382400
C	7.04868500	-0.56459900	-0.77824800
C	6.30025900	-2.06340500	-2.28424900
N	5.91876500	-1.14878700	-0.24521300
C	5.43506300	-2.05904100	-1.15675900
C	5.99698900	-2.90567900	-3.37035600
C	4.29406300	-2.86119700	-1.08019600
C	4.84795500	-3.68463600	-3.31079400
C	4.00420500	-3.65275000	-2.17770700
C	2.44336600	5.27413400	-3.14651700
C	1.82882300	5.38149800	-1.75032200
N	0.78456100	4.37102100	-1.56866100
C	-0.53101800	4.58782700	-1.55265600
N	-1.01362500	5.81029900	-1.18188200
N	-1.37914200	3.65207200	-1.96284400
C	-2.66548400	2.56963700	4.32806500
C	-3.86625800	2.04598100	3.55011700
O	-4.79333900	3.13634400	3.45909600
C	-3.42420100	1.54043400	2.19372800
S	-2.15510100	0.30120500	2.18718900
C	-3.90482200	2.06027000	1.04497300
S	-3.22070600	1.58122900	-0.50784600
C	-5.05871700	3.03531300	1.05634400
C	-5.74522500	2.98396800	2.42163600
C	1.52844100	1.68460100	-4.30247100
C	2.20914000	1.17061400	-3.04668000
O	3.29133500	2.06220600	-2.74616200
C	1.26277600	1.06745800	-1.86827600
S	-0.40172500	0.60376300	-2.18635800
C	1.68112900	1.36336300	-0.61113900
S	0.56958500	1.24197200	0.74885000
C	3.10581800	1.78519600	-0.31568700
C	3.98355100	1.64788100	-1.56498500
W	-1.39351000	0.05942400	-0.00601400
O	1.37906100	-1.79304600	-0.65664600
C	-0.44540700	-1.83124100	0.96967100
C	0.10963800	-1.98815100	-0.31157200
C	-4.95083900	-3.96687200	-0.10012700
O	-5.12197600	-4.14724200	1.10402700
N	-4.64445700	-4.96181300	-0.97815200
N	-6.61493000	-2.29787600	-0.42849900
C	-7.46571200	-1.78530900	-1.35889800
O	-7.17610000	-1.64602400	-2.54370600
C	-4.47702500	-6.34803800	-0.57898700
C	-8.81731000	-1.37213900	-0.81711200
H	5.55781900	1.83130500	4.78742400
H	3.01107300	-0.97175000	4.38845400
H	2.70879000	-2.64244100	3.88051800
H	4.78708300	-2.50044300	5.28754600
H	5.56390200	-0.53915400	3.26717100
H	8.13932500	-0.41868400	-3.89711000
H	9.12390400	-1.64361300	-3.10135700
H	7.58434700	0.19837700	-0.22809700
H	5.34985100	-0.82810300	0.55119100
H	6.64215900	-2.93625100	-4.24570000
H	4.58986100	-4.32883700	-4.14796700
H	3.65773100	-2.84809600	-0.20524900
H	3.11062000	-4.27089100	-2.16256800
H	2.88488000	4.28518100	-3.28960300
H	1.68410400	5.44302600	-3.91671600
H	2.59026200	5.23113400	-0.97854400
H	1.39124900	6.37076100	-1.59424300
H	1.07665000	3.38896000	-1.62587000
H	-2.01800900	5.91013600	-1.16848200
H	-0.52059900	6.30050100	-0.45015500

H	-2.27353800	3.51902500	-1.48353200
H	-0.99501600	2.72872600	-2.24075400
H	-4.18869100	-1.49668500	0.80570500
H	-4.77835700	-0.52073800	-0.55995300
H	-2.15028300	3.33760700	3.74349500
H	-1.95992900	1.76498200	4.54045200
H	-4.34399700	1.22688500	4.11869100
H	-5.77219200	2.78455200	0.26012600
H	-6.29114100	2.03141200	2.52974400
H	1.03481900	2.64606600	-4.12972000
H	0.77640800	0.97535500	-4.65127800
H	2.62766600	0.17059200	-3.24946900
H	3.51492300	1.15992000	0.48724500
H	4.31667300	0.60912700	-1.68459100
H	0.21917400	-1.60009600	1.79342300
H	-2.99785500	3.01244700	5.27357100
H	-4.71150000	4.06092300	0.85929900
H	-6.46451800	3.80174000	2.54115500
H	2.27544000	1.82138000	-5.09168700
H	3.22839200	6.02924100	-3.26769000
H	4.87550700	2.27809500	-1.49519200
H	3.11720800	2.82260600	0.05688600
H	7.08858800	1.56118500	5.63699200
H	6.94852600	1.19506400	3.89267700
H	9.11431600	0.01294500	-2.48720400
H	5.19851200	-2.98446500	3.63332200
H	-5.17497800	-2.65840200	-1.82933900
H	1.94079500	-1.66971100	0.17530200
H	-1.29490600	-2.45833800	1.21515400
H	-9.59701400	-1.72889200	-1.49457300
H	-9.01868300	-1.74325300	0.19209300
H	-8.87300900	-0.27870100	-0.80297100
H	-0.45514300	-2.48947600	-1.09064100
H	-4.43202800	-4.69795800	-1.92852000
H	-6.88823100	-2.38249300	0.54029500
H	-4.80932100	-6.43002300	0.45663100
H	-5.08154900	-7.00745300	-1.21108600
H	-3.42877800	-6.66412800	-0.63714700

Int1-Displacement-0.1-Structure1 optimized

C	6.47524100	-0.37313500	4.94328500
C	5.98613300	-1.80984200	4.92774300
O	5.69999700	-2.42910000	5.94922600
N	5.87804800	-2.30573100	3.65811500
C	4.87944100	-3.32654300	3.37462500
C	3.52709700	-2.68562100	3.02189800
C	3.62055700	-1.75087600	1.80128000
O	4.52984500	-0.85265300	1.80230200
O	2.80178000	-1.94282400	0.87129300
C	-5.19441700	-2.23402000	-1.44862200
C	-4.18473100	-1.54011800	-0.55090400
S	-2.54615500	-1.49180800	-1.35902000
C	8.37741500	0.34284000	-3.13493700
C	7.19218100	-0.22760900	-2.40174800
C	6.89252000	-0.01760800	-1.07171400
C	6.14400600	-1.08668000	-2.90631400
N	5.73908700	-0.67403300	-0.71192800
C	5.25897500	-1.33795500	-1.81701600
C	5.84006900	-1.68321700	-4.14826600
C	4.11424900	-2.14031900	-1.93095400
C	4.70582800	-2.48197300	-4.26577100
C	3.84300000	-2.71191300	-3.16521600
C	2.28678000	6.13022600	-1.41070000
C	1.28184800	5.92559700	-0.27632700
N	0.35034000	4.84570800	-0.60398800
C	-0.97713700	4.90853900	-0.62331000
N	-1.62143700	5.95468300	-0.02792800
N	-1.69575500	4.00534200	-1.28963200
C	-2.62398500	1.18439800	4.88590600
C	-3.81373000	0.82262100	4.00200300
O	-4.78072300	1.85992500	4.19643900
C	3.36474100	0.70292400	2.55575800
S	-2.11496400	-0.48583600	2.24195400
C	-3.84223400	1.52266600	1.58139600
S	-3.14548700	1.53205800	-0.01066700
C	-5.02003400	2.43027300	1.86519000
C	-5.72029300	1.97002700	3.14245400
C	1.40069700	2.98369600	-3.68006200
C	2.10094000	2.15165600	-2.61011900
O	3.16870600	2.95279300	-2.09347500
C	1.15207100	1.72823900	-1.49911800
S	-0.42531500	1.09624300	-2.00035000
C	1.49694700	1.86365600	-0.19241200
S	0.31725900	1.59128200	1.10520500
C	2.90074700	2.25150900	0.22422200
C	3.81827200	2.30110300	-0.99861900
W	-1.17098400	-0.11698600	0.11720300
O	1.95149800	-4.37258500	-0.09106400
C	-0.07254800	-1.69969000	0.78794700
C	0.34542200	-1.36727800	-0.40036900
C	-5.13394900	-3.79388500	-1.37438800
O	-5.65542000	-4.36639700	-0.41567700
N	-4.58612100	-4.47080200	-2.42155400
N	-6.56088400	-1.92790600	-1.01803800
C	-7.40276800	-1.09816400	-1.69467300
O	-7.06871700	-0.43183500	-2.66990200
C	-4.54442300	-5.93870200	-2.48412300
C	-8.82935700	-1.05122800	-1.15033500
H	5.67872200	0.27730700	4.56475500
H	3.17709500	-2.10889700	3.88755000
H	2.78779900	-3.46306200	2.80939500
H	4.78832400	-3.96282400	4.25818700
H	5.83296200	-1.58255600	2.93533300
H	8.07495600	0.97943500	-3.97745100
H	9.02496400	-0.44186000	-3.54913500
H	7.43325400	0.57267900	-0.34273800
H	5.27748300	-0.67504900	0.21727800
H	6.48445400	-1.52229400	-5.01019200
H	4.47565400	-2.93891600	-5.22558400
H	3.47377400	-2.28062200	-1.06942800
H	2.96470700	-3.34010100	-3.28644500
H	2.79516200	5.19259500	-1.65163100
H	1.78072800	6.48840000	-2.31251800
H	1.79821100	5.67562000	0.65788400
H	0.70646000	6.83953200	-0.10536900
H	0.75528800	3.92687200	-0.81835400
H	-2.62948000	5.94652000	-0.07739700
H	-1.23332600	6.31406200	0.83160300

H	-2.57925500	3.70095600	-0.87813000
H	-1.21088200	3.18203500	-1.69621600
H	-4.09999600	-2.05574600	0.41131400
H	-4.53407000	-0.52398900	-0.37754300
H	-2.14319800	2.09156300	4.50871300
H	-1.88647100	0.37969600	4.89616900
H	-4.24966000	-0.13473900	4.34024900
H	-5.71481300	2.41479600	1.01594200
H	-6.22997700	1.00792700	2.96791100
H	0.91587700	3.86636400	-3.25147000
H	0.64483700	2.39003600	-4.19732300
H	2.53215900	1.25326000	-3.08318000
H	3.28377700	1.50452300	0.93092700
H	4.10767900	1.28582500	-1.29464000
H	2.18177200	-3.52370500	0.34507700
H	-2.96395900	1.36572000	5.91132900
H	-4.68430100	3.46997200	1.98953900
H	-6.47039300	2.69641300	3.47304700
H	2.13990700	3.32578000	-4.41155100
H	3.03361100	6.87468500	-1.11552000
H	4.73105800	2.86907800	-0.79613300
H	2.89373400	3.21696500	0.75485900
H	6.73196200	-0.07762900	5.96192000
H	7.34366500	-0.23688200	4.29053900
H	8.99075600	0.95440300	-2.46486000
H	5.22764600	-3.95052200	2.54246900
H	-5.09121200	-1.87049400	-2.47427300
H	2.76972400	-4.61851600	-0.53874000
H	0.10655300	-2.38253400	1.60548600
H	-9.50988400	-1.43171600	-1.91806100
H	-8.97022900	-1.62851500	-0.23239900
H	-0.09864000	-0.00842600	-0.96323500
H	1.04992000	-1.63034000	-1.17388100
H	-4.05679600	-3.93927800	-3.09866800
H	-6.91437800	-2.54614400	-0.29883200
H	-5.26331800	-6.31460100	-1.75626300
H	-4.81828000	-6.27399300	-3.48869400
H	-3.54992100	-6.32410600	-2.23322100

Int1-Displacement-0.1-Structure2 optimized

C	6.34573700	0.56861000	4.96142300
C	5.91725500	-0.88335300	5.13647000
O	5.86325900	-1.41948700	6.24263500
N	5.59147600	-1.48375700	3.96186400
C	4.74697500	-2.66821000	3.90221300
C	3.35217700	-2.29765800	3.37502500
C	3.42064500	-1.68738800	1.96222800
O	4.20011300	-0.68489600	1.79810500
O	2.72628900	-2.22201700	1.07032500
C	-5.26509900	-2.29066400	-1.19118200
C	-4.20671700	-1.54968100	-0.38712300
S	-2.56463700	-1.64261100	-1.18643500
C	8.44512400	-0.28581000	-3.03423400
C	7.28196600	-0.63288500	-2.18244800
C	6.93088100	-0.18925600	-0.92654500
C	6.26354700	-1.54489300	-2.59357100
N	5.74166900	-0.76720900	-0.53364200
C	5.31403500	-1.59810100	-1.54197000
C	6.07642300	-2.31561000	-3.75457900
C	4.16658000	-2.38686800	-1.62522200
C	4.94798600	-3.11533200	-3.83613400
C	4.01445100	-3.13614100	-2.77845600
C	2.38665500	5.86235200	-2.32278600
C	1.47295400	5.81563400	-1.09728100
N	0.54876100	4.68503200	-1.18926600
C	-0.77919800	4.73450200	-1.22946200
N	-1.43448200	5.85901000	-0.81568100
N	-1.48642200	3.73193800	-1.74545000
C	-2.78483500	2.02798800	4.63597800
C	-3.92660600	1.52387200	3.75948000
O	-4.89312400	2.57876200	3.72425800
C	3.40799100	1.16157100	2.37837900
S	-2.17067100	-0.07814500	2.31731300
C	-3.84272600	1.79283600	1.25502500
S	-3.09450600	1.49909200	-0.28393700
C	-5.03184400	2.72804000	1.32044900
C	-5.78673400	2.49664700	2.62804400
C	1.44882200	2.46958000	-3.97565700
C	2.16634700	1.75975400	-2.82835300
O	3.21455800	2.63750000	-2.40261600
C	1.23118700	1.43449400	-1.67172000
S	-0.31523800	0.67795300	-2.07984100
C	1.56490100	1.74853100	-0.39481300
S	0.38501300	1.61266700	0.92187100
C	2.95798700	2.20724100	-0.01860700
C	3.87709100	2.13339500	-1.23910000
W	-1.17015600	-0.13942100	0.18692500
O	1.90256500	-4.51717000	-0.22016700
C	-0.19416500	-1.63025200	1.18430300
C	0.17798100	-1.65107900	-0.06246900
C	-5.27578100	-3.85388200	-0.91733800
O	-5.97602900	-4.28019000	0.00511300
N	-4.57633100	-4.69553200	-1.73100100
N	-6.58780400	-1.87224400	-0.77133900
C	-7.44643500	-1.20109600	-1.58440900
O	-7.13079500	-0.67284100	-2.64565200
C	-4.57925600	-6.16735800	-1.55681600
C	-8.86506800	-1.19522600	-1.05350500
H	5.46741900	1.21409500	5.07648100
H	2.89952100	-1.56789900	4.05838200
H	2.71137300	-3.18314800	3.34410700
H	4.69425700	-3.09034700	4.90932100
H	5.41767700	-0.88182700	3.15102500
H	8.13269100	0.16174700	-3.98782000
H	9.04650600	-1.17012200	-3.28672900
H	7.44671800	0.50538000	-0.27627800
H	5.21840700	-0.64422300	0.35066400
H	6.80092100	-2.28286600	-4.56514300
H	4.77062400	-3.72581700	-4.71805400
H	3.44374800	-2.39336600	-0.81881300
H	3.12610200	-3.75757300	-2.87421300
H	2.91452300	4.91339300	-2.44578700
H	1.80394400	6.05453800	-3.22901900
H	2.06161500	5.71356100	-0.17867000
H	0.89001100	6.73706300	-1.01784200
H	0.95946900	3.74835700	-1.27366500
H	-2.44227400	5.83511100	-0.86675100
H	-1.05357000	6.35435300	-0.02324700

H	-2.38102500	3.49003300	-1.31516400
H	-1.00355700	2.86368900	-2.03330200
H	-4.14379300	-1.95448100	0.62877700
H	-4.52113400	-0.51012700	-0.32647600
H	-2.28230600	2.86663100	4.14553400
H	-2.05092800	1.23901300	4.81262300
H	-4.38938900	0.63644000	4.22827400
H	-5.68770900	2.55409300	0.45828100
H	-6.28992100	1.51600100	2.60463200
H	0.94686700	3.37878000	-3.63340400
H	0.70381600	1.81284000	-4.42897000
H	2.61718000	0.82762500	-3.20762800
H	3.34426100	1.54493500	0.76689200
H	4.19050000	1.09764400	-1.41358100
H	2.11468800	-3.78978800	0.40016200
H	-3.17794800	2.36780200	5.60015600
H	-4.70416400	3.77646200	1.27000400
H	-6.54892900	3.26553000	2.79327200
H	2.18118100	2.75220600	-4.73840200
H	3.12100800	6.66707900	-2.20891800
H	4.77603300	2.74282800	-1.10645900
H	2.93594900	3.22577900	0.40146100
H	7.06321600	0.83320600	5.74134900
H	6.78143000	0.76296200	3.97751400
H	9.11601900	0.43064500	-2.54587600
H	5.20544100	-3.41910200	3.24522800
H	-5.15608600	-2.06858700	-2.25614100
H	2.74599600	-4.67102200	-0.66305400
H	-0.05361700	-2.11636000	2.13928800
H	-9.41741100	-2.03424500	-1.49214500
H	-8.91109700	-1.28827000	0.03509500
H	-9.36336900	-0.27336300	-1.36055800
H	0.78258500	-2.20592800	-0.76400200
H	-3.89486600	-4.28393400	-2.35516800
H	-6.96125900	-2.44986200	-0.02549700
H	-5.45080400	-6.42061000	-0.95407500
H	-4.64413100	-6.64781400	-2.53659900
H	-3.67450500	-6.50912100	-1.04288800

Int1-Displacement-0.1-Structure3 optimized

C	6.32253200	0.45865300	4.85367000
C	5.90857600	-0.97724400	5.05034600
O	5.62451600	-1.45951100	6.14277300
N	5.84652300	-1.64640100	3.85868300
C	4.83035800	-2.66823700	3.71558900
C	3.46967800	-2.06333900	3.31937900
C	3.54239500	-1.29374100	1.98915900
O	4.44323900	-0.38983400	1.87967300
O	2.74032300	-1.61520200	1.08093700
C	-5.26368800	-2.44009000	-1.30098400
C	-4.36132800	-1.39071900	-0.66570800
S	-2.64475000	-1.58177200	-1.27419700
C	8.48526600	-0.23185400	-2.97841800
C	7.25763300	-0.66392500	-2.22418000
C	6.88285300	-0.20801600	-0.97869900
C	6.22995600	-1.59959700	-2.62273100
N	5.70127200	-0.78181600	-0.57397500
C	5.27492100	-1.63663600	-1.56397600
C	5.99422700	-2.41546700	-3.74893500
C	4.11893300	-2.43011200	-1.60690800
C	4.85427700	-3.21345700	-3.79056800
C	3.91691400	-3.22203400	-2.72860100
C	2.44968200	5.73972100	-2.44760000
C	1.53871300	5.75227900	-1.21963300
N	0.58989200	4.63991300	-1.27305500
C	-0.73745500	4.71514000	-1.25401700
N	-1.35171900	5.85820600	-0.82739500
N	-1.48528000	3.72046900	-1.72505400
C	-2.66928500	1.95882500	4.68144600
C	-3.85900800	1.52071700	3.83260100
O	-4.78055000	2.61606100	3.84413400
C	-3.40078400	1.16061000	2.42983100
S	-2.21245900	-0.12114800	2.31075300
C	-3.84708700	1.82313000	1.32989100
S	-3.15084100	1.53155400	-0.23475500
C	-4.99680100	2.80142300	1.44702900
C	-5.71331300	2.58524900	2.77897600
C	1.50758800	2.30719900	-4.02255400
C	2.17355400	1.66025600	-2.81080300
O	3.20654400	2.55813500	-2.38933000
C	1.20090000	1.38942500	-1.67065100
S	-0.36010800	0.67106600	-2.09648900
C	1.52147700	1.70225000	-0.39068200
S	0.32572900	1.56916500	0.91132100
C	2.90465300	2.17479800	0.00294300
C	3.84801000	2.09300000	-1.19804600
W	-1.24998800	-0.15406800	0.15898700
O	2.00781900	-4.23155700	0.61990300
C	-0.29448600	-1.68612500	1.11552600
C	0.09614600	-1.66007300	-0.12490100
C	-5.05101000	-3.86619500	-0.83755300
O	-5.42736600	-4.23980700	0.27442800
N	-4.55999000	-4.69127100	-1.78656400
N	-6.65973400	-2.16250500	-0.93101600
C	-7.48725900	-1.33610700	-1.62417100
O	-7.16279600	-0.76359200	-2.66109900
C	-4.45362300	-6.10020300	-1.54286600
C	-8.87937600	-1.16277800	-1.01754500
H	5.52369700	0.98491400	4.31952700
H	3.14586400	-1.37842400	4.11316500
H	2.72446400	-2.85830900	3.22842700
H	4.74897600	-3.19853800	4.66737700
H	5.80626700	-1.02017600	3.05176800
H	8.23522600	0.23374600	-3.94134600
H	9.15517400	-1.07379900	-3.20018400
H	7.38884000	0.50519200	-0.34031500
H	5.19335600	-0.58776900	0.30981700
H	6.69543200	-2.42302200	-4.58096500
H	4.67678800	-3.84136000	-4.66070800
H	3.41534700	-2.39617400	-0.78461800
H	3.03176400	-3.84896300	-2.79351300
H	2.96415200	4.78036300	-2.53856200
H	1.86681700	5.90869300	-3.35850700
H	2.12902700	5.66981900	-0.29971000
H	0.97426200	6.68751700	-1.17046100
H	0.97778000	3.69200000	-1.34074000
H	-2.36104900	5.85347400	-0.83542600
H	-0.92797100	6.35459200	-0.05761400

H	-2.36368000	3.49569000	-1.25305200
H	-1.02943000	2.84394300	-2.03484700
H	-4.38005000	-1.49495900	0.42280700
H	-4.75053700	-0.41224800	-0.94075500
H	-2.14300300	2.78135000	4.18865200
H	-1.96806800	1.13415700	4.82320700
H	-4.34522200	0.64618900	4.30207400
H	-5.69055200	2.66158200	0.60833800
H	-6.25811200	1.62659000	2.76272200
H	0.98885500	3.23077000	-3.74876000
H	0.78288300	1.62644400	-4.47333700
H	2.63850000	0.71004000	-3.12275200
H	3.29432700	1.53300800	0.80334500
H	4.18241700	1.06007700	-1.34265400
H	2.18045900	-3.30014500	0.88206200
H	-3.01799000	2.30005800	5.66204800
H	-4.63219800	3.83733800	1.39311600
H	-6.43672600	3.38288100	2.97922800
H	2.27301500	2.55221300	-4.76540900
H	3.19446200	6.53876100	-2.36402800
H	4.73346600	2.72075500	-1.05885000
H	2.86205800	3.20031600	0.40505700
H	6.49997100	0.94030800	5.81700900
H	7.22543900	0.53407300	4.23800300
H	9.05863600	0.49920100	-2.39887700
H	5.14743500	-3.39324500	2.95563600
H	-5.19509500	-2.35875500	-2.38958400
H	2.82777000	-4.48803700	0.18080700
H	-0.16462500	-2.20071300	2.05706700
H	-9.62507900	-1.37617100	-1.78790800
H	-9.06462600	-1.80212300	-0.14997000
H	-9.00531100	-0.11732700	-0.72072500
H	0.72940700	-2.16800000	-0.83578200
H	-4.14131500	-4.28422400	-2.60953300
H	-6.95828100	-2.60594700	-0.07222600
H	-5.05440300	-6.32983200	-0.66259700
H	-4.82949800	-6.66996700	-2.40019900
H	-3.42052400	-6.41269500	-1.34461300

Int1-Displacement-0.1-Structure4 optimized

C	6.32920200	0.44223500	5.04182100
C	5.94634800	-1.01456800	5.13919300
O	5.79138800	-1.59856900	6.20920300
N	5.76245900	-1.56965100	3.90867300
C	4.84320600	-2.67722600	3.76254600
C	3.44991100	-2.18278800	3.33475600
C	3.50641700	-1.46578000	1.97594600
O	4.33117400	-0.49307700	1.86144800
O	2.77390400	-1.89675300	1.05682700
C	-5.17521800	-2.49683000	-1.23244700
C	-4.26039500	-1.52694900	-0.50015200
S	-2.57506000	-1.61943400	-1.20539400
C	8.51036600	-0.11514700	-2.88941600
C	7.27753800	-0.58059000	-2.16829800
C	6.88585500	-0.18600000	-0.90728200
C	6.26232700	-1.50192600	-2.62303100
N	5.70489200	-0.78748200	-0.54337600
C	5.29636000	-1.59689300	-1.57858000
C	6.04857100	-2.26315500	-3.79090300
C	4.15032700	-2.39895100	-1.67316100
C	4.91685700	-3.06778400	-3.88510000
C	3.96945100	-3.13594600	-2.83466500
C	2.43543500	5.78297000	-2.10765700
C	1.38382400	5.76739700	-0.99874400
N	0.43366200	4.68111400	-1.23086500
C	-0.89196500	4.75020000	-1.17497000
N	-1.49742500	5.84176500	-0.62429100
N	-1.64735400	3.80653700	-1.73754000
C	-2.78831100	1.84372800	4.68164500
C	-3.93920500	1.35377900	3.80914100
O	-4.92580600	2.39039100	3.83549400
C	-3.44042500	1.05759200	2.40538600
S	-2.17521400	-0.14843100	2.27762300
C	-3.90512500	1.72745500	1.31750700
S	-3.17029100	1.52291500	-0.24327900
C	-5.10959800	2.63664900	1.44240500
C	-5.83638400	2.33699600	2.75197300
C	1.46987600	2.45689300	-4.03301600
C	2.13458300	1.74119000	-2.86001400
O	3.21923400	2.57499800	-2.44150800
C	1.16800900	1.48248700	-1.71178400
S	-0.40990400	0.79463100	-2.13324100
C	1.50492200	1.78453200	-0.43173100
S	0.31083300	1.69581800	0.87858200
C	2.90927500	2.20422600	-0.05178200
C	3.84110900	2.06969500	-1.25676900
W	-1.20834400	-0.09507800	0.12933400
O	1.93124300	-4.36906300	0.19024100
C	-0.15227100	-1.58384300	1.04423400
C	0.24662000	-1.48535500	-0.19091100
C	-5.00423100	-3.94811400	-0.89655600
O	-5.42449000	-4.43412100	0.15457300
N	-4.48364400	-4.66908900	-1.90591800
N	-6.58913800	-2.21520200	-0.86689700
C	-7.40136600	-1.33129300	-1.51623200
O	-7.03656300	-0.67258300	-2.48624000
C	-4.39140400	-6.08165100	-1.75894300
C	-8.84056100	-1.19622600	-0.97464500
H	5.43358200	1.03295000	4.81720300
H	3.07203800	-1.48950800	4.09677200
H	2.75671600	-3.02547000	3.26294300
H	4.79399800	-3.19873800	4.72163100
H	5.63216800	-0.90579800	3.13968400
H	8.26994600	0.39578800	-3.83173500
H	9.18092200	-0.94698200	-3.14522600
H	7.38082500	0.49836200	-0.22983300
H	5.18224700	-0.63387100	0.33971300
H	6.76047700	-2.22390100	-4.61287900
H	4.75437700	-3.65410600	-4.78665100
H	3.44163700	-2.41773300	-0.85538100
H	3.09098000	-3.76766300	-2.93676400
H	2.91600800	4.80589200	-2.20343800
H	1.97519400	6.03297900	-3.06850300
H	1.85714400	5.63240000	-0.01817000
H	0.83085500	6.71120300	-0.97839300
H	0.82483300	3.74103400	-1.36433800
H	-2.50663400	5.83357500	-0.60602200
H	-1.05429800	6.26369200	0.17849300

H	-2.50848400	3.53296900	-1.25889600
H	-1.17917300	2.95492800	-2.09414000
H	-4.22713500	-1.76570700	0.56737300
H	-4.66217400	-0.52462000	-0.63509700
H	-2.30894300	2.70834600	4.21361900
H	-2.03871600	1.06094500	4.81400400
H	-4.37553800	0.43952300	4.25082500
H	-5.77849500	2.48624700	0.58568500
H	-6.32221300	1.34872900	2.69625800
H	1.01464200	3.40050400	-3.71750800
H	0.69501800	1.83073200	-4.47940900
H	2.54310800	0.77868400	-3.21118000
H	3.27178300	1.55373300	0.75459100
H	4.11728800	1.01980200	-1.40523500
H	2.15854900	-3.52580100	0.63703800
H	-3.16731600	2.14061800	5.66545800
H	-4.80239800	3.69238800	1.42953400
H	-6.60947400	3.08388200	2.96171200
H	2.22466000	2.68117400	-4.79322300
H	3.19959900	6.53534800	-1.88590400
H	4.76144800	2.64552100	-1.12155800
H	2.91430600	3.23413600	0.34005900
H	6.74798500	0.78694200	5.98944400
H	7.04857300	0.62177100	4.23677400
H	9.08092700	0.58670900	-2.27203500
H	5.22749900	-3.38452400	3.01625100
H	-5.08971800	-2.31950900	-2.30771900
H	2.75739500	-4.61392200	-0.24356100
H	0.00476900	-2.12456500	1.96643600
H	-9.53428900	-1.41603100	-1.79018800
H	-9.05819100	-1.85285100	-0.12740400
H	-8.99915400	-0.15714900	-0.67427300
H	0.91477400	-1.92261500	-0.91606700
H	-3.99304300	-4.19113400	-2.64708300
H	-6.92301100	-2.74339300	-0.07109000
H	-5.23011900	-6.42348700	-1.15072500
H	-4.43438100	-6.56683700	-2.73919700
H	-3.46616100	-6.39957300	-1.25942200

Int1-Displacement-0.1-Structure5 optimized

C	6.27933400	0.86985600	4.82314500
C	5.93785300	-0.59724800	5.05804800
O	6.06917600	-1.12634000	6.16264000
N	5.46467500	-1.21346700	3.95093500
C	4.77399700	-2.49191500	3.96744500
C	3.34074200	-2.32879100	3.45412700
C	3.27370200	-1.75640000	2.02344700
O	4.03827700	-0.76672100	1.74791200
O	2.46320200	-2.28961600	1.23470500
C	-5.32631000	-2.24401600	-1.00088600
C	-4.14174700	-1.65894700	-0.23171500
S	-2.64277800	-1.58379700	-1.29519000
C	8.43864400	-0.32690800	-2.99566000
C	7.26998100	-0.73197600	-2.14792000
C	6.99761100	-0.32439300	-0.85797300
C	6.20019800	-1.62379200	-2.51844400
N	5.83608300	-0.90459000	-0.40033800
C	5.32403900	-1.69633200	-1.40053700
C	5.87749300	-2.36965600	-3.67025300
C	4.14860300	-2.45287800	-1.40082000
C	4.71630000	-3.13478200	-3.67473800
C	3.85905200	-3.17321300	-2.54993300
C	2.42871300	5.75927600	-2.57379100
C	1.57362000	5.70699700	-1.30657500
N	0.66498000	4.56116800	-1.34972300
C	-0.66429600	4.59076200	-1.31221300
N	-1.30821100	5.70065100	-0.84316100
N	-1.38709900	3.58915900	-1.80205100
C	-2.65147600	2.29103400	4.55605700
C	-3.82231000	1.80980100	3.70604800
O	-4.72735400	2.91368700	3.61012700
C	-3.33803000	1.34458000	2.34367000
S	-2.13747700	0.06887900	2.33165700
C	-3.79247600	1.89511600	1.18650500
S	-3.10587000	1.45020800	-0.34646700
C	-4.96090000	2.85771600	1.20595400
C	-5.66760300	2.77644400	2.55815300
C	1.49768700	2.28061400	-4.09663000
C	2.21092500	1.59448700	-2.93264700
O	3.24825300	2.49271500	-2.51871000
C	1.27981600	1.28222400	-1.76606400
S	-0.26792600	0.50561100	-2.12607300
C	1.63281700	1.61462600	-0.50102200
S	0.46793300	1.49794400	0.82795100
C	3.03065600	2.06284700	-0.13362700
C	3.93482600	1.99390700	-1.36592300
W	-1.18461600	-0.15942600	0.19201600
O	1.81156100	-4.55013400	-0.22355900
C	-0.37093500	-1.67917100	1.28279100
C	-0.03753900	-1.84037000	0.03295400
C	-5.45910300	-3.80922900	-0.84980500
O	-6.46622500	-4.28583500	-0.31470200
N	-4.45935200	-4.59694400	-1.32561600
N	-6.59611000	-1.71949800	-0.55022200
C	-7.40534000	-1.06304900	-1.43858900
O	-7.01063500	-0.48735300	-2.44470000
C	-4.50362300	-6.06587700	-1.22125400
C	-8.86343000	-1.16597300	-1.06412700
H	5.47113700	1.49252000	5.22328600
H	2.79606200	-1.64701800	4.12123800
H	2.81909400	-3.28989000	3.46510700
H	4.79603000	-2.87030500	4.99350200
H	5.19498100	-0.66801300	3.12609700
H	8.11978900	0.15680900	-3.92884000
H	9.05847300	-1.18708500	-3.28310900
H	7.56562600	0.34566600	-0.22531200
H	5.31851100	-0.76181200	0.47778000
H	6.52409700	-2.34525700	-4.54485100
H	4.45741200	-3.71015300	-4.56048400
H	3.48844200	-2.46483000	-0.54142800
H	2.94424800	-3.75882700	-2.58579800
H	2.97513200	4.82152800	-2.70702900
H	1.80069100	5.92331300	-3.45450300
H	2.20647600	5.62435500	-0.41563200
H	0.97829200	6.61871800	-1.20926500
H	1.08453200	3.63481600	-1.47826600
H	-2.31679800	5.65755400	-0.82753500
H	-0.88795600	6.18298500	-0.06246100

H	-2.26423000	3.33661100	-1.33856900
H	-0.92126600	2.72629300	-2.12371500
H	-3.92535900	-2.23355900	0.67591600
H	-4.42052900	-0.64966000	0.06408900
H	-2.09503100	3.06630200	4.02102700
H	-1.96937900	1.46812400	4.78053100
H	-4.33505800	0.97823700	4.22377900
H	-5.65450500	2.61230000	0.39211100
H	-6.20916100	1.81989000	2.64260100
H	0.99566200	3.19713400	-3.77627800
H	0.75268200	1.61452800	-4.53688200
H	2.67289600	0.66059400	-3.29249700
H	3.41162400	1.38861300	0.64289500
H	4.25312500	0.96281600	-1.55583000
H	1.96834000	-3.84476900	0.42773100
H	-3.02398700	2.70940400	5.49673700
H	-4.61700700	3.88800900	1.03343300
H	-6.39165000	3.58859800	2.68207100
H	2.23298300	2.54490400	-4.86349500
H	3.14741600	6.58205000	-2.50350400
H	4.83019700	2.61122800	-1.24673100
H	3.02251000	3.07780100	0.29502700
H	7.19019200	1.12110100	5.37245700
H	6.41069400	1.11459000	3.76576200
H	9.08596500	0.37988100	-2.46528500
H	5.31226100	-3.21490400	3.33782900
H	-5.21950600	-1.98521500	-2.05990200
H	2.69135200	-4.73919000	-0.57310700
H	-0.25870200	-2.10889500	2.26880900
H	-9.24355300	-2.14504800	-1.37761300
H	-9.01776100	-1.08014100	0.01600600
H	-9.43597800	-0.39102500	-1.57665100
H	0.47754400	-2.50534900	-0.64627400
H	-3.60730100	-4.14533000	-1.64333000
H	-7.07320000	-2.38819700	0.04968800
H	-5.50898500	-6.33908900	-0.90249000
H	-4.28388700	-6.51720700	-2.19334700
H	-3.77797300	-6.43127100	-0.48637700

Int1-Displacement-0.1-Structure6 optimized

C	6.39619000	0.52155300	4.88329200
C	6.00819000	-0.93776100	5.01084100
O	5.98350500	-1.52615100	6.09065100
N	5.67073000	-1.48391900	3.81351900
C	4.80928200	-2.64632600	3.73637500
C	3.39014300	-2.24064100	3.30036600
C	3.40034100	-1.57230400	1.91424000
O	4.16612200	-0.55449600	1.77094900
O	2.69360400	-2.07787600	1.01515800
C	-5.19217500	-2.40953400	-1.26355800
C	-4.29809400	-1.35872900	-0.62599300
S	-2.60941400	-1.48024500	-1.32653900
C	8.47285200	-0.08173900	-2.90757200
C	7.26574300	-0.52463800	-2.15101300
C	6.85291500	-0.10883200	-0.90409800
C	6.28304200	-1.46904700	-2.60424400
N	5.67295100	-0.72437100	-0.55300600
C	5.30010300	-1.55796300	-1.58074100
C	6.12896600	-2.25029400	-3.76579300
C	4.17127900	-2.37555100	-1.69207100
C	5.01984600	-3.07933600	-3.87376800
C	4.05152600	-3.13457100	-2.84498400
C	2.22573700	5.83257600	-2.19142500
C	1.23805100	5.73611800	-1.02609000
N	0.31284500	4.61390800	-1.20628500
C	-0.99099500	4.68256200	-1.45245600
N	-1.67728500	5.83581100	-1.19894700
N	-1.64018800	3.66319200	-2.01755900
C	-2.72824100	1.81524100	4.76252800
C	-3.89330400	1.41247800	3.86501600
O	-4.81443900	2.50776500	3.89174400
C	-3.39409200	1.10605500	2.46401000
S	-2.20060000	-0.16697600	2.33083300
C	-3.81389500	1.80634500	1.37575900
S	-3.07771400	1.56711300	-0.17517800
C	-4.96807300	2.77878800	1.49842100
C	-5.71917300	2.51440000	2.80237300
C	1.51500200	2.48779900	-3.90713600
C	2.20386000	1.81140100	-2.72422800
O	3.22600300	2.70897300	-2.28027000
C	1.24231700	1.48083700	-1.59076700
S	-0.28647300	0.70974500	-2.03780300
C	1.55470200	1.76429600	-0.30260300
S	0.37603000	1.53904400	1.00177300
C	2.92574900	2.26324400	0.10126800
C	3.87163000	2.22376600	-1.10019900
W	-1.20483800	-0.14892800	0.19677800
O	1.93566900	-4.45248800	-0.17365100
C	-0.29838900	-1.72521400	1.12648000
C	0.08809400	-1.69829800	-0.11533700
C	-4.93785500	-3.84765600	-0.84872300
O	-5.21101100	-4.24203800	0.28522000
N	-4.54685000	-4.65600800	-1.85979500
N	-6.58925600	-2.17271600	-0.86082800
C	-7.48328100	-1.45107700	-1.59060600
O	-7.21406900	-0.92997400	-2.66955800
C	-4.43720100	-6.07684900	-1.67679100
C	-8.87835300	-1.32673100	-0.97554800
H	5.49050500	1.13705800	4.93471800
H	2.98158100	-1.53688600	4.03650500
H	2.74049100	-3.11952000	3.26612300
H	4.79948200	-3.11982700	4.72163800
H	5.46667500	-0.83779500	3.04522200
H	8.20782900	0.39426400	-3.86173600
H	9.13942900	-0.92064200	-3.15115500
H	7.32536800	0.59629400	-0.23216300
H	5.11964700	-0.59447700	0.31461500
H	6.86635500	-2.20587200	-4.56450300
H	4.88727100	-3.69014600	-4.76364800
H	3.43192500	-2.38965200	-0.90112400
H	3.18243800	-3.77780500	-2.96197000
H	2.77330300	4.89464600	-2.31015300
H	1.69890400	6.05174100	-3.12560600
H	1.76891400	5.58596600	-0.08039900
H	0.66140800	6.66018400	-0.93557500
H	0.72485200	3.67107000	-1.20628600
H	-2.66674500	5.82359600	-1.39630600
H	-1.40232800	6.37799000	-0.39370500

H	-2.58791200	3.47902300	-1.69531700
H	-1.13538400	2.76479400	-2.16401300
H	-4.26450300	-1.50538100	0.45678100
H	-4.72582000	-0.38089400	-0.84248200
H	-2.18929700	2.65626700	4.31705900
H	-2.03097300	0.98497500	4.89037800
H	-4.39361100	0.52142400	4.28625600
H	-5.64003900	2.66908600	0.63756400
H	-6.26171200	1.55643600	2.73771700
H	0.97993800	3.39012200	-3.59961000
H	0.80377600	1.80674700	-4.37864500
H	2.67958600	0.87963300	-3.07375400
H	3.31858100	1.60781100	0.88884200
H	4.21996600	1.19882300	-1.26938900
H	2.12913700	-3.68742900	0.40732800
H	-3.10289500	2.11763300	5.74641100
H	-4.60172300	3.81521100	1.49210500
H	-6.44894600	3.30384800	3.01192500
H	2.26980600	2.77489400	-4.64600100
H	2.93967200	6.64188200	-2.00266500
H	4.74812000	2.86027600	-0.94460900
H	2.86204400	3.27885500	0.52366400
H	7.04913300	0.80625500	5.71126900
H	6.89225000	0.73801500	3.93283700
H	9.06073600	0.64367600	-2.33424200
H	5.22042000	-3.37083000	3.02070200
H	-5.15787600	-2.29555100	-2.35064600
H	2.78664300	-4.62035000	-0.59645700
H	-0.18967300	-2.25906400	2.06003300
H	-9.61209200	-1.68940600	-1.70045300
H	-8.99807500	-1.87571000	-0.03737900
H	-9.08884800	-0.26822800	-0.79790000
H	0.68777300	-2.23392600	-0.83584600
H	-4.22284500	-4.23097500	-2.71536800
H	-6.85248300	-2.59708400	0.01852300
H	-4.93458900	-6.32748600	-0.73931600
H	-4.92186600	-6.61102700	-2.50181400
H	-3.39330400	-6.40795600	-1.61191400

Int1-Displacement-0.1-Structure7 optimized

C	6.34817700	0.43938500	5.12031300
C	5.93028800	-1.04302000	5.12305300
O	6.02189200	-1.72032700	6.14740100
N	5.47132100	-1.50476300	3.93105800
C	4.75728300	-2.77469900	3.74814000
C	3.33688500	-2.50207700	3.24516700
C	3.35562200	-1.80486600	1.87348700
O	4.07113400	-0.75006900	1.76198500
O	2.68877600	-2.33309700	0.95730900
C	-5.23329300	-2.23910000	-1.19628600
C	-4.12720200	-1.68149800	-0.30862000
S	-2.54119400	-1.62329900	-1.22310400
C	8.37912400	0.00660900	-2.98524900
C	7.23102100	-0.44875000	-2.16014100
C	6.87031500	-0.08922500	-0.87990800
C	6.24448800	-1.37860400	-2.61548600
N	5.70973400	-0.73597700	-0.51194000
C	5.30435400	-1.52381200	-1.56342300
C	6.06910000	-2.09623200	-3.81284200
C	4.17943600	-2.34129600	-1.68144000
C	4.96536000	-2.92725700	-3.92837200
C	4.03696400	-3.03471300	-2.86966600
C	2.39862800	5.83953100	-2.19438100
C	1.45605700	5.81586600	-0.98960900
N	0.52200400	4.69420500	-1.09263700
C	-0.80625000	4.74994200	-1.09625200
N	-1.44492100	5.86989400	-0.64706800
N	-1.52977400	3.75880100	-1.61224200
C	-2.79210900	1.84750500	4.74270200
C	-3.91963200	1.35679200	3.84073200
O	-4.90427900	2.39453000	3.83599700
C	3.39086400	1.05129400	2.44939500
S	-2.12185400	-0.15042700	2.34839300
C	-3.85148300	1.69457600	1.34192800
S	-3.11455700	1.44793400	-0.20986000
C	-5.06451100	2.59648500	1.43644400
C	-5.80379000	2.31749700	2.74359700
C	1.40433800	2.60921400	-3.92474100
C	2.12932000	1.83072200	-2.82608100
O	3.21034700	2.66183000	-2.39103400
C	1.21221100	1.47721800	-1.66255200
S	-0.33923300	0.72670000	-2.06175700
C	1.56661500	1.75716800	-0.38331300
S	0.40519600	1.58998100	0.94761100
C	2.96945100	2.19166600	-0.01604100
C	3.87093900	2.11098700	-1.24827400
W	-1.14881600	-0.14794500	0.20615400
O	1.88318000	-4.56622300	-0.44003100
C	-0.16886600	-1.66159900	1.15986800
C	0.17838800	-1.66705500	-0.09439800
C	-5.34043200	-3.80793700	-1.15592900
O	-6.24020000	-4.34181700	-0.49947300
N	-4.46398700	-4.55169300	-1.87901400
N	-6.55326900	-1.78989000	-0.75859700
C	-7.34647000	-0.98767000	-1.53103900
O	-6.94051700	-0.32465200	-2.47934500
C	-4.54396300	-6.02205500	-1.88246500
C	-8.81794700	-0.99900500	-1.12589800
H	5.63362100	1.00301600	5.72876800
H	2.81982200	-1.86190400	3.97110700
H	2.77989300	-3.43851000	3.15352300
H	4.75637300	-3.29194400	4.71151800
H	5.23990000	-0.84700100	3.18239400
H	8.04654600	0.49666000	-3.91059700
H	9.02447600	-0.82925000	-3.28906400
H	7.36286000	0.59008100	-0.19619700
H	5.16811700	-0.65242000	0.36431700
H	6.78335300	-1.99898600	-4.62740600
H	4.80268100	-3.49479200	-4.84137200
H	3.46013500	-2.40425900	-0.87444000
H	3.16512800	-3.67372700	-2.99463400
H	2.91383600	4.88236900	-2.30433100
H	1.84020600	6.03829000	-3.11432500
H	2.02354500	5.71916600	-0.05665000
H	0.87958400	6.74345400	-0.93437200
H	0.92568900	3.75608600	-1.19697700
H	-2.45371300	5.85520300	-0.67533700
H	-1.04006600	6.35415700	0.14022000

H	-2.41827000	3.51394900	-1.17336800
H	-1.05636200	2.89688600	-1.93372500
H	-4.00387700	-2.27778200	0.60231900
H	-4.41930600	-0.67367300	-0.02213300
H	-2.30186700	2.71304700	4.28777000
H	-2.04526300	1.06542900	4.89407800
H	-4.36942400	0.44520100	4.27494900
H	-5.72102400	2.42496300	0.57464200
H	-6.28421200	1.32622900	2.70131400
H	0.92383900	3.50873700	-3.53179600
H	0.63998200	1.98701900	-4.39494600
H	2.54513000	0.90439500	-3.25606500
H	3.35016600	1.51476100	0.75941800
H	4.14446900	1.06902500	-1.44815300
H	2.09366900	-3.87059200	0.21608400
H	-3.19686700	2.14347500	5.71640900
H	-4.76290700	3.65344200	1.40755300
H	-6.58217900	3.06452000	2.93156000
H	2.12827000	2.91429900	-4.68680100
H	3.14246400	6.63336300	-2.06621700
H	4.79243400	2.68550300	-1.11639800
H	2.97077500	3.20741600	0.41128800
H	7.32855700	0.52806400	5.59545400
H	6.38413200	0.87918000	4.12005700
H	9.01122800	0.72335200	-2.44839600
H	5.29829000	-3.40269600	3.02803800
H	-5.08649300	-1.88577000	-2.22105200
H	2.72951100	-4.70333100	-0.88281900
H	-0.01914100	-2.17002900	2.10174700
H	-9.34299100	-1.76224900	-1.71124600
H	-8.96355400	-1.22141500	-0.06491900
H	-9.25951800	-0.02926900	-1.36219400
H	0.75403500	-2.22241700	-0.81955100
H	-3.63959000	-4.09563200	-2.25126200
H	-7.01448300	-2.48721300	-0.18088000
H	-5.59322300	-6.31391400	-1.94456500
H	-3.99951000	-6.39919900	-2.75036500
H	-4.11593100	-6.45641400	-0.97186600

Int1-Displacement-0.1-Structur8 optimized

C	6.39820500	0.95441500	4.96309700
C	5.97151900	-0.51073600	5.16526000
O	6.00653300	-1.03315600	6.27979700
N	5.57262500	-1.13353400	4.02763800
C	4.84057300	-2.40256100	3.97625400
C	3.43242200	-2.17104400	3.41089900
C	3.40162600	-1.48829000	2.02340000
O	4.23785100	-0.54634000	1.79982900
O	2.53773700	-1.89363700	1.21232100
C	-5.37399200	-2.37969600	-0.99691400
C	-4.15051800	-1.76676700	-0.28917400
S	-2.70065200	-1.59679500	-1.41157300
C	8.49199800	-0.40209600	-3.08129100
C	7.31171600	-0.76016300	-2.22523500
C	6.98563200	-0.20832700	-1.00393800
C	6.27752900	-1.72435200	-2.51297900
N	5.81661600	-0.75001600	-0.51905700
C	5.35930800	-1.67537200	-1.42713800
C	6.01579500	-2.62966000	-3.56185700
C	4.19763700	-2.45459000	-1.37137000
C	4.87986700	-3.42976600	-3.49926200
C	3.97392100	-3.33884000	-2.41468800
C	2.42431400	5.70706000	-2.65352100
C	1.47767400	5.70013800	-1.45179600
N	0.60269400	4.52827600	-1.49493600
C	-0.72872700	4.51698600	-1.48841800
N	-1.41808900	5.62804500	-1.09422900
N	-1.40650600	3.46714800	-1.94141100
C	-2.65903200	2.39711300	4.56232300
C	-3.80690800	1.94540300	3.66410900
O	-4.67793800	3.07254700	3.53345600
C	-3.31370200	1.44702700	2.31299700
S	-2.15902900	0.12914700	2.32048100
C	-3.78177000	1.95126700	1.13981600
S	-3.16704700	1.38805400	-0.38820700
C	-4.92286400	2.94657200	1.13218400
C	-5.62538700	2.92814200	2.48900500
C	1.56531000	2.17762600	-4.14648300
C	2.23251800	1.54720300	-2.92336400
O	3.23291300	2.48315000	-2.50213500
C	1.27257700	1.24370700	-1.77342400
S	-0.24214400	0.40814700	-2.13957300
C	1.58461100	1.60366000	-0.50463000
S	0.41330400	1.43698500	0.80790900
C	2.95109500	2.12287800	-0.11101600
C	3.89417900	2.04628300	-1.31134600
W	-1.24983600	-0.19170500	0.16031900
O	1.90108300	-4.41347800	0.28050600
C	-0.50232900	-1.73330200	1.27285300
C	-0.17096800	-1.92045800	0.02959500
C	-5.47814900	-3.90550400	-0.85003300
O	-6.49558900	-4.43573200	-0.38713200
N	-4.42260900	-4.64115200	-1.24590600
N	-6.60267600	-1.86687500	-0.45423800
C	-7.37908100	-1.05796200	-1.22948100
O	-6.96775100	-0.35164100	-2.14120700
C	-4.49608300	-6.07752500	-1.06710100
C	-8.82305900	-1.20963500	-0.86593100
H	5.66967300	1.60060700	5.46339900
H	2.87195300	-1.53231500	4.10665000
H	2.89470500	-3.12042200	3.33233600
H	4.80515300	-2.81075100	4.98989600
H	5.37374400	-0.57641500	3.19150200
H	8.18475700	-0.01157900	-4.06079900
H	9.13952300	-1.26772800	-3.27598900
H	7.51622500	0.54829100	-0.44013600
H	5.31952000	-0.55203400	0.36216800
H	6.69240200	-2.70387900	-4.41063400
H	4.67535700	-4.13077400	-4.30509300
H	3.49632300	-2.33807200	-0.55248400
H	3.07816100	-3.95441000	-2.40437600
H	2.98338500	4.76982300	-2.70748200
H	1.86202000	5.82734200	-3.58458400
H	2.04526400	5.68647600	-0.51385100
H	0.85352300	6.59789800	-1.45032600
H	1.05094700	3.60916800	-1.55587800
H	-2.42509300	5.55495300	-1.10196700
H	-1.03210300	6.16882700	-0.33461900

H	-2.28875100	3.20762800	-1.49011500
H	-0.90201700	2.61053900	-2.21716900
H	-3.87343400	-2.35096800	0.59605600
H	-4.44864000	-0.77408600	0.04252900
H	-2.07124200	3.17056600	4.05935000
H	-1.99891600	1.55981500	4.79865900
H	-4.36132300	1.13153500	4.16785400
H	-5.62633000	2.69589400	0.32878900
H	-6.19198800	1.98959700	2.60590700
H	1.03680100	3.09916400	-3.88554500
H	0.84874700	1.48505300	-4.59399200
H	2.72987800	0.61232600	-3.23045500
H	3.34388200	1.49421300	0.69861400
H	4.25072100	1.01913900	-1.44626000
H	2.05115300	-3.56048900	0.74317100
H	-3.05977400	2.80842900	5.49438100
H	-4.55016600	3.96133800	0.92898600
H	-6.32685100	3.76312200	2.58935400
H	2.33300100	2.42159900	-4.88663700
H	3.12958100	6.54038800	-2.56669100
H	4.76532900	2.69636500	-1.18495600
H	2.88510600	3.15179700	0.27776800
H	7.36487500	1.11154500	5.44924100
H	6.46542000	1.24569000	3.91172800
H	9.10794200	0.36544400	-2.60059600
H	5.38819900	-3.11422300	3.34413400
H	-5.32502000	-2.10919700	-2.05900600
H	2.76143100	-4.59739700	-0.11591100
H	-0.41652400	-2.14324000	2.26949800
H	-9.20768500	-2.13461100	-1.31145700
H	-8.96881100	-1.27910100	0.21646300
H	-9.40855200	-0.37358000	-1.25412200
H	0.33178600	-2.60849100	-0.63447700
H	-3.55388400	-4.18082900	-1.49950600
H	-7.10438300	-2.59261000	0.05269900
H	-5.35824100	-6.48355000	-1.60348000
H	-3.58301100	-6.53183400	-1.45749400
H	-4.60464600	-6.34435200	-0.01018700

Int1-Displacement-0.1-Structure9 optimized

C	6.47029700	0.10093400	4.93725600
C	5.99283100	-1.32909400	5.01688700
O	5.76473500	-1.90512600	6.07706000
N	5.81434200	-1.87314200	3.77611100
C	4.78745200	-2.88179100	3.60764200
C	3.43518200	-2.23452200	3.25560000
C	3.53689800	-1.48125300	1.92128900
O	4.39705100	-0.53673000	1.84566700
O	2.81494100	-1.87191400	0.97492900
C	-5.31326900	-2.19388200	-1.22745500
C	-4.14612000	-1.73628600	-0.35266000
S	-2.56687000	-1.65945000	-1.27887300
C	8.47390700	-0.10557500	-2.98617400
C	7.23118600	-0.55889300	-2.27146600
C	6.85622100	-0.19018800	-0.99763600
C	6.19084900	-1.44316900	-2.74398100
N	5.66286100	-0.77302000	-0.64180700
C	5.23040000	-1.54684500	-1.69488800
C	5.95185900	-2.16641900	-3.93104200
C	4.07157100	-2.33001300	-1.80060900
C	4.80363300	-2.94560800	-4.03885100
C	3.86585200	-3.02961000	-2.98093600
C	2.37328500	6.00353700	-1.94914500
C	1.38639200	5.90537300	-0.78449400
N	0.47052600	4.78220000	-0.98511600
C	-0.85838300	4.80803400	-0.91859300
N	-1.49256200	5.87959400	-0.35844300
N	-1.58678500	3.84284200	-1.47405500
C	-2.65473600	1.59721800	4.76862500
C	-3.81375500	1.13490500	3.88827600
O	-4.80195600	2.16674500	3.96788600
C	-3.34160900	0.88672600	2.46348500
S	-2.09006000	-0.32151200	2.26107400
C	-3.83340000	1.59016600	1.40526300
S	-3.15306300	1.42982100	-0.18485100
C	-5.03296900	2.49625500	1.58957200
C	-5.73408900	2.14902100	2.90096600
C	1.49628000	2.72457700	-3.87288300
C	2.16475800	1.95007800	-2.73952500
O	3.21091300	2.79436100	-2.24724300
C	1.19518600	1.57817400	-1.62279000
S	-0.36765500	0.88679800	-2.09880900
C	1.51278300	1.80711200	-0.32213400
S	0.31657200	1.59792500	0.97003300
C	2.89771800	2.24707500	0.10341200
C	3.84399800	2.23040400	-1.09635500
W	-1.15739800	-0.16450600	0.10249900
O	1.99066300	-4.38340300	0.18316100
C	-0.09449800	-1.70749700	0.91068500
C	0.32375400	-1.49715100	-0.30380800
C	-5.47414600	-3.76548500	-1.31068600
O	-6.50853400	-4.29553100	-0.88882600
N	-4.48664100	-4.52536700	-1.84568500
N	-6.57847400	-1.74312500	-0.69429400
C	-7.35678800	-0.87392600	-1.40486100
O	-6.94039500	-0.10124300	-2.25922300
C	-4.62983000	-5.99347500	-1.90894800
C	-8.81554200	-1.01069000	-1.04389300
H	5.65116500	0.73051700	4.57167600
H	3.15794600	-1.53915200	4.05706000
H	2.66075000	-3.00246000	3.17726000
H	4.71733600	-3.44624700	4.54053200
H	5.74502600	-1.18367200	3.02313500
H	8.24314300	0.43519200	-3.91407100
H	9.12193700	-0.94744400	-3.26529000
H	7.37074800	0.46369600	-0.30484600
H	5.16217200	-0.64003900	0.25697000
H	6.65783200	-2.11804800	-4.75763800
H	4.62235800	-3.50180200	-4.95573000
H	3.37834700	-2.36865100	-0.97091900
H	2.97789700	-3.64641400	-3.09294700
H	2.89793500	5.05560300	-2.09310400
H	1.84896400	6.25137100	-2.87717700
H	1.92130900	5.76842100	0.16327100
H	0.79482000	6.82188800	-0.70571600
H	0.88763000	3.85924200	-1.14660900
H	-2.50095000	5.84022100	-0.33248100
H	-1.05808000	6.30859400	0.44531600

H	-2.45696800	3.55714900	-1.02190300
H	-1.10992800	3.00731900	-1.85948500
H	-4.01458500	-2.39074800	0.51699200
H	-4.39477000	-0.74069200	0.00665000
H	-2.18424700	2.48198200	4.33002200
H	-1.89993500	0.81363200	4.86205400
H	-4.24094900	0.20358100	4.30272700
H	-5.71745600	2.37987700	0.74047900
H	-6.21948700	1.16265100	2.81958200
H	0.99644700	3.62426300	-3.50247400
H	0.75577000	2.10391200	-4.38152400
H	2.61477500	1.03029200	-3.14921600
H	3.27827800	1.55521600	0.86572400
H	4.15844000	1.20332700	-1.31501300
H	2.21809700	-3.51826200	0.58680400
H	-3.02702900	1.85263400	5.76626000
H	-4.72159700	3.55066600	1.61227800
H	-6.50358700	2.88672900	3.15193300
H	2.25789900	3.03042000	-4.59668400
H	3.10733200	6.79069400	-1.74716100
H	4.74131800	2.82878600	-0.91190400
H	2.86151000	3.24618200	0.56694000
H	6.78230400	0.45082200	5.92288900
H	7.30069900	0.20886700	4.23158000
H	9.06338700	0.56569000	-2.35288900
H	5.08027800	-3.57962300	2.81329300
H	-5.19034800	-1.77454300	-2.23187100
H	2.78887400	-4.60749300	-0.31033000
H	0.05566300	-2.32026900	1.78765900
H	-9.23261300	-1.88192400	-1.56218900
H	-8.96000300	-1.16218700	0.03015800
H	-9.36501900	-0.12334500	-1.36299100
H	1.01365600	-1.85310000	-1.05244300
H	-3.60012000	-4.09009000	-2.07472900
H	-7.07976600	-2.51128200	-0.25359900
H	-5.47527700	-6.26373100	-2.54768300
H	-3.70999100	-6.40893100	-2.32303200
H	-4.80579800	-6.40960000	-0.91280600

Int1-Displacement-0.1-Structure10 optimized

C	6.43878400	0.58639500	5.04322400
C	5.96772300	-0.87722300	5.12772600
O	5.98859300	-1.48900400	6.19614900
N	5.54696000	-1.39367500	3.94540300
C	4.77799300	-2.63333500	3.79484100
C	3.38084700	-2.31782700	3.24374300
C	3.38588400	-1.53847300	1.90877500
O	4.22705300	-0.58411800	1.77535900
O	2.54834700	-1.88697700	1.04526900
C	-5.26588200	-2.36339400	-1.14946900
C	-4.08810000	-1.73916700	-0.38805200
S	-2.64388000	-1.48277500	-1.49748700
C	8.46148100	-0.17789400	-3.09980000
C	7.30509700	-0.57310500	-2.24187700
C	6.96232400	-0.08390600	-0.99977500
C	6.30019700	-1.54066200	-2.58409900
N	5.80090800	-0.67464300	-0.55183100
C	5.37222100	-1.56440200	-1.50825100
C	6.08554600	-2.38824600	-3.68801000
C	4.23100000	-2.37141200	-1.51658000
C	4.97023600	-3.21550300	-3.68910100
C	4.05264200	-3.19709100	-2.61380800
C	2.35818400	5.83385400	-2.33521100
C	1.44242200	5.77283400	-1.11078500
N	0.54631500	4.61795800	-1.19030600
C	-0.78350100	4.63348900	-1.24269400
N	-1.46995400	5.74446500	-0.84360600
N	-1.46065800	3.60955500	-1.75404100
C	-2.75422800	2.04127700	4.70042800
C	-3.89163700	1.63935800	3.76905900
O	-4.78230200	2.75727900	3.71429100
C	-3.37008100	1.25657700	2.39382100
S	-2.17824300	-0.02529200	2.33017200
C	-3.82377200	1.84592300	1.25627900
S	-3.15643200	1.42577400	-0.29407400
C	-4.98335300	2.81813600	1.30593800
C	-5.70853400	2.68056600	2.64415000
C	1.47987400	2.46287700	-3.98638100
C	2.19015300	1.74974200	-2.83522400
O	3.21192400	2.64528900	-2.38296700
C	1.25795300	1.37705000	-1.68696900
S	-0.25855800	0.56761800	-2.08855000
C	1.58830500	1.66175200	-0.40431100
S	0.43425800	1.40600600	0.91209000
C	2.96074800	2.16266100	-0.00827600
C	3.88395000	2.13762400	-1.22661300
W	-1.23131500	-0.17973600	0.17181700
O	1.92412800	-4.39364000	0.07737200
C	-0.48110700	-1.78553800	1.18586700
C	-0.13475000	-1.88395600	-0.06377900
C	-5.36764900	-3.89020100	-0.97843600
O	-6.33010600	-4.40894200	-0.40278600
N	-4.37163000	-4.63922400	-1.49513700
N	-6.54661900	-1.85081800	-0.67729300
C	-7.36146300	-1.10213600	-1.48130300
O	-6.98795500	-0.51504800	-2.49001200
C	-4.44256300	-6.08070700	-1.33500500
C	-8.81086900	-1.08512600	-1.01805100
H	5.72194200	1.21397500	5.58266800
H	2.83697400	-1.71266700	3.98124200
H	2.81652400	-3.24274000	3.09392000
H	4.72459100	-3.11571200	4.77456200
H	5.36429900	-0.76374500	3.15890600
H	8.13294300	0.23609700	-4.06278900
H	9.11431000	-1.03069600	-3.33113600
H	7.47100300	0.65674500	-0.39622000
H	5.29171600	-0.52260200	0.33238000
H	6.78067800	-2.39455300	-4.52481000
H	4.78976400	-3.87781600	-4.53232500
H	3.51035400	-2.31818300	-0.70908200
H	3.17126600	-3.83302500	-2.65218600
H	2.91021000	4.89821700	-2.45023200
H	1.77306800	6.00499900	-3.24410900
H	2.03236800	5.69521500	-0.19058500
H	0.83565200	6.67946900	-1.04036600
H	0.97897300	3.69185300	-1.27314700
H	-2.47649400	5.69535100	-0.90279700
H	-1.10760600	6.25768700	-0.05398000

H	-2.35874200	3.34933100	-1.33931800
H	-0.95775100	2.75538700	-2.04374800
H	-3.79817900	-2.35360200	0.47179000
H	-4.42377700	-0.77276100	-0.01574600
H	-2.17561400	2.85556600	4.25454100
H	-2.08358700	1.19854900	4.88006700
H	-4.43430900	0.78053000	4.20627900
H	-5.66913100	2.62010500	0.47288600
H	-6.26068400	1.72669000	2.67604700
H	0.95896900	3.36031800	-3.64201600
H	0.75091200	1.79999100	-4.45747500
H	2.66728100	0.83386600	-3.22168100
H	3.36564100	1.49961900	0.76703100
H	4.22441900	1.11436800	-1.41992100
H	2.06947300	-3.54399400	0.54835600
H	-3.16116700	2.38145700	5.65842200
H	-4.62546800	3.85151800	1.18972700
H	-6.42636300	3.49342700	2.79694900
H	2.22015500	2.76359100	-4.73398000
H	3.07027600	6.65878300	-2.22448800
H	4.76561800	2.76887500	-1.08004000
H	2.90341100	3.17443500	0.42469500
H	7.40260500	0.67662000	5.55124100
H	6.52859800	0.95473000	4.01803200
H	9.08128900	0.58280500	-2.61233800
H	5.30782200	-3.31156800	3.11278400
H	-5.18194000	-2.10358600	-2.21040900
H	2.78487200	-4.56939100	-0.32185800
H	-0.40590700	-2.26589400	2.15155500
H	-9.33873000	-1.93766400	-1.46064100
H	-8.90352700	-1.15647900	0.06957300
H	-9.29025300	-0.16928600	-1.36790200
H	0.37583900	-2.52190500	-0.77000900
H	-3.52556200	-4.18767600	-1.82417500
H	-7.01004500	-2.51646900	-0.06475200
H	-5.38908300	-6.45414200	-1.73422100
H	-3.61418600	-6.53956700	-1.87876600
H	-4.38387200	-6.37417800	-0.28092600

Int1-Displacement-0.15-Structure1 optimized

C	6.54982100	-0.06929800	4.89315100
C	6.10690500	-1.51778900	4.91399200
O	6.05639000	-2.18468500	5.94597500
N	5.75057900	-1.95634200	3.67841200
C	4.83058600	-3.06258400	3.51574500
C	3.42502400	-2.55264500	3.14959400
C	3.42546800	-1.72822400	1.84791000
O	4.25615500	-0.75562600	1.77917900
O	2.63103000	-2.06745900	0.94207100
C	-5.24439900	-2.20088000	-1.32035200
C	-4.08749600	-1.58891600	-0.52277900
S	-2.62100100	-1.30541700	-1.59123600
C	8.21852700	0.15367000	-3.19868300
C	7.13494900	-0.32379600	-2.31028600
C	6.85812800	-0.04639300	-0.99067800
C	6.11329000	-1.20690800	-2.76698000
N	5.71193200	-0.70752200	-0.59834100
C	5.23221400	-1.41408800	-1.67589300
C	5.87579000	-1.82467000	-4.00638200
C	4.08975100	-2.20452200	-1.80139700
C	4.75596500	-2.62919800	-4.13038400
C	3.88504600	-2.79833500	-3.03502400
C	2.37959700	5.95755100	-1.64365800
C	1.41116100	5.77954000	-0.47319900
N	0.48240000	4.67807500	-0.73498700
C	-0.83991400	4.75089900	-0.84728600
N	-1.50987000	5.83550400	-0.35851300
N	-1.52728800	3.81598600	-1.50259400
C	-2.64680300	1.43910900	4.88011600
C	-3.81373000	1.13208300	3.94961000
O	-4.71689200	2.23546500	4.06089400
C	-3.32231900	0.93027400	2.52687600
S	-2.12985200	-0.32669200	2.28658400
C	-3.77301400	1.68569600	1.48877500
S	-3.09533800	1.50852500	-0.09877300
C	-4.92799400	2.64441800	1.69056900
C	-5.64832100	2.30828800	2.99554300
C	1.48322400	2.83580300	-3.73645400
C	2.20277300	2.01226000	-2.66984500
O	3.24768800	2.84200200	-2.15159500
C	1.27181000	1.55539600	-1.55454900
S	-0.27143200	0.84154400	-2.03430700
C	1.61538500	1.70637000	-0.25310400
S	0.45609300	1.36393000	1.04340000
C	2.99890200	2.14642700	0.17275700
C	3.91511800	2.22046400	-1.04994900
W	-1.17705500	-0.17982900	0.13847100
O	1.92114800	-4.43224600	-0.32648900
C	-0.35707100	-1.87144700	0.93540100
C	0.02029400	-1.76981400	-0.30473900
C	-5.34276400	-3.67379000	-1.17772000
O	-6.01536700	-4.22906600	-0.30547700
N	-4.66153500	-4.34063900	-2.11732800
N	-6.54150000	-1.68163800	-0.80991200
C	-7.47195300	-1.03822800	-1.58467300
O	-7.23844200	-0.59430600	-2.70341700
C	-4.71417300	-5.74779600	-1.99732700
C	-8.87219200	-0.88949700	-0.95230600
H	5.66560700	0.57497200	4.96234700
H	3.05529600	-1.92035500	3.96709000
H	2.73809400	-3.39531900	3.03294900
H	4.81262000	-3.62395900	4.45358800
H	5.57012900	-1.23881100	2.96984400
H	7.82027500	0.69548700	-4.06746600
H	8.81845000	-0.67646700	-3.59670500
H	7.39751700	0.58041200	-0.29250000
H	5.21257400	-0.64670400	0.30635200
H	6.55383000	-1.66991100	-4.84241000
H	4.53469800	-3.12578500	-5.07163500
H	3.39699800	-2.31202800	-0.97619100
H	3.00060100	-3.41979300	-3.16293100
H	2.89805000	5.02136700	-1.86396800
H	1.84111400	6.27441000	-2.54244700
H	1.95617800	5.56155400	0.45194800
H	0.83341700	6.69321600	-0.31050500
H	0.89413000	3.75038400	-0.89369400
H	-2.51251700	5.83424900	-0.47409400
H	-1.17206600	6.24770400	0.49836000

H	-2.43800700	3.54435900	-1.12920100
H	-1.03320800	2.97215800	-1.84549700
H	-3.81760700	-2.23006500	0.32244800
H	-4.43075900	-0.63282400	-0.13216000
H	-2.09159600	2.30553900	4.50913000
H	-1.96354800	0.58972800	4.93990200
H	-4.33003800	0.21810200	4.29646500
H	-5.61805800	2.57984400	0.84002100
H	-6.19574900	1.35705800	2.88986100
H	0.97602800	3.70154700	-3.30177300
H	0.74239600	2.22662800	-4.25816700
H	2.65641500	1.12657800	-3.14507300
H	3.40081800	1.41217400	0.88283300
H	4.24056900	1.21574200	-1.33969200
H	2.09247200	-3.66763500	0.26302600
H	-3.02049500	1.66398900	5.88476700
H	-4.56352200	3.68085500	1.73318500
H	-6.36925500	3.08653500	3.26733100
H	2.21474300	3.20065100	-4.46430100
H	3.11903600	6.72754800	-1.39802400
H	4.80663900	2.82233700	-0.85001700
H	2.95876200	3.11494100	0.69691800
H	7.19173900	0.13701700	5.75235700
H	7.07715800	0.18912700	3.97036900
H	8.91004700	0.83199800	-2.68510700
H	5.19319700	-3.73773900	2.72906200
H	-5.18471900	-1.89440600	-2.36750100
H	2.76227900	-4.54149900	-0.78654700
H	-0.26571300	-2.48195300	1.82269800
H	-9.55886000	-1.57337700	-1.46111200
H	-8.89036700	-1.10221300	0.12012900
H	-9.22166200	0.12955600	-1.13020900
H	0.57799600	-2.27964400	-1.07601700
H	-3.95545300	-3.86901200	-2.66538400
H	-6.88654500	-2.23242000	-0.03135500
H	-5.75406900	-6.08483400	-1.97996800
H	-4.21028800	-6.21636600	-2.84773000
H	-4.24142800	-6.11072500	-1.07575700

Int1-Displacement-0.15-Structure2 optimized

C	6.43411700	0.21139500	5.09143600
C	6.03738600	-1.29740700	5.02509300
O	6.31800800	-2.03571400	5.97071000
N	5.39722500	-1.71594300	3.89956100
C	4.84707100	-3.07360300	3.65387400
C	3.43929300	-2.96756700	3.07393200
C	3.43449900	-2.27704300	1.69673300
O	4.08397400	-1.18144900	1.59435900
O	2.79483000	-2.84532400	0.78372500
C	-5.17353800	-2.22074000	-1.24036300
C	-4.10740600	-1.65983300	-0.30943100
S	-2.46079300	-1.68760300	-1.10799800
C	8.43172400	0.33527300	-3.01321600
C	7.24246800	-0.23665000	-2.28678700
C	6.93573000	-0.04830000	-0.95355500
C	6.19661000	-1.08387000	-2.81478600
N	5.77667600	-0.70999800	-0.61761100
C	5.30622500	-1.35260200	-1.73780300
C	5.89918200	-1.66248300	-4.06738500
C	4.16436700	-2.15449600	-1.85837400
C	4.76766900	-2.46260600	-4.19696600
C	3.90393700	-2.71141300	-3.10000000
C	2.19751100	6.12014200	-1.71455300
C	1.16171400	5.96117200	-0.60318000
N	0.27093200	4.84278400	-0.90729100
C	-1.05754200	4.84195700	-0.86303300
N	-1.72141100	5.86865200	-0.25781500
N	-1.75985100	3.89548600	-1.48562700
C	-2.61995600	1.48813400	4.77550800
C	-3.81681900	1.03036900	3.94968000
O	-4.80218400	2.06111600	4.06607400
C	3.37138300	0.80314200	2.51709800
S	-2.07745400	-0.36091600	2.31120100
C	-3.85946900	1.54250700	1.48603400
S	-3.13954300	1.46743800	-0.09451100
C	-5.06259000	2.43642300	1.69779600
C	-5.74801900	2.06477300	3.01145000
C	1.41418000	2.73596500	-3.80298400
C	2.11589600	2.01172800	-2.65976200
O	3.15096200	2.88326900	-2.19213700
C	1.15277600	1.66112400	-1.53600800
S	-0.40540800	0.96322600	-2.01262300
C	1.46520900	1.92138300	-0.23919400
S	0.26613900	1.74379900	1.05462100
C	2.85181200	2.37664500	0.16681000
C	3.79614300	2.34378600	-1.03637100
W	-1.12059200	-0.11391700	0.17515600
O	2.15883400	-4.90320500	-0.98084900
C	0.06803200	-1.56911200	0.97844700
C	0.49364900	-1.29053000	-0.22068200
C	-5.26899800	-3.73591800	-1.17872200
O	-5.96522700	-4.29977600	-0.33037600
N	-4.59441000	-4.40971600	-2.13027600
N	-6.51689800	-1.75108600	-0.83968100
C	-7.37932400	-1.13531200	-1.71162000
O	-7.03212600	-0.64954300	-2.78219500
C	-4.64338900	-5.84721400	-2.10652200
C	-8.84702300	-1.09722900	-1.25983900
H	5.96315500	0.64514400	5.97747500
H	2.80866100	-2.39432100	3.76602000
H	3.00308000	-3.96406000	2.96264100
H	4.86152100	-3.60542400	4.60929100
H	5.12401100	-1.07018900	3.15672600
H	8.13235600	0.98730300	-3.84482300
H	9.06916900	-0.45011900	-3.44097200
H	7.47885700	0.52176000	-0.21048900
H	5.28205400	-0.77364200	0.28403500
H	6.54658800	-1.48949400	-4.92467100
H	4.54059300	-2.90841100	-5.16275300
H	3.53337000	-2.33862900	-0.99362100
H	3.02725100	-3.34037600	-3.22963300
H	2.73931900	5.18473100	-1.88120300
H	1.71272500	6.40644600	-2.65288700
H	1.65148500	5.78196000	0.36187400
H	0.55735700	6.86798600	-0.51008900
H	0.71160200	3.93938700	-1.10768400
H	-2.72899200	5.80685800	-0.25010700
H	-1.30822100	6.26321500	0.57438500

H	-2.61198200	3.55979100	-1.03035100
H	-1.24810500	3.08038400	-1.86826500
H	-4.05516900	-2.23063900	0.62436800
H	-4.37986200	-0.63367700	-0.07823100
H	-2.15658600	2.36103200	4.30694800
H	-1.87164000	0.69763800	4.85201400
H	-4.22882800	0.09662400	4.37291500
H	-5.75796600	2.33021900	0.85551000
H	-6.23593300	1.08061100	2.91785000
H	0.89706200	3.63367700	-3.45018300
H	0.68483300	2.08298000	-4.28518100
H	2.57920600	1.08921400	-3.04736000
H	3.23026000	1.70311100	0.94537500
H	4.11906300	1.31483600	-1.23775000
H	2.27615400	-4.28893200	-0.23072600
H	-2.94707700	1.76285800	5.78448500
H	-4.75701100	3.49229900	1.73250500
H	-6.51342300	2.79837400	3.28576400
H	2.15683100	3.04279500	-4.54622100
H	2.91610500	6.90132000	-1.44570600
H	4.68888100	2.95279700	-0.86589200
H	2.81271000	3.38344900	0.61210100
H	7.51766300	0.27207000	5.22344500
H	6.14106500	0.78356200	4.20653900
H	9.05367300	0.93047900	-2.33622000
H	5.50410000	-3.61534500	2.96022000
H	-5.00921800	-1.86147300	-2.25866800
H	2.98839600	-4.79737600	-1.46213500
H	0.26564200	-2.19529200	1.83662700
H	-9.39464400	-1.89088900	-1.77911000
H	-8.97009900	-1.23658400	-0.18210300
H	-9.27758300	-0.13995000	-1.55917500
H	1.24677400	-1.55610100	-0.94654800
H	-3.89140700	-3.92601900	-2.67186200
H	-6.92357900	-2.33952400	-0.12007200
H	-5.67812200	-6.17016000	-1.97595000
H	-4.25860100	-6.24071100	-3.05061600
H	-4.05366700	-6.27100800	-1.28427300

Int1-Displacement-0.15-Structure3 optimized

C	6.21901300	0.81345900	4.93279900
C	5.83662700	-0.64338300	5.16579600
O	5.62840300	-1.09853600	6.28839600
N	5.73345300	-1.35295600	4.00458500
C	4.86738700	-2.52466600	3.92129300
C	3.47080300	-2.12433700	3.42496300
C	3.50145300	-1.45405000	2.03753100
O	4.35993600	-0.52598800	1.84107400
O	2.68121900	-1.87035200	1.18760800
C	-5.33007000	-2.37416800	-1.05076800
C	-4.24892700	-1.73183600	-0.18488400
S	-2.63158200	-1.75902800	-1.05430800
C	8.47031200	-0.32096100	-3.12769000
C	7.29401600	-0.72419500	-2.28024500
C	6.98518900	-0.21104000	-1.03738000
C	6.25522700	-1.68541200	-2.57754900
N	5.83119300	-0.77334900	-0.54386900
C	5.35964700	-1.67312900	-1.47085900
C	5.96171500	-2.56145300	-3.64453400
C	4.20165200	-2.45860200	-1.40974300
C	4.82496100	-3.36291000	-3.57946800
C	3.94236800	-3.31098900	-2.47134700
C	2.53957700	5.61997000	-2.75482700
C	1.64610200	5.74069700	-1.51832500
N	0.71763000	4.61187000	-1.44548700
C	-0.60672800	4.66461500	-1.31928000
N	-1.20328100	5.81782800	-0.89579100
N	-1.36786300	3.63839800	-1.68301700
C	-2.79263200	2.33868800	4.47381600
C	-3.94983200	1.75561900	3.66677200
O	-4.91885400	2.80165600	3.55250200
C	-3.45343300	1.27196900	2.31478200
S	-2.21820400	0.03179400	2.33960500
C	-3.90252800	1.80738400	1.14628300
S	-3.16893500	1.40079300	-0.37398900
C	-5.10025600	2.73387900	1.14655100
C	-5.83113300	2.61787700	2.48272700
C	1.47315000	2.24864200	-4.05709600
C	2.15539400	1.56237000	-2.87242800
O	3.20958200	2.44320600	-2.46535400
C	1.20316100	1.29312400	-1.71188100
S	-0.35488300	0.54142000	-2.09343300
C	1.52692400	1.66552000	-0.44735700
S	0.32806700	1.62505100	0.85731300
C	2.92035600	2.12286800	-0.07160600
C	3.85248100	1.98064900	-1.27393500
W	-1.22270700	-0.16152200	0.21773700
O	1.97772600	-4.39757900	0.30521200
C	-0.25305900	-1.59926900	1.29527400
C	0.13020200	-1.67642300	0.05386200
C	-5.39148000	-3.93797900	-0.99528600
O	-6.41780000	-4.50652000	-0.60472700
N	-4.32156200	-4.64644600	-1.42641700
N	-6.66932100	-1.94864600	-0.68310300
C	-7.33006800	-1.01930800	-1.43365800
O	-6.77738300	-0.22328300	-2.18528900
C	-4.35855400	-6.11308800	-1.43179000
C	-8.83778300	-1.09345000	-1.29260700
H	5.32709000	1.37025900	4.62352500
H	3.03081300	-1.42258100	4.14553500
H	2.81930500	-3.00110400	3.37029600
H	4.81644600	-2.97521800	4.91563800
H	5.61672200	-0.78876900	3.15729600
H	8.15719800	0.09993800	-4.09266100
H	9.13009100	-1.16976100	-3.35307000
H	7.52219400	0.53305800	-0.46284300
H	5.34475200	-0.57740200	0.34639200
H	6.61525100	-2.61303200	-4.51298100
H	4.60363800	-4.03701200	-4.40382700
H	3.53192300	-2.36408900	-0.56359700
H	3.04975600	-3.93042300	-2.45362300
H	3.05892000	4.65941000	-2.76323900
H	1.94351800	5.69932700	-3.66904300
H	2.25496200	5.76515300	-0.60625300
H	1.06131800	6.66435700	-1.55421000
H	1.11609000	3.67095200	-1.51271200
H	-2.20938600	5.79968300	-0.81563800
H	-0.72402000	6.35627200	-0.18949000

H	-2.22967800	3.42888100	-1.17644100
H	-0.93592200	2.75656800	-2.00349500
H	-4.14820700	-2.23559100	0.78296200
H	-4.54631300	-0.69963600	-0.01013000
H	-2.29958400	3.12796800	3.89909500
H	-2.05504200	1.56909200	4.71039500
H	-4.40145800	0.91406300	4.22298700
H	-5.76573400	2.47360000	0.31439900
H	-6.32892800	1.63713000	2.55687300
H	0.97078800	3.17103200	-3.75488800
H	0.73088200	1.58730500	-4.50912500
H	2.59898000	0.61199300	-3.21229000
H	3.29284400	1.49223700	0.74605400
H	4.15048600	0.93432400	-1.40099800
H	2.14149800	-3.54517300	0.76206700
H	-3.16993900	2.76667400	5.40879000
H	-4.78546300	3.77621300	0.99280400
H	-6.59460700	3.39528900	2.59193300
H	2.22778800	2.49949100	-4.80881800
H	3.27876900	6.42812400	-2.75505600
H	4.75976300	2.58114000	-1.15842300
H	2.90575500	3.16011000	0.30057100
H	6.60075200	1.24576400	5.85944600
H	6.96535300	0.91871500	4.13953600
H	9.07425100	0.43757100	-2.61866300
H	5.31588000	-3.25701400	3.23876700
H	-5.14955000	-2.06237200	-2.08686300
H	2.83515900	-4.59827300	-0.08926500
H	-0.11342700	-2.03490400	2.27448400
H	-9.22911300	-1.81065700	-2.02334900
H	-9.15060800	-1.42169200	-0.29689600
H	-9.27406100	-0.11674100	-1.50965900
H	0.74676600	-2.25504800	-0.61663600
H	-3.45079200	-4.15550500	-1.60448800
H	-7.21409300	-2.71921300	-0.30237400
H	-5.24276000	-6.45810300	-1.97335500
H	-3.45795900	-6.47991000	-1.92705900
H	-4.40190600	-6.51817600	-0.41503400

Int1-Displacement-0.15-Structure4 optimized

C	6.23523400	-0.63118600	4.94561900
C	5.89374300	-2.09100000	4.82928900
O	5.61971900	-2.80504500	5.78912900
N	5.86771500	-2.49064400	3.52047400
C	4.86974500	-3.47305100	3.15619800
C	3.50683400	-2.81451500	2.86789100
C	3.59342100	-1.78758700	1.72566700
O	4.46996000	-0.86125200	1.83559200
O	2.82735000	-1.93591600	0.74377000
C	-5.33832600	-2.03453600	-1.45542300
C	-4.12307500	-1.73125000	-0.56964000
S	-2.57907300	-1.45851900	-1.52972500
C	8.30431800	0.49106500	-3.06594500
C	7.20668300	-0.04793100	-2.24001300
C	6.87177200	0.11524400	-0.91608100
C	6.21735400	-0.89066400	-2.81372600
N	5.71375600	-0.58209400	-0.63251300
C	5.29197700	-1.20238800	-1.78555100
C	6.06051000	-1.38014900	-4.11924000
C	4.17885700	-1.99987600	-2.05174000
C	4.96329300	-2.17873800	-4.38313200
C	4.05233700	-2.46441000	-3.35041700
C	2.23654600	6.16052900	-1.11223700
C	1.19371700	5.89164100	-0.02524400
N	0.31006200	4.79206800	-0.41783900
C	-1.01556200	4.82342800	-0.51161600
N	-1.71935300	5.84401800	0.06034300
N	-1.67258100	3.91366800	-1.23109400
C	-2.64396400	1.02616700	4.99086500
C	-3.78366200	0.73802700	4.01705100
O	-4.73021900	1.79541200	4.19655400
C	-3.28822500	0.64691600	2.57974100
S	-2.04703300	-0.54138500	2.24722200
C	-3.78942200	1.43796200	1.58891400
S	-3.13888700	1.38997900	-0.01995400
C	-4.97910000	2.33557200	1.85785800
C	-5.67386100	1.89182500	3.14385000
C	1.52113100	3.25460100	-3.49025800
C	2.19148100	2.31654400	-2.48710100
O	3.24231200	3.08262400	-1.88846500
C	1.23405300	1.77340200	-1.42676200
S	-0.29148700	1.05859500	-1.98351900
C	1.54864400	1.83750600	-0.10800300
S	0.37004800	1.41004200	1.14313800
C	2.92332100	2.25085600	0.37409200
C	3.87100000	2.37605200	-0.81801600
W	-1.14293700	-0.20186000	0.09843100
O	2.10513800	-4.38989600	-0.28107800
C	-0.12969900	-1.84210800	0.77508800
C	0.21964400	-1.61233400	-0.45601600
C	-5.52480000	-3.58687200	-1.75962200
O	-6.55928100	-4.14825800	-1.38274200
N	-4.55683200	-4.26868300	-2.43172100
N	-6.56257100	-1.64262600	-0.81611200
C	-7.36968100	-0.73634000	-1.44411400
O	-6.98544300	0.12498600	-2.22458000
C	-4.66491700	-5.71939800	-2.72234600
C	-8.80622300	-0.98109300	-1.09977300
H	5.38586700	-0.04516200	4.57710200
H	3.16009700	-2.31074300	3.77919200
H	2.77505200	-3.58228700	2.60172400
H	4.78174500	-4.18684900	3.97875700
H	5.80886100	-1.70456100	2.86722800
H	7.92297600	1.09801700	-3.89864200
H	8.90889600	-0.30916700	-3.51488500
H	7.37141900	0.68269200	-0.14179900
H	5.21780900	-0.61406800	0.27979000
H	6.78184800	-1.13307300	-4.89431800
H	4.79314600	-2.58254700	-5.37766500
H	3.45602900	-2.22416900	-1.27905900
H	3.19056500	-3.08758300	-3.58505700
H	2.78941600	5.24894700	-1.35341400
H	1.75527400	6.52400200	-2.02537400
H	1.68085600	5.63031600	0.92127900
H	0.58395700	6.78235400	0.14815800
H	0.75381700	3.88962700	-0.63323800
H	-2.72239100	5.81408100	-0.04808500
H	-1.39006600	6.20226800	0.94440000

H	-2.57785900	3.59371900	-0.88838700
H	-1.14463800	3.11544300	-1.62975000
H	-3.94812300	-2.53272500	0.15757100
H	-4.35892300	-0.82364600	-0.01912700
H	-2.12516700	1.94378300	4.69854300
H	-1.92143100	0.20737100	4.99713400
H	-4.26760200	-0.21659300	4.29512100
H	-5.67208500	2.29586200	1.00864400
H	-6.18145600	0.92610000	2.98460600
H	1.03978700	4.09664300	-2.98576700
H	0.76674300	2.72250100	-4.07452000
H	2.63731900	1.46637300	-3.02978800
H	3.31053900	1.48385300	1.05662400
H	4.17538200	1.38094800	-1.16105000
H	2.28301300	-3.53997700	0.17877200
H	-3.04584300	1.15378700	6.00113700
H	-4.65395300	3.38066700	1.96304100
H	-6.42454900	2.62102900	3.46648400
H	2.27922700	3.65257400	-4.17143200
H	2.94137900	6.92459500	-0.76741500
H	4.77304100	2.93938700	-0.56140200
H	2.87441100	3.19298400	0.94307900
H	6.43805400	-0.36384600	5.98478800
H	7.09898500	-0.36734200	4.32645500
H	8.99075800	1.12690500	-2.49383500
H	5.20576300	-4.02646700	2.27031400
H	-5.24144400	-1.47926200	-2.39405100
H	2.86624300	-4.47985300	-0.86698700
H	0.04261000	-2.48783900	1.62423300
H	-9.16364800	-1.85037900	-1.66408000
H	-8.93915000	-1.20229900	-0.03613100
H	-9.41935000	-0.11831800	-1.36744300
H	0.83299600	-1.99323900	-1.25765000
H	-3.67663400	-3.79569500	-2.60752600
H	-7.05011100	-2.45509600	-0.44517500
H	-5.72161800	-5.98319100	-2.69784000
H	-4.24747800	-5.91916900	-3.71211400
H	-4.12834100	-6.31613000	-1.97649400

Int1-Displacement-0.15-Structure5 optimized

C	6.61406000	-0.18112500	4.94899600
C	6.11986900	-1.61706800	4.94457200
O	6.09673800	-2.30934400	5.96174800
N	5.69671200	-2.01488300	3.71895400
C	4.79837300	-3.13911000	3.54109300
C	3.39627200	-2.65470900	3.13124700
C	3.39426000	-1.81137800	1.83735900
O	4.25188400	-0.86369800	1.76200100
O	2.55688000	-2.10465900	0.95396300
C	-5.25607400	-2.17889500	-1.32346200
C	-4.05869400	-1.55346600	-0.59734600
S	-2.69265200	-1.13906400	-1.75408800
C	8.35740200	0.12811300	-3.06372900
C	7.16841800	-0.36156700	-2.29640200
C	6.83036800	-0.05139000	-0.99599200
C	6.13520000	-1.24165000	-2.77634000
N	5.65128900	-0.66512900	-0.63807100
C	5.20453900	-1.39861400	-1.71176100
C	5.89230700	-1.92230800	-3.98619800
C	4.04931600	-2.18117000	-1.82202900
C	4.75886600	-2.71920300	-4.09557700
C	3.84505400	-2.84406900	-3.02261300
C	2.23045400	6.16012400	-1.56042800
C	1.34232200	5.85253600	-0.35424400
N	0.44890100	4.72910400	-0.64240800
C	-0.87596000	4.76635400	-0.75355600
N	-1.57939300	5.80337700	-0.21192400
N	-1.53482400	3.84384700	-1.45290800
C	-2.49706900	1.34259900	4.91414300
C	-3.68305000	1.11922100	3.98500100
O	-4.54347600	2.25007100	4.14678100
C	3.22518400	0.94968300	2.54682400
S	-2.06319600	-0.32291400	2.24006000
C	-3.70733500	1.72095800	1.53679600
S	-3.10968500	1.53208300	-0.08474400
C	-4.83901400	2.69480800	1.78971100
C	-5.51357400	2.36170300	3.12012000
C	1.45660800	2.98775600	-3.74446400
C	2.19290700	2.15571700	-2.69708300
O	3.20969400	2.99962200	-2.14477100
C	1.27561100	1.63465200	-1.59800000
S	-0.25243000	0.89984300	-2.08843700
C	1.62627300	1.73617400	-0.29378000
S	0.49497400	1.29841600	0.99158700
C	3.00347900	2.18654000	0.14472500
C	3.90691500	2.34635000	-1.07969600
W	-1.19185900	-0.15151400	0.05065400
O	1.84349700	-4.38027400	-0.45073900
C	-0.43036300	-1.90275900	0.77906600
C	-0.13535100	-1.81111500	-0.48406500
C	-5.29886600	-3.69978200	-1.14796200
O	-5.94545500	-4.21393600	-0.23225900
N	-4.61090100	-4.42507300	-2.05768500
N	-6.51896400	-1.69810400	-0.72781600
C	-7.55945900	-1.17676800	-1.45428100
O	-7.46138700	-0.79921600	-2.61615000
C	-4.57605800	-5.86611400	-1.94511100
C	-8.89855900	-1.08788400	-0.69793400
H	5.77222500	0.48638600	5.16623800
H	2.98485400	-2.03873000	3.94175100
H	2.73056400	-3.51052500	2.98914800
H	4.76537500	-3.69375100	4.48266400
H	5.51812400	-1.29614000	3.01091400
H	8.06428300	0.69760700	-3.95619800
H	8.99229500	-0.69768200	-3.41268600
H	7.35818400	0.57747800	-0.29032700
H	5.15921400	-0.64038800	0.27287100
H	6.58238700	-1.82893400	-4.82213200
H	4.56433200	-3.25105100	-5.02394600
H	3.35129100	-2.23615200	-0.99403600
H	2.95715100	-3.46025700	-3.14111000
H	2.79086700	5.27131600	-1.86114700
H	1.62523200	6.49438000	-2.40892900
H	1.94936300	5.59422200	0.51996500
H	0.73769100	6.72399900	-0.09058500
H	0.88887500	3.82644400	-0.85551300
H	-2.58216600	5.77018700	-0.32331000
H	-1.25391800	6.18092100	0.66557400

H	-2.43123800	3.51763800	-1.08282000
H	-1.01407500	3.03533700	-1.83338400
H	-3.69518300	-2.22308100	0.18897600
H	-4.40775400	-0.63669500	-0.12433600
H	-1.90922100	2.19949900	4.57227000
H	-1.84855800	0.46462500	4.93363800
H	-4.23151300	0.21340600	4.30394600
H	-5.56354900	2.64538000	0.96716500
H	-6.08924000	1.42591700	3.02592500
H	0.93210800	3.83281100	-3.28928900
H	0.72733000	2.37525600	-4.27845100
H	2.67695200	1.30004100	-3.19697000
H	3.42361400	1.42589300	0.81529500
H	4.25910900	1.36538100	-1.41863600
H	2.00679400	-3.63736000	0.16900000
H	-2.85356000	1.54241400	5.93005500
H	-4.45834500	3.72597000	1.82288000
H	-6.20294800	3.15449700	3.42933300
H	2.17927500	3.38443700	-4.46434900
H	2.93765600	6.95762900	-1.30778100
H	4.78176800	2.96486700	-0.85786500
H	2.94587600	3.12499300	0.71896200
H	7.35953700	-0.05117200	5.73662200
H	7.03966600	0.11763500	3.98706100
H	8.98387600	0.78346100	-2.44886600
H	5.19427300	-3.81385100	2.76976700
H	-5.27194000	-1.88934900	-2.37705600
H	2.69948900	-4.48827000	-0.88212600
H	-0.32420600	-2.52769800	1.65416200
H	-9.54380800	-1.90820200	-1.02933600
H	-8.78602500	-1.14709400	0.38810700
H	-9.38410400	-0.14801300	-0.96723900
H	0.33937000	-2.33925800	-1.29761500
H	-3.96591900	-3.94580400	-2.67191900
H	-6.76691500	-2.23088400	0.09919400
H	-5.46393700	-6.18062400	-1.39737400
H	-4.57721200	-6.32104500	-2.94044100
H	-3.69056200	-6.21917400	-1.40135700

Int1-Displacement-0.15-Structure6 optimized

C	6.10918500	0.53213900	5.10588000
C	5.73090600	-0.94115100	5.18986700
O	5.62515900	-1.52889500	6.26525100
N	5.50832900	-1.50089900	3.97011700
C	4.69343900	-2.69763100	3.81235100
C	3.29610800	-2.32513100	3.29595000
C	3.36904600	-1.63659400	1.92153900
O	4.14681000	-0.62590500	1.81273700
O	2.68328800	-2.12573100	0.99670900
C	-5.17997100	-2.33994600	-1.16126200
C	-4.03981900	-1.79080500	-0.30075300
S	-2.52153200	-1.58326300	-1.31473200
C	8.47081900	-0.03484900	-2.89141500
C	7.28620100	-0.49817500	-2.11172200
C	6.88682700	-0.09198000	-0.85670400
C	6.31225800	-1.45717800	-2.55218400
N	5.72280800	-0.72853700	-0.48911000
C	5.34675000	-1.56354500	-1.51491000
C	6.15155100	-2.23681300	-3.71425500
C	4.22508700	-2.39177100	-1.61421500
C	5.05132700	-3.07897200	-3.80890500
C	4.09738000	-3.14706700	-2.76702900
C	2.34386900	5.77226600	-2.20358500
C	1.32130600	5.77386500	-1.06491100
N	0.39770700	4.64652000	-1.20063400
C	-0.92888600	4.69457100	-1.26706700
N	-1.59308700	5.82290600	-0.88085100
N	-1.62316000	3.68306300	-1.78638400
C	-2.84447000	1.89086500	4.77429600
C	-3.93804800	1.40781100	3.82747000
O	-4.92352100	2.44395600	3.79727600
C	-3.37908100	1.10466800	2.44575300
S	-2.09511300	-0.08044400	2.35926600
C	-3.85812700	1.70459900	1.32114200
S	-3.13858500	1.40394400	-0.22934400
C	-5.08511100	2.58977000	1.39208800
C	-5.82135500	2.33475600	2.70610800
C	1.47856800	2.62013600	-3.97299700
C	2.16968200	1.82905200	-2.85917200
O	3.26447000	2.64020800	-2.42250200
C	1.23950900	1.49005500	-1.69796600
S	-0.29861400	0.70362800	-2.08554100
C	1.58575800	1.77907900	-0.41897600
S	0.42552700	1.59242600	0.91068100
C	2.98329500	2.22407000	-0.04355700
C	3.89885400	2.10052200	-1.26082000
W	-1.14468200	-0.13033600	0.20338400
O	1.92089000	-4.49804700	-0.17903000
C	-0.21354700	-1.65117000	1.19075100
C	0.12308600	-1.70341300	-0.06523800
C	-5.30516000	-3.89965600	-1.14379600
O	-6.24816200	-4.43984600	-0.55674700
N	-4.38774300	-4.62974700	-1.82645900
N	-6.48646900	-1.86645600	-0.72720400
C	-7.23067000	-1.03734600	-1.52069100
O	-6.77062100	-0.36199400	-2.43463000
C	-4.48556200	-6.09383100	-1.88706100
C	-8.71372500	-1.04883400	-1.19242300
H	5.19554400	1.13593000	5.15136300
H	2.82371200	-1.64494900	4.01609000
H	2.67224200	-3.21894100	3.20832200
H	4.63912500	-3.19268500	4.78544500
H	5.35314000	-0.86310900	3.18388400
H	8.17832800	0.43646700	-3.83975100
H	9.14610200	-0.86260500	-3.14862600
H	7.35858800	0.61891100	-0.19039000
H	5.17025600	-0.60876400	0.37826100
H	6.87632100	-2.17997100	-4.52361800
H	4.91297300	-3.68796400	-4.69914600
H	3.49190500	-2.41029300	-0.81805800
H	3.23121200	-3.79565900	-2.87663800
H	2.86525700	4.81399100	-2.26335900
H	1.85080000	5.95640300	-3.16300600
H	1.82505900	5.70282800	-0.09368500
H	0.74073900	6.70065000	-1.07223100
H	0.81273200	3.70783600	-1.25656400
H	-2.59932000	5.80309800	-0.95569300
H	-1.22526000	6.33616800	-0.09391700

H	-2.52651700	3.44899200	-1.37549100
H	-1.12533500	2.81417700	-2.05417500
H	-3.82816000	-2.43842600	0.55727700
H	-4.35754800	-0.81951800	0.07428700
H	-2.34441700	2.76662800	4.35050900
H	-2.09817400	1.11054900	4.93773600
H	-4.40214400	0.49358300	4.24161300
H	-5.73880100	2.38581800	0.53533200
H	-6.29228700	1.33809400	2.68712200
H	1.01218900	3.53122400	-3.59144000
H	0.70781300	2.01204100	-4.45235700
H	2.56877100	0.89151500	-3.28096700
H	3.35363000	1.57122800	0.75711100
H	4.15483000	1.04944500	-1.43427800
H	2.11843200	-3.73047500	0.39785100
H	-3.28436900	2.16826200	5.73790100
H	-4.79833900	3.64967800	1.33567000
H	-6.60696200	3.07847600	2.87650300
H	2.22188000	2.90372500	-4.72422700
H	3.07839500	6.56800700	-2.03835400
H	4.82917300	2.66051500	-1.12853000
H	2.98364000	3.25344600	0.34917800
H	6.73458600	0.79784400	5.96088900
H	6.62966000	0.77889000	4.17629600
H	9.05812200	0.70037000	-2.33002800
H	5.18009400	-3.38597500	3.10935400
H	-5.03544600	-1.98961500	-2.18842100
H	2.76973900	-4.66920100	-0.60480100
H	-0.07951200	-2.13884700	2.14594100
H	-9.20405600	-1.83052200	-1.78393100
H	-8.90981800	-1.25067300	-0.13523300
H	-9.15262200	-0.08891400	-1.47007900
H	0.66994300	-2.29892200	-0.78093000
H	-3.55114800	-4.16567400	-2.16044800
H	-6.98725600	-2.57384700	-0.19592200
H	-5.53417000	-6.36941100	-2.00883500
H	-3.90526400	-6.44967100	-2.74082400
H	-4.10732500	-6.56809800	-0.97403300

Int1-Displacement-0.15-Structure7 optimized

C	6.28763000	0.53102100	4.95722700
C	5.82888900	-0.89548600	5.14619100
O	5.62102800	-1.39499800	6.24940200
N	5.64522300	-1.52549100	3.95216600
C	4.67672200	-2.59601800	3.85433200
C	3.31494500	-2.06940300	3.36569500
C	3.42090300	-1.41746900	1.97609600
O	4.29168100	-0.48736000	1.83901300
O	2.67607900	-1.84792800	1.06666800
C	-5.38639700	-2.21349200	-1.15361700
C	-4.16034100	-1.69353800	-0.39181400
S	-2.65487400	-1.57921900	-1.43745600
C	8.48765300	-0.13586300	-2.95351700
C	7.29762900	-0.59131300	-2.16732800
C	6.92335400	-0.16163200	-0.91229200
C	6.29866700	-1.54586600	-2.57380100
N	5.76003200	-0.77598000	-0.51039200
C	5.35030800	-1.62140800	-1.51483100
C	6.09260600	-2.34497100	-3.71629600
C	4.21034300	-2.43174200	-1.57646500
C	4.97424900	-3.16896300	-3.77289300
C	4.03757900	-3.20668300	-2.71285100
C	2.47723100	5.69299400	-2.12020400
C	1.47664600	5.65814700	-0.96258300
N	0.52604000	4.55803200	-1.13477800
C	-0.79624600	4.64263500	-1.23662800
N	-1.44322600	5.77610200	-0.83646500
N	-1.50333200	3.66473700	-1.80239700
C	-2.61719200	2.04352800	4.63038900
C	-3.78250700	1.56686100	3.76746900
O	-4.71923800	2.64803300	3.73795500
C	3.30749600	1.17531700	2.37673000
S	-2.12384800	-0.11037700	2.27892700
C	-3.77318800	1.78738200	1.25277800
S	-3.10821800	1.42132700	-0.30742200
C	-4.94182000	2.74684500	1.33642200
C	-5.65328500	2.56162400	2.67536400
C	1.45777000	2.57302300	-3.97281700
C	2.16425400	1.74735800	-2.89639700
O	3.26243000	2.54574100	-2.44639400
C	1.24376500	1.37521700	-1.73953800
S	-0.30243900	0.61870000	-2.14591700
C	1.59678600	1.62954300	-0.45560000
S	0.44126600	1.41229700	0.86962000
C	2.99458500	2.07027000	-0.07643600
C	3.90266000	1.97686800	-1.30111200
W	-1.19562600	-0.21660300	0.11469100
O	1.97695300	-4.37535800	0.18389500
C	-0.34197400	-1.79865600	1.08472600
C	0.01847100	-1.83289800	-0.16451800
C	-5.53076300	-3.77444000	-1.11695600
O	-6.60428900	-4.28581400	-0.77428200
N	-4.46916700	-4.54861900	-1.43591800
N	-6.59240900	-1.73129000	-0.55356100
C	-7.36652500	-0.86900900	-1.27002200
O	-6.95556500	-0.06485300	-2.09587200
C	-4.57751100	-6.00738400	-1.31064800
C	-8.80054100	-1.12756300	-0.96371400
H	5.43002600	1.14495600	4.65882900
H	2.94668400	-1.32498500	4.08298700
H	2.59069900	-2.88744800	3.32014600
H	4.58422000	-3.05382400	4.84238500
H	5.56311400	-0.90732300	3.14024600
H	8.19735000	0.32869700	-3.90570200
H	9.16328300	-0.96576600	-3.20247000
H	7.41575900	0.55467200	-0.26687500
H	5.22546400	-0.60942400	0.36199900
H	6.79770300	-2.31752200	-4.54445600
H	4.80924400	-3.78880200	-4.65108200
H	3.49097100	-2.41541800	-0.76744000
H	3.16121700	-3.84517300	-2.79098800
H	2.97202900	4.72637600	-2.23898700
H	1.96991300	5.93753800	-3.05868300
H	1.99570900	5.52447900	-0.00662500
H	0.91808500	6.59669300	-0.90935600
H	0.91827700	3.61193800	-1.21891700
H	-2.44726400	5.78305200	-0.93857100
H	-1.08516400	6.25784800	-0.02546500

H	-2.42076600	3.44138000	-1.41614500
H	-1.02552500	2.79039300	-2.08171000
H	-3.95485600	-2.31479400	0.48756000
H	-4.41673900	-0.69596400	-0.04347000
H	-2.10241500	2.87229400	4.13580900
H	-1.89908900	1.23697400	4.79358100
H	-4.26409200	0.69668100	4.25025500
H	-5.62975600	2.56277000	0.50220500
H	-6.17705800	1.59183500	2.69247200
H	1.00535200	3.47599300	-3.55641800
H	0.67496300	1.98463500	-4.45688800
H	2.55874500	0.82404400	-3.35253800
H	3.37614100	1.40506400	0.70897600
H	4.15624700	0.93073300	-1.50331800
H	2.14419800	-3.51987100	0.63487500
H	-2.99037800	2.38817900	5.60045100
H	-4.59676300	3.78722900	1.24900600
H	-6.39270100	3.35038600	2.84981900
H	2.18822400	2.87617700	-4.72933300
H	3.23376200	6.46201500	-1.92969000
H	4.83423500	2.53257200	-1.16039700
H	2.99224900	3.09226100	0.33614500
H	6.69358800	0.92416900	5.89145000
H	7.04002900	0.61526000	4.16691900
H	9.07161400	0.60293200	-2.39394300
H	5.04298600	-3.36562300	3.16239800
H	-5.33111400	-1.86522200	-2.19203100
H	2.83355200	-4.58464500	-0.20775700
H	-0.23413400	-2.30217100	2.03512500
H	-9.10860000	-2.05083300	-1.46797200
H	-8.96966700	-1.26812200	0.10852100
H	-9.43533200	-0.31260400	-1.31925700
H	0.57854900	-2.41828200	-0.87821300
H	-3.56950200	-4.11017400	-1.60881900
H	-7.10875100	-2.50004500	-0.13168500
H	-5.38126000	-6.38284700	-1.94938000
H	-3.62942100	-6.45254300	-1.61705200
H	-4.79959800	-6.29696500	-0.27860200

Int1-Displacement-0.15-Structure8 optimized

C	6.17175700	0.95219800	4.96740100
C	5.81221800	-0.52245000	5.19631800
O	5.89429800	-1.02943500	6.31596700
N	5.41035500	-1.17501300	4.07853100
C	4.76085600	-2.48500700	4.06956600
C	3.36174000	-2.37175500	3.45453800
C	3.38805600	-1.84857300	2.00382100
O	4.12218100	-0.82962500	1.76033500
O	2.68460600	-2.45688000	1.16825500
C	-5.17001300	-2.42892900	-1.20718900
C	-4.29713700	-1.38954500	-0.54456700
S	-2.56126100	-1.65887400	-1.06298900
C	8.48650100	-0.28130900	-2.97065600
C	7.27137400	-0.71916500	-2.19620500
C	6.91897500	-0.28037200	-0.93582700
C	6.23655300	-1.64947200	-2.59153700
N	5.74047000	-0.85787600	-0.52422500
C	5.30111600	-1.69816100	-1.51943500
C	5.97731700	-2.45866800	-3.71879000
C	4.14254600	-2.48511400	-1.53765400
C	4.83689500	-3.25706400	-3.73852000
C	3.92036600	-3.27185400	-2.65658600
C	2.40942100	5.72838400	-2.81264900
C	1.59880000	5.77888900	-1.51809900
N	0.68960800	4.63564500	-1.44543300
C	-0.64003300	4.67065100	-1.40893200
N	-1.28032200	5.81430200	-1.02291400
N	-1.36393500	3.63542800	-1.82035900
C	-2.81850900	2.29904700	4.53890800
C	-3.96719300	1.75644300	3.69625100
O	-4.92277800	2.81752800	3.59773700
C	-3.44457900	1.31328300	2.34250500
S	-2.21267700	0.06416400	2.36269300
C	-3.85735600	1.89354200	1.18655700
S	-3.07802900	1.52896500	-0.32302600
C	-5.03867000	2.83988300	1.18754800
C	-5.80755400	2.68788300	2.49895600
C	1.53096800	2.12432900	-4.06396800
C	2.22422800	1.56219800	-2.82492400
O	3.22386500	2.51927800	-2.44711600
C	1.26427300	1.31925800	-1.66814400
S	-0.28178000	0.55103900	-2.05069100
C	1.58042400	1.71207300	-0.40915100
S	0.38259200	1.66457600	0.89512100
C	2.96207600	2.20967100	-0.04194100
C	3.89712900	2.11617600	-1.25063900
W	-1.18973100	-0.11231000	0.24675900
O	1.79704000	-4.64738000	-0.23837500
C	-0.22379800	-1.54963000	1.33343600
C	0.13020900	-1.66604900	0.08700100
C	-5.03842200	-3.86191800	-0.67360100
O	-5.45645200	-4.15068900	0.44766400
N	-4.55264700	-4.77595000	-1.55190700
N	-6.64808300	-2.10454000	-0.91741600
C	-7.53743600	-1.38777500	-1.69614400
O	-7.21506400	-0.89809900	-2.77306900
C	-4.44983400	-6.18607400	-1.21796900
C	-9.04896700	-1.17764500	-1.20607400
H	5.42709600	1.57545900	5.47319400
H	2.76136400	-1.68209900	4.06249800
H	2.86393200	-3.34532200	3.45992300
H	4.72195200	-2.84298400	5.10216500
H	5.19382700	-0.65664400	3.22283600
H	8.21811200	0.20257700	-3.91948300
H	9.14378100	-1.12481900	-3.22168400
H	7.44083100	0.41970600	-0.29564700
H	5.22326100	-0.74340600	0.36257700
H	6.66005400	-2.46234000	-4.56610700
H	4.64083500	-3.87963800	-4.60867900
H	3.46022000	-2.46382700	-0.69418500
H	3.02506100	-3.88531100	-2.70934000
H	2.94957400	4.78141600	-2.88611800
H	1.75201500	5.82411700	-3.68233400
H	2.26101700	5.75985900	-0.64518800
H	1.00835900	6.69751700	-1.46760200
H	1.10660800	3.70244300	-1.51303800
H	-2.28891600	5.77531900	-1.00285300
H	-0.85656400	6.35359800	-0.28241600

H	-2.23784100	3.41148700	-1.33683100
H	-0.89517800	2.75549800	-2.09299200
H	-4.37182400	-1.46705600	0.54375100
H	-4.64149000	-0.40851000	-0.86339500
H	-2.30423900	3.09727100	3.99609200
H	-2.09587400	1.51304000	4.76677600
H	-4.43919600	0.90274100	4.21545400
H	-5.68885500	2.62232300	0.33078100
H	-6.32283200	1.71344800	2.52322900
H	0.97624900	3.03958700	-3.83616400
H	0.83266500	1.39486100	-4.47842600
H	2.72568800	0.61734300	-3.09208800
H	3.35439600	1.58393400	0.76966200
H	4.26709500	1.09085400	-1.36628000
H	2.02444300	-3.96069500	0.42059100
H	-3.20587300	2.70598900	5.47932600
H	-4.70330000	3.88157000	1.07986400
H	-6.56157100	3.47351100	2.61599000
H	2.28469400	2.36142500	-4.82129400
H	3.13097200	6.55226700	-2.83435400
H	4.76122600	2.77920300	-1.14389700
H	2.91199400	3.24056400	0.34386200
H	7.14023100	1.15707100	5.43183200
H	6.20678400	1.23225600	3.91127400
H	9.07889500	0.43519000	-2.39190200
H	5.36707600	-3.19581400	3.49135400
H	-5.05339300	-2.38359400	-2.29290000
H	2.64496800	-4.81316700	-0.66806900
H	-0.07663900	-1.96564100	2.32014800
H	-9.69423800	-1.60414900	-1.97644800
H	-9.27455300	-1.63140800	-0.23686100
H	-9.22018000	-0.10055300	-1.16197800
H	0.71898900	-2.27459100	-0.58356300
H	-4.09099200	-4.43383000	-2.38220900
H	-6.95913500	-2.50658600	-0.04141800
H	-5.07219800	-6.36093700	-0.34011400
H	-4.80710900	-6.79904400	-2.05174300
H	-3.41922200	-6.47429300	-0.98021500

Int1-Displacement-0.15-Structure9 optimized

C	6.39616100	0.81870900	4.85333800
C	5.93958200	-0.60752800	5.08599200
O	5.89472400	-1.11426900	6.20602300
N	5.56828600	-1.22200000	3.93364800
C	4.67040600	-2.35845000	3.94065600
C	3.27031200	-1.94598800	3.45151000
C	3.30615800	-1.37773200	2.02041800
O	4.11972900	-0.41124000	1.80287400
O	2.56528300	-1.90472100	1.16149300
C	-5.36090100	-2.42011700	-0.96036600
C	-4.14964300	-1.78221000	-0.25237600
S	-2.69615500	-1.62545900	-1.37790000
C	8.53757900	-0.50228700	-2.77531500
C	7.26244000	-0.86857400	-2.06438200
C	6.81630800	-0.30291600	-0.88869700
C	6.25394000	-1.83574600	-2.44005900
N	5.60438300	-0.83129400	-0.51187100
C	5.23492600	-1.77077600	-1.44579400
C	6.08127600	-2.76199000	-3.49081400
C	4.07595800	-2.55864500	-1.47950300
C	4.94323100	-3.56394500	-3.51798100
C	3.94077800	-3.46541100	-2.52081300
C	2.49027500	5.78565900	-2.63892100
C	1.48222400	5.77888400	-1.48834500
N	0.63661300	4.58771400	-1.56088900
C	-0.69276600	4.53965300	-1.49112500
N	-1.38981400	5.62730200	-1.04819400
N	-1.36366600	3.48105500	-1.93251500
C	-2.61895600	2.34717900	4.56518500
C	-3.77042800	1.91735700	3.65981600
O	-4.63074800	3.05396900	3.54130500
C	-3.28471400	1.42823800	2.30170800
S	-2.13165600	0.10971100	2.29409500
C	-3.75855700	1.94124000	1.13360800
S	-3.15924700	1.38572900	-0.40375100
C	-4.89399400	2.94317900	1.14099600
C	-5.58663600	2.92299800	2.50287600
C	1.70375600	2.20604700	-4.15192500
C	2.31337300	1.60874000	-2.88182200
O	3.27403500	2.57625400	-2.43575500
C	1.31235800	1.30444600	-1.76274300
S	-0.18261100	0.43823000	-2.15967600
C	1.58060300	1.68050100	-0.48799400
S	0.38158200	1.50194100	0.79630900
C	2.91855200	2.24000800	-0.05376500
C	3.90617600	2.17623700	-1.21692600
W	-1.22485400	-0.18436500	0.13215400
O	1.86089500	-4.43562800	0.29136100
C	-0.43556200	-1.70929900	1.23684800
C	-0.11742100	-1.89183400	-0.01040500
C	-5.49798600	-3.94543100	-0.75676300
O	-6.49892700	-4.42724100	-0.21392500
N	-4.50857800	-4.73415400	-1.22700700
N	-6.61283200	-1.86939400	-0.49535700
C	-7.31453500	-1.01065400	-1.28880900
O	-6.82946000	-0.35853200	-2.20600800
C	-4.63716700	-6.17898200	-1.09306400
C	-8.78255800	-0.99296000	-0.94978200
H	5.52644200	1.48420900	4.90343600
H	2.87155200	-1.17965900	4.12845800
H	2.59622200	-2.80671000	3.47328300
H	4.63290100	-2.74771400	4.96146500
H	5.39417200	-0.63168800	3.11490400
H	8.34995800	-0.11071700	-3.78431100
H	9.21075300	-1.36251000	-2.89144600
H	7.29282200	0.45875600	-0.28443700
H	5.05073000	-0.60665800	0.33558800
H	6.83058100	-2.85425400	-4.27445300
H	4.81743500	-4.27803900	-4.32870400
H	3.32330300	-2.43691200	-0.70976700
H	3.05305300	-4.08964000	-2.57695200
H	3.06418600	4.85623400	-2.65355000
H	1.97546500	5.88578300	-3.59930900
H	2.00209200	5.79694400	-0.52226500
H	0.83780100	6.66136500	-1.53777900
H	1.10772400	3.68269400	-1.64007900
H	-2.39351900	5.52564900	-1.00416100
H	-0.98087900	6.16660300	-0.29951500

H	-2.22752000	3.19926200	-1.45829100
H	-0.85331800	2.63785100	-2.23630300
H	-3.86729500	-2.34776800	0.64275000
H	-4.45649600	-0.78527000	0.05943700
H	-2.02174900	3.11976900	4.07206500
H	-1.96827700	1.50030600	4.79324300
H	-4.33330900	1.10363700	4.15448000
H	-5.60487800	2.70169700	0.34132100
H	-6.15990100	1.98834400	2.61917700
H	1.14955500	3.12518900	-3.93863900
H	1.02027400	1.49531300	-4.62275600
H	2.84427200	0.67915700	-3.14551300
H	3.29780900	1.63170200	0.77717100
H	4.29971500	1.15941700	-1.32454600
H	2.03879900	-3.58841100	0.75245000
H	-3.01778700	2.75204200	5.50080200
H	-4.51615300	3.95647000	0.93985700
H	-6.28078800	3.76290700	2.61263000
H	2.50767300	2.44498500	-4.85384100
H	3.17759800	6.63055600	-2.52617500
H	4.75090500	2.85669700	-1.06979700
H	2.80867900	3.27134600	0.31856600
H	7.09553200	1.11667800	5.63772800
H	6.86389300	0.95267100	3.87388900
H	9.08257600	0.26810200	-2.21987000
H	5.06580600	-3.15327900	3.29394200
H	-5.27521800	-2.20330100	-2.03229800
H	2.70607500	-4.63004800	-0.13199100
H	-0.33267900	-2.11858900	2.23199000
H	-9.28213600	-1.81434100	-1.47687800
H	-8.96433600	-1.12296700	0.12126000
H	-9.23124100	-0.05514000	-1.28300900
H	0.38656300	-2.57528900	-0.67781900
H	-3.64702200	-4.31236100	-1.55578600
H	-7.14912000	-2.55287700	0.03367500
H	-5.58368700	-6.51093000	-1.52755400
H	-3.80793900	-6.65684600	-1.61837100
H	-4.62139400	-6.48876200	-0.04245400

Int1-Displacement-0.15-Structure10 optimized

C	6.39427200	-0.41510300	4.71171800
C	6.15756400	-1.88899700	4.73151300
O	5.99804100	-2.54804400	5.75209800
N	6.04287100	-2.38374900	3.45400800
C	4.92921900	-3.28493200	3.27370200
C	3.59566600	-2.53092900	3.09549000
C	3.65269900	-1.70835300	1.80268000
O	4.49432100	-0.74707600	1.76567800
O	2.93738500	-2.08232400	0.83885200
C	-5.27614400	-2.09885800	-1.49529900
C	-4.24282800	-1.59166700	-0.50177200
S	-2.58968200	-1.53580900	-1.28836900
C	8.29151800	0.35580900	-3.21808000
C	7.15455400	-0.20367400	-2.43027800
C	6.84813100	0.00578300	-1.10361900
C	6.14761500	-1.09128300	-2.93677100
N	5.71672500	-0.69437200	-0.74817200
C	5.26604500	-1.37547700	-1.85612100
C	5.90685300	-1.67401600	-4.19478200
C	4.16163200	-2.22362300	-2.00096800
C	4.81007300	-2.51141300	-4.34411000
C	3.95271500	-2.77917000	-3.25378800
C	2.45626300	6.05701900	-1.48954100
C	1.47703800	5.92542000	-0.32257400
N	0.50038700	4.87310600	-0.60179500
C	-0.81318000	4.92436900	-0.39914300
N	-1.34971500	5.93598400	0.34211100
N	-1.62720400	4.05238000	-0.99193100
C	-2.59785400	1.06395600	4.97417300
C	-3.78434600	0.73707500	4.07184100
O	-4.74473200	1.77472200	4.29131600
C	-3.33932800	0.65255100	2.62027700
S	-2.07814600	-0.51462900	2.27073900
C	-3.84515300	1.47455500	1.66232800
S	-3.17625500	1.51265500	0.05579200
C	-5.03154000	2.36320000	1.96935500
C	-5.70469400	1.88778900	3.25554300
C	1.31768700	3.04244100	-3.70838400
C	2.01124500	2.14631700	-2.68295800
O	3.12908000	2.88754400	-2.18461100
C	1.08169400	1.73197600	-1.54931500
S	-0.52083300	1.13241000	-2.00851900
C	1.46336700	1.85033300	-0.24962100
S	0.30620000	1.60675400	1.07603800
C	2.88864000	2.18976300	0.13399900
C	3.77592000	2.19868000	-1.11065900
W	-1.18979300	-0.11490300	0.12441500
O	1.48012000	-4.35255100	1.24667200
C	-0.06039400	-1.70077200	0.74632300
C	0.37051800	-1.30275300	-0.41747600
C	-5.27368700	-3.70372500	-1.64989600
O	-6.07226500	-4.34921500	-0.96755100
N	-4.44102100	-4.31928100	-2.54832300
N	-6.65030000	-1.80317400	-1.06427700
C	-7.48364600	-0.94400200	-1.73295700
O	-7.10075700	-0.16333000	-2.59787300
C	-4.38328800	-5.79962600	-2.77145100
C	-8.97139700	-1.00467800	-1.33403300
H	5.50860200	0.07313300	4.29067700
H	3.43470000	-1.87574600	3.95932500
H	2.77271500	-3.24742600	3.03746400
H	4.88532700	-3.93881300	4.14794100
H	5.97434700	-1.63754700	2.75982700
H	7.94414400	0.94810700	-4.07572400
H	8.93874900	-0.43378100	-3.62407500
H	7.36615900	0.61381000	-0.37290300
H	5.23925600	-0.67201700	0.17339500
H	6.56886200	-1.47126100	-5.03394000
H	4.60567800	-2.97024600	-5.30853800
H	3.51817100	-2.42446800	-1.15232900
H	3.10553900	-3.44520000	-3.40113700
H	2.91870200	5.09433100	-1.72241200
H	1.93913700	6.41358800	-2.38562800
H	2.01383700	5.68830600	0.60493000
H	0.93559900	6.86349900	-0.16705500
H	0.86680300	3.95838800	-0.88657600
H	-2.35133400	5.91992400	0.46630100
H	-0.82047300	6.26170000	1.13743500

H	-2.44665300	3.71430000	-0.48289300
H	-1.21337200	3.26551300	-1.52050600
H	-4.19306700	-2.22800100	0.38872400
H	-4.53415100	-0.58693400	-0.19990600
H	-2.11116400	1.98142400	4.63087500
H	-1.86364600	0.25625100	4.96151800
H	-4.22882000	-0.22632300	4.38141400
H	-5.73916800	2.34018200	1.13117500
H	-6.21027900	0.92323700	3.08297400
H	0.88319500	3.92958700	-3.23824800
H	0.52126400	2.49840600	-4.21998200
H	2.38590500	1.24317600	-3.19357700
H	3.26290800	1.43472800	0.83713400
H	4.00806000	1.17227900	-1.41756400
H	2.00155700	-3.53766500	1.03599600
H	-2.94446700	1.21222200	6.00242800
H	-4.71048100	3.40801700	2.09046200
H	-6.45390500	2.60580300	3.60563700
H	2.05110600	3.37473300	-4.44968600
H	3.24077100	6.77732100	-1.23539900
H	4.72060200	2.71985900	-0.93180600
H	2.93042500	3.15845800	0.65763000
H	6.58927900	-0.03274700	5.71602300
H	7.23498500	-0.15261600	4.05902400
H	8.92230400	1.00954400	-2.60536000
H	5.10480200	-3.92164400	2.39660200
H	-5.12382400	-1.61327300	-2.46273900
H	2.13320900	-5.06143300	1.21894000
H	0.09733700	-2.43784400	1.52082300
H	-9.53620100	-1.42725500	-2.17063200
H	-9.16067400	-1.60314100	-0.43852100
H	-9.32667600	0.01558600	-1.17365100
H	1.10526300	-1.50360200	-1.18272700
H	-3.71161300	-3.75082600	-2.96043800
H	-7.05964200	-2.56648500	-0.53522000
H	-5.26173900	-6.22979700	-2.29146800
H	-4.39860200	-6.00329500	-3.84509000
H	-3.47766900	-6.22327800	-2.32664500

Int1-Displacement-0.2-Structure1 optimized

C	6.43108300	-0.37755600	5.10137800
C	6.06890400	-1.84511700	4.82990200
O	6.22851900	-2.70951600	5.69227200
N	5.57299500	-2.07176000	3.58751300
C	4.87657700	-3.29461600	3.18533100
C	3.42421800	-2.96717200	2.81248700
C	3.34242700	-1.96655600	1.64297600
O	4.02529000	-0.88925000	1.74618800
O	2.63167200	-2.28199900	0.66323000
C	-5.30895400	-2.06736200	-1.39790700
C	-4.17767700	-1.49117400	-0.55774200
S	-2.65652200	-1.27375500	-1.56272700
C	8.27795300	0.44594100	-2.90087000
C	7.20157700	-0.04296700	-2.03486000
C	6.79744100	0.17907900	-0.74034500
C	6.27570300	-0.93454400	-2.61913800
N	5.63715800	-0.53513600	-0.49439700
C	5.29808800	-1.21471200	-1.64033500
C	6.24223500	-1.47275200	-3.91290000
C	4.22036500	-2.03562800	-1.95281600
C	5.18792300	-2.30454300	-4.22081700
C	4.21812500	-2.54643400	-3.23729700
C	2.15102500	6.25541600	-1.12297100
C	1.11201100	5.84289700	-0.07655600
N	0.26025600	4.75733200	-0.56988000
C	-1.04933400	4.80159600	-0.79368400
N	-1.79585600	5.83153700	-0.29665000
N	-1.64793200	3.89578900	-1.57013600
C	-2.67649400	0.90816300	4.98448500
C	-3.82561700	0.74438400	3.99649300
O	-4.70569200	1.84995100	4.21577300
C	3.30931700	0.69513700	2.56757700
S	-2.11182400	-0.52800800	2.21873500
C	-3.74296200	1.56003200	1.60768900
S	-3.04319400	1.55851300	0.02305300
C	-4.88908300	2.50606900	1.89877300
C	-5.62604200	2.04890900	3.15683200
C	1.50216700	3.04754000	-3.61489900
C	2.20609100	2.23772200	-2.53101300
O	3.19063100	3.10335100	-1.95362900
C	1.25590600	1.71443300	-1.46010200
S	-0.27048400	0.99610000	-2.00343500
C	1.57736100	1.80517300	-0.14646900
S	0.42047200	1.37322000	1.12151600
C	2.93973700	2.26794400	0.32338100
C	3.87227600	2.46021600	-0.87407900
W	-1.15362100	-0.18351600	0.10085400
O	1.92790200	-4.41094200	-0.93376200
C	-0.25551900	-1.88960900	0.76464500
C	0.10501900	-1.68181300	-0.46847400
C	-5.28022300	-3.66063700	-1.53897200
O	-6.08623400	-4.32560900	-0.88086400
N	-4.42034600	-4.25917800	-2.41289600
N	-6.60925700	-1.80664200	-0.79904000
C	-7.52164500	-0.97582600	-1.38375100
O	-7.24622900	-0.14133400	-2.23952800
C	-4.38079200	-5.73187700	-2.62282200
C	-8.94601700	-1.19835700	-0.89570900
H	5.72774500	0.02455700	5.83792500
H	2.92344500	-2.53352300	3.68750400
H	2.89128000	-3.87932200	2.53017600
H	4.93101100	-3.99761300	4.02111200
H	5.27899300	-1.27983700	3.00937600
H	7.87749500	0.97022900	-3.77891200
H	8.89685900	-0.37695700	-3.28382600
H	7.23859800	0.79442900	0.03243300
H	5.07297500	-0.56893400	0.37192600
H	7.01681900	-1.23541500	-4.63655500
H	5.08934100	-2.76070400	-5.20193800
H	3.43354300	-2.24100000	-1.23940000
H	3.37882300	-3.18867100	-3.50576800
H	2.73216300	5.38781000	-1.44793300
H	1.66291600	6.69222500	-1.99978800
H	1.60192200	5.49884300	0.84035400
H	0.48217300	6.69607400	0.18733900
H	0.72158800	3.85951600	-0.76135600
H	-2.78814900	5.79133000	-0.47736300
H	-1.54147400	6.19505100	0.60976600

H	-2.59188900	3.62162300	-1.30442100
H	-1.11214200	3.05403500	-1.86493300
H	-3.96286900	-2.13009600	0.30488800
H	-4.50807400	-0.51916700	-0.19402400
H	-2.08993500	1.79628300	4.73216400
H	-2.01586400	0.03935200	4.96124700
H	-4.37344400	-0.18935400	4.22228900
H	-5.57250000	2.53628300	1.04100600
H	-6.18779000	1.12296100	2.95004000
H	0.96304300	3.89970900	-3.18999900
H	0.79182500	2.42562000	-4.16311900
H	2.72090700	1.38340100	-3.00211200
H	3.35318900	1.50279400	0.99257400
H	4.25804400	1.49091300	-1.20980500
H	2.11298100	-3.75302200	-0.23016800
H	-3.07310700	1.02427600	5.99870400
H	-4.51058800	3.52706700	2.04933200
H	-6.33682900	2.80713300	3.50213100
H	2.24730100	3.43492800	-4.31659900
H	2.83021200	7.00161300	-0.69754700
H	4.72552100	3.09759600	-0.62259200
H	2.85247600	3.19558900	0.91117900
H	7.42978700	-0.33513800	5.54426900
H	6.40056200	0.24969800	4.20671400
H	8.96040300	1.14439300	-2.39936300
H	5.39011100	-3.74948000	2.32775200
H	-5.29438600	-1.60202500	-2.38860400
H	2.78461100	-4.51067800	-1.36631900
H	-0.13139800	-2.55976300	1.60341800
H	-9.43539700	-1.93230600	-1.54604600
H	-8.98621600	-1.57300200	0.13113200
H	-9.50131700	-0.26130900	-0.96619600
H	0.68072700	-2.11352800	-1.27346400
H	-3.66518900	-3.69516900	-2.78572000
H	-6.96112800	-2.61863400	-0.29851700
H	-5.36077700	-6.12865200	-2.35933600
H	-4.15915100	-5.93295200	-3.67338100
H	-3.62018700	-6.20522800	-1.99271400

Int1-Displacement-0.2-Structure2 optimized

C	6.39064800	-0.33153900	4.79241400
C	6.16267900	-1.81269200	4.72181800
O	6.02903900	-2.52961800	5.70797900
N	6.04825200	-2.23836000	3.42331200
C	5.03649000	-3.24377700	3.18059300
C	3.63846400	-2.61175700	3.03941400
C	3.61071200	-1.70540800	1.80190700
O	4.40400000	-0.70197200	1.79450000
O	2.87414000	-2.04856700	0.84397300
C	-5.19694000	-2.11232600	-1.56183700
C	-4.23329300	-1.47027600	-0.59830100
S	-2.55038400	-1.56378100	-1.29609300
C	8.12709700	0.27590300	-3.30156700
C	7.05605200	-0.18246900	-2.39900400
C	6.75986700	0.07154400	-1.08050300
C	6.07165000	-1.08537000	-2.87721800
N	5.63047200	-0.63284900	-0.70901500
C	5.19338000	-1.35203300	-1.79788000
C	5.89948300	-1.67402200	-4.13876900
C	4.12103200	-2.22908000	-1.95915600
C	4.83406800	-2.53736800	-4.30384000
C	3.98112000	-2.79195300	-3.21576100
C	2.42519700	6.16723000	-1.70853800
C	1.62150600	5.96605500	-0.42337800
N	0.68110500	4.85879900	-0.58864500
C	-0.63224300	4.87877800	-0.37743800
N	-1.18680600	5.88361400	0.36229200
N	-1.42960300	3.98368600	-0.95292300
C	-2.62580200	1.39215100	4.74112400
C	-3.84562200	0.90886700	3.96278300
O	-4.84599700	1.92140700	4.12048700
C	3.42966200	0.70143500	2.52049000
S	-2.18647200	-0.51174800	2.26560100
C	-3.87367000	1.51406400	1.52728800
S	-3.11353500	1.52116500	-0.03652500
C	-5.05599800	2.42678900	1.77220100
C	-5.77137900	1.99260500	3.04983800
C	1.16480800	2.91116900	-3.67065100
C	1.97256600	2.10711300	-2.65416000
O	3.00930300	2.96487300	-2.16057100
C	1.09646000	1.62470300	-1.51192100
S	-0.48064600	0.98133800	-1.97274000
C	1.48047500	1.77402600	-0.21779900
S	0.33504300	1.51628400	1.11364300
C	2.88749400	2.19194100	0.15114400
C	3.74484700	2.32428500	-1.11006300
W	-1.18499800	-0.17953500	0.16422900
O	1.54998500	-4.42564100	1.14078300
C	-0.12111100	-1.78487600	0.84918300
C	0.34094300	-1.43147200	-0.31740300
C	-5.14986900	-3.69436600	-1.52510900
O	-5.72928500	-4.27461700	-0.60574400
N	-4.53425500	-4.37882800	-2.53547200
N	-6.62826500	-1.83519800	-1.13993700
C	-7.51181900	-0.92510800	-1.67611600
O	-7.19865000	-0.13594700	-2.56129200
C	-4.45745700	-5.85980300	-2.58398000
C	-8.99791200	-0.89165300	-1.12228900
H	5.48036100	0.17762700	4.45678000
H	3.42032400	-2.02923100	3.94215600
H	2.88308000	-3.39413600	2.93401200
H	5.05757000	-3.94667300	4.01678500
H	5.91128700	-1.46681700	2.76717700
H	7.72201300	0.79618100	-4.18045900
H	8.72259100	-0.56452800	-3.68405800
H	7.26976000	0.70414900	-0.36570700
H	5.15480700	-0.60222600	0.21269500
H	6.58633600	-1.45466600	-4.95231700
H	4.64854500	-3.02321800	-5.25812700
H	3.45315500	-2.45175500	-1.13653300
H	3.15297400	-3.48241100	-3.37061900
H	2.91809300	5.23792400	-2.00265300
H	1.76899400	6.48278900	-2.52556900
H	2.28893800	5.74965000	0.41946600
H	1.05330500	6.86770300	-0.17765000
H	1.06522100	3.96644300	-0.90866800
H	-2.18605600	5.83655900	0.49922200
H	-0.66045800	6.21267300	1.15842400

H	-2.24912800	3.63241900	-0.44881100
H	-1.01556800	3.20721100	-1.48927500
H	-4.25637700	-1.97387600	0.37348100
H	-4.52416100	-0.43013400	-0.47163800
H	-2.20750200	2.27959800	4.25779000
H	-1.85435800	0.62089200	4.77881100
H	-4.22169800	-0.03395000	4.39706100
H	-5.73760200	2.38852400	0.91291700
H	-6.26900100	1.02171300	2.89226300
H	0.63265900	3.74228000	-3.19881200
H	0.43403100	2.27576100	-4.17231200
H	2.43940300	1.24789000	-3.16386700
H	3.32659000	1.43253700	0.81157700
H	4.07890600	1.33658500	-1.44800400
H	2.00134000	-3.55931400	0.98555000
H	-2.91341000	1.65287300	5.76604700
H	-4.72856000	3.47161300	1.87573100
H	-6.53293700	2.71975900	3.35095000
H	1.84311200	3.32827100	-4.42264700
H	3.18350800	6.94273000	-1.55686100
H	4.63175000	2.93996000	-0.93355900
H	2.87100600	3.13496200	0.72142300
H	6.62902400	-0.02347700	5.81244200
H	7.19690300	-0.01567100	4.12109600
H	8.82684600	0.96727800	-2.81605600
H	5.28242200	-3.80355600	2.26920600
H	-5.06882200	-1.71233300	-2.57006500
H	2.23090800	-5.07828800	0.93946400
H	0.00721100	-2.50818200	1.64200500
H	-9.66396400	-1.07346800	-1.96853900
H	-9.19606200	-1.62102400	-0.33176900
H	-9.18283700	0.11733200	-0.74796800
H	1.07407100	-1.67256400	-1.07139000
H	-3.93908300	-3.84971000	-3.15840400
H	-6.95990700	-2.51914400	-0.46969800
H	-5.23304600	-6.24522300	-1.92273300
H	-4.63150300	-6.19869600	-3.60862800
H	-3.48134100	-6.21740500	-2.23958900

Int1-Displacement-0.2-Structure3 optimized

C	6.22286400	-0.00142900	4.94923400
C	5.85578500	-1.46429900	5.08244700
O	5.70547300	-2.02007000	6.16855900
N	5.68779800	-2.05640200	3.86811900
C	4.81490300	-3.20500000	3.73146400
C	3.42277800	-2.77849000	3.23155100
C	3.48970900	-2.05834000	1.87068600
O	4.28746800	-1.05997200	1.78519000
O	2.77430300	-2.49823500	0.94476000
C	-5.24739000	-2.32034000	-1.30323800
C	-4.26613600	-1.52046100	-0.45603200
S	-2.58685700	-1.61634600	-1.18271800
C	8.58271400	0.17286000	-2.75445100
C	7.30572900	-0.40937000	-2.16334000
C	6.92248000	-0.20319100	-0.85205900
C	6.25336400	-1.24092100	-2.73894300
N	5.73139900	-0.82169700	-0.56701400
C	5.29764100	-1.46539700	-1.70177500
C	5.96615400	-1.84544100	-3.98602900
C	4.12388000	-2.22308500	-1.85788900
C	4.80573300	-2.60621800	-4.14710200
C	3.87170900	-2.80587000	-3.09355000
C	2.59574800	6.09392500	-1.84071200
C	1.63389400	5.94446500	-0.66187900
N	0.70619400	4.84091900	-0.90641500
C	-0.61510800	4.85484000	-0.74399400
N	-1.20435300	5.87702100	-0.05744800
N	-1.38475400	3.93785300	-1.32403800
C	-2.89435300	1.58606800	4.75980200
C	-4.01236300	1.17612200	3.80733900
O	-4.98221300	2.22664500	3.86042500
C	-3.46203200	0.96018300	2.40711800
S	-2.19459900	-0.24366800	2.25975200
C	-3.89161500	1.68826600	1.34271000
S	-3.12238900	1.55637900	-0.21285900
C	-5.09064600	2.60317400	1.47999400
C	-5.86047000	2.24418100	2.74913900
C	1.54922400	2.68807600	-3.83338100
C	2.20183800	1.92676600	-2.68110100
O	3.23608600	2.77945500	-2.17170700
C	1.21855200	1.56594600	-1.57240800
S	-0.35560800	0.91498000	-2.06097300
C	1.53162900	1.79101900	-0.26908200
S	0.31466300	1.64761100	1.01254200
C	2.92767600	2.18415200	0.16613600
C	3.87483000	2.19146400	-1.03482200
W	-1.18741700	-0.10261700	0.13169200
O	1.82577100	-4.45965400	-0.75637400
C	-0.11169700	-1.61102400	0.99649300
C	0.27565800	-1.47646700	-0.23926500
C	-5.18849900	-3.79400700	-1.15685000
O	-5.68547100	-4.40399500	-0.20866400
N	-4.65286100	-4.38462900	-2.23350700
N	-6.66068700	-1.97073200	-0.91402200
C	-7.47716100	-1.08787300	-1.57551700
O	-7.09260500	-0.41157000	-2.52463700
C	-4.67274100	-5.79476900	-2.25015700
C	-8.95555500	-0.94990200	-1.08556800
H	5.31712800	0.57597500	4.73072300
H	2.97748300	-2.09983000	3.97055800
H	2.77185800	-3.65186600	3.13463100
H	4.74804900	-3.69288900	4.70731200
H	5.54556100	-1.41872900	3.07832600
H	8.38046500	0.84665100	-3.59756200
H	9.26211000	-0.60591800	-3.12543500
H	7.44086500	0.36138600	-0.08684000
H	5.21155200	-0.84287200	0.33170600
H	6.64541700	-1.72377600	-4.82763700
H	4.61233800	-3.05812200	-5.11780700
H	3.45588100	-2.33421000	-1.01057600
H	2.97187000	-3.39336900	-3.24801500
H	3.10454600	5.14774900	-2.04349200
H	2.05441000	6.39342500	-2.74322700
H	2.18875200	5.75611500	0.26588000
H	1.05034600	6.85932500	-0.52413500
H	1.11291600	3.93455000	-1.15251000
H	-2.20736200	5.82269500	0.04598300
H	-0.71139900	6.23437300	0.74788400

H	-2.22084200	3.60661400	-0.83331500
H	-0.94204300	3.13497400	-1.79815600
H	-4.23478300	-1.90453000	0.56910500
H	-4.60066900	-0.48506500	-0.44141100
H	-2.38192700	2.47138100	4.37225400
H	-2.16274200	0.78351900	4.87178900
H	-4.48198100	0.24321100	4.16900600
H	-5.73400300	2.50629300	0.59659700
H	-6.35596900	1.26692400	2.62624000
H	1.04676700	3.59491800	-3.48237200
H	0.81325900	2.06244900	-4.34207100
H	2.66503900	1.00749100	-3.07566100
H	3.28528200	1.45702200	0.90640000
H	4.19009700	1.17005000	-1.27746400
H	2.06344200	-3.86817000	-0.01438100
H	-3.31301500	1.82388800	5.74349300
H	-4.77286000	3.65472000	1.53154900
H	-6.63053300	2.98919200	2.97574900
H	2.32070100	2.98234500	-4.55139700
H	3.34512000	6.85993800	-1.61651100
H	4.77209700	2.78628700	-0.83956300
H	2.91296200	3.16537300	0.66727900
H	6.65311000	0.36347800	5.88406100
H	6.92694500	0.16993700	4.12929100
H	9.11950000	0.74576700	-1.99205000
H	5.25515200	-3.92290400	3.02694300
H	-5.14297100	-2.01280800	-2.34628600
H	2.67451400	-4.60261900	-1.19245500
H	0.05991200	-2.18117700	1.89825700
H	-9.60888100	-1.19814700	-1.92544500
H	-9.20212000	-1.58555000	-0.23021300
H	-9.12436800	0.09681700	-0.82249100
H	0.93783500	-1.90100700	-0.97849000
H	-4.08350800	-3.84920000	-2.87152000
H	-7.03806000	-2.57028400	-0.19084300
H	-5.66395800	-6.15177400	-1.96001200
H	-4.44553300	-6.16302700	-3.25502400
H	-3.95025900	-6.24142500	-1.55374800

Int1-Displacement-0.2-Structure4 optimized

C	6.60826400	1.36916300	4.52099000
C	6.09294400	0.00222300	4.98156700
O	6.37025500	-0.43031300	6.10166700
N	5.33114800	-0.65477400	4.07572100
C	4.63073800	-1.90539200	4.35046500
C	3.19557000	-1.84066700	3.81944500
C	3.21056400	-1.74116300	2.28493400
O	3.83242100	-0.73393900	1.79678000
O	2.66839500	-2.67256800	1.65446500
C	-5.36232800	-2.03132100	-0.85581100
C	-4.14121700	-1.60812900	-0.04021400
S	-2.59342200	-1.73341300	-1.01718800
C	8.12787000	-0.89944900	-3.00787500
C	6.99793300	-1.12235100	-2.07743800
C	6.72491100	-0.58637200	-0.83747300
C	5.92959700	-2.01533500	-2.38381900
N	5.53867200	-1.09871500	-0.35442700
C	5.03459300	-1.97169300	-1.28652700
C	5.66230100	-2.84047000	-3.48995800
C	3.86256700	-2.72600600	-1.26170700
C	4.50325100	-3.59731300	-3.47131200
C	3.62996900	-3.52647200	-2.36572000
C	2.65895800	5.40616600	-3.35266400
C	1.91863500	5.54839400	-2.02239700
N	1.01934600	4.41137400	-1.83289100
C	-0.29023300	4.45000800	-1.59342600
N	-0.85704600	5.59593900	-1.11278600
N	-1.07145600	3.42169000	-1.89946300
C	-2.55547500	2.96723800	4.27543400
C	-3.71130200	2.31752900	3.52060000
O	-4.66026300	3.36264400	3.28705800
C	-3.22368700	1.67462200	2.23251100
S	-2.03082100	0.39629500	2.39096500
C	-3.68004100	2.06590200	1.01355300
S	-2.99187700	1.42675700	-0.45223900
C	-4.85265600	3.01838600	0.90607900
C	-5.58053100	3.07859200	2.24742200
C	1.28472600	1.80080000	-4.34743800
C	2.10052400	1.22156100	-3.18847500
O	3.15050600	2.16525500	-2.92246500
C	1.27125100	0.99922100	-1.92960100
S	-0.27732200	0.17849100	-2.10599900
C	1.69660300	1.46519100	-0.72959400
S	0.61411700	1.49730700	0.66577900
C	3.10915000	1.95626900	-0.50194200
C	3.92570500	1.77197000	-1.78139300
W	-1.11530300	-0.15791800	0.28330200
O	1.54315400	-4.66525800	0.09836600
C	-0.28963100	-1.53279200	1.55165500
C	-0.01929400	-1.88419900	0.32803700
C	-5.71643100	-3.61640700	-0.63847700
O	-6.87843900	-3.91241900	-0.36253400
N	-4.72881700	-4.57242300	-0.71409200
N	-6.52455200	-1.30247000	-0.44888100
C	-7.51087000	-1.05405200	-1.37173900
O	-7.32726100	-0.98518600	-2.57760300
C	-4.92663900	-6.04097100	-0.44905900
C	-8.84793100	-0.90541200	-0.70931200
H	6.21027200	2.13720400	5.19133500
H	2.69132800	-0.96610900	4.24863500
H	2.65040600	-2.74179400	4.11226100
H	4.65909300	-2.06341200	5.43267500
H	5.04793500	-0.23838200	3.18788100
H	7.78512900	-0.51845900	-3.97979100
H	8.67687100	-1.82882700	-3.21359600
H	7.29512300	0.12783100	-0.25760100
H	5.01904800	-0.88063200	0.51182600
H	6.34842800	-2.87980300	-4.33288900
H	4.25550600	-4.24702900	-4.30687400
H	3.19694500	-2.69030700	-0.40763100
H	2.71563100	-4.11615600	-2.38572200
H	3.17449400	4.44484600	-3.40502800
H	1.95728800	5.46482200	-4.19034700
H	2.62907500	5.59208800	-1.18790200
H	1.32535900	6.46696900	-2.00488300
H	1.42270100	3.48344000	-1.97338900
H	-1.84944200	5.55803000	-0.92915500
H	-0.32038000	6.12752400	-0.44313600

H	-1.89552400	3.19567600	-1.33009100
H	-0.65448300	2.55062100	-2.24345200
H	-4.04278400	-2.20952800	0.87121300
H	-4.29208900	-0.57268300	0.25570100
H	-2.05632400	3.69745700	3.63184700
H	-1.82261000	2.21915800	4.58555600
H	-4.18155400	1.54907500	4.16100100
H	-5.52907300	2.68245300	0.11087000
H	-6.10280000	2.12603800	2.43568500
H	0.79696100	2.74118600	-4.07481600
H	0.51416000	1.09462400	-4.66306600
H	2.55408400	0.27018900	-3.51000900
H	3.54895600	1.36664700	0.31155000
H	4.23628400	0.72708700	-1.89527700
H	1.87702000	-4.01416500	0.74691400
H	-2.93446000	3.48258400	5.16413200
H	-4.51268600	4.02759500	0.63144700
H	-6.32376000	3.88257600	2.26602000
H	1.95071700	1.99914400	-5.19313100
H	3.39248200	6.21209600	-3.46104100
H	4.82306300	2.39780900	-1.78649400
H	3.11533000	3.00904200	-0.17671000
H	7.69776600	1.38535600	4.61706800
H	6.33324100	1.61692700	3.49195800
H	8.85452500	-0.17739000	-2.61680300
H	5.15914600	-2.74891500	3.88347200
H	-5.20804600	-1.84270400	-1.92024500
H	2.34600600	-4.94916600	-0.35516400
H	-0.14934600	-1.81864300	2.58509200
H	-9.21314100	-1.90442300	-0.44590100
H	-8.78593200	-0.31504000	0.21060800
H	-9.56073400	-0.43833100	-1.39110500
H	0.43638400	-2.66927400	-0.26113800
H	-3.78304100	-4.25316600	-0.89815600
H	-6.88058700	-1.59052000	0.45397000
H	-5.98702500	-6.18613100	-0.24329400
H	-4.63147500	-6.62057600	-1.32797100
H	-4.32922100	-6.34931100	0.41357800

Int1-Displacement-0.2-Structure5 optimized

C	6.51060400	-0.75991200	4.90895800
C	6.09445400	-2.19203700	4.83670900
O	5.84304100	-2.88282600	5.81774300
N	5.93854100	-2.59328700	3.53414600
C	4.74887400	-3.37262600	3.28931300
C	3.51212200	-2.47767100	3.07656700
C	3.68952600	-1.64047000	1.80143400
O	4.64439300	-0.79191200	1.79199200
O	2.93282400	-1.88983000	0.82705400
C	-5.41704700	-2.03227000	-1.53165900
C	-4.15030800	-1.76768300	-0.69276800
S	-2.61455200	-1.46198500	-1.65252400
C	8.36165200	0.51224300	-3.24028300
C	7.21211400	-0.09881300	-2.48470200
C	6.93916300	0.06195300	-1.14203700
C	6.17149100	-0.96160200	-2.99251000
N	5.81063100	-0.63501500	-0.77628800
C	5.31770700	-1.27188200	-1.89285200
C	5.85764500	-1.51247500	-4.25176900
C	4.18903200	-2.09638400	-2.01575900
C	4.73840300	-2.32889200	-4.37920400
C	3.90805700	-2.62073700	-3.27026400
C	2.49891000	6.16076800	-0.82666400
C	1.44600800	5.84531300	0.23730800
N	0.51174400	4.83602900	-0.25983800
C	-0.80911300	4.81613500	-0.09186600
N	-1.40112000	5.70152400	0.76068300
N	-1.57542400	4.00866500	-0.82246500
C	-2.75925900	0.98987500	4.91587300
C	-3.85403100	0.58067600	3.92805800
O	-4.89960200	1.54157600	4.10335200
C	-3.34406100	0.53285400	2.49046100
S	-2.07628700	-0.62024400	2.12379500
C	-3.86449900	1.33548700	1.51735500
S	-3.18046600	1.38754100	-0.07735500
C	-5.11736500	2.14503300	1.77622000
C	-5.81419200	1.60248500	3.02137500
C	1.39964200	3.32884900	-3.54500500
C	2.08283600	2.33630200	-2.60447800
O	3.17450300	3.04575000	-2.01045700
C	1.14239400	1.78679500	-1.53569000
S	-0.44119400	1.19101700	-2.06601800
C	1.50074800	1.79276300	-0.22509200
S	0.32772900	1.41166500	1.05128600
C	2.90897900	2.12318700	0.22186500
C	3.81805900	2.26740800	-0.99764400
W	-1.18300000	-0.18465100	-0.02323900
O	1.75712200	-4.35612600	0.96466500
C	-0.12525400	-1.84929800	0.51753700
C	0.32655300	-1.41391100	-0.62390000
C	-5.61277100	-3.45649400	-1.99036600
O	-6.71695300	-4.01374300	-1.92340900
N	-4.52557000	-4.09133200	-2.44139600
N	-6.57210100	-1.73936600	-0.72810900
C	-7.16957400	-0.53636800	-0.96980500
O	-6.58677100	0.52428300	-1.14562500
C	-4.69186000	-5.49103400	-2.68217700
C	-8.61903100	-0.75933100	-1.16266800
H	5.68332100	-0.13766800	4.55016000
H	3.38958200	-1.81953800	3.94505800
H	2.62737000	-3.11065100	2.98523200
H	4.60051500	-4.03436700	4.14523200
H	5.96585800	-1.81410200	2.87322300
H	8.01873200	1.16067000	-4.05802900
H	9.01045900	-0.25004000	-3.69278800
H	7.48603400	0.63723300	-0.40564200
H	5.36450000	-0.65074800	0.16050200
H	6.48235700	-1.30220800	-5.11746400
H	4.49510400	-2.75246600	-5.35092300
H	3.57363800	-2.28998300	-1.14399200
H	3.04296300	-3.26497100	-3.40414200
H	2.97925500	5.24525500	-1.18398400
H	2.04007700	6.65958900	-1.68543500
H	1.92473500	5.47991000	1.15513300
H	0.87673500	6.74492100	0.49022000
H	0.91636800	3.97587600	-0.64189000
H	-2.40362000	5.62806200	0.85642600
H	-0.90632400	5.92805800	1.61096600

H	-2.41301600	3.60292600	-0.39828100
H	-1.12660600	3.29488800	-1.41995100
H	-3.97767900	-2.59321400	0.00775000
H	-4.36694300	-0.87641600	-0.11049900
H	-2.35152600	1.96515500	4.63473800
H	-1.94587700	0.26013300	4.91973100
H	-4.23977500	-0.41680100	4.20708600
H	-5.77495200	2.07627500	0.90186500
H	-6.23872500	0.60748500	2.81055700
H	0.96182600	4.16376900	-2.98938800
H	0.60795100	2.84003300	-4.11686600
H	2.48523900	1.49758200	-3.19719000
H	3.28987600	1.31533000	0.85963200
H	4.07524400	1.27924000	-1.39707900
H	2.14199900	-3.44704200	0.89748200
H	-3.18090500	1.06028200	5.92347000
H	-4.87494900	3.20722300	1.92685700
H	-6.62918900	2.25854000	3.34490400
H	2.14140000	3.73426500	-4.23978100
H	3.26282000	6.82401400	-0.40874600
H	4.74858000	2.78642300	-0.75084900
H	2.91995600	3.03995000	0.83357300
H	6.76721200	-0.47491800	5.93168100
H	7.36420400	-0.55420800	4.25351800
H	8.98487400	1.12169500	-2.57730800
H	4.88611400	-4.00767400	2.40504300
H	-5.38164200	-1.36610200	-2.40666200
H	2.29705500	-4.87858300	0.36010800
H	0.01348900	-2.62919700	1.25245000
H	-8.76629100	-1.23762700	-2.13797000
H	-9.03684400	-1.43308400	-0.40731500
H	-9.18474800	0.17627800	-1.15033800
H	1.04792600	-1.59956400	-1.40576500
H	-3.60962400	-3.65534900	-2.38301900
H	-7.21183600	-2.53043800	-0.76846900
H	-5.42943100	-5.66813300	-3.47072700
H	-3.73751400	-5.92345000	-2.99334300
H	-5.04204000	-6.01354500	-1.78490100

Int1-Displacement-0.2-Structure6 optimized

C	6.53738100	1.69047600	4.74494900
C	6.07158500	0.28282000	5.07594800
O	6.14215500	-0.17304200	6.21783900
N	5.57218900	-0.37739300	4.00569400
C	4.78872200	-1.59031400	4.12433200
C	3.36777100	-1.37511200	3.58096700
C	3.36332300	-0.98408700	2.09170900
O	4.15347400	-0.04010100	1.73716300
O	2.60911200	-1.61913700	1.32100800
C	-5.19961800	-2.56322000	-0.68856900
C	-4.05986100	-1.81849100	0.01523300
S	-2.57395100	-1.76827800	-1.05728500
C	8.50502800	-0.93615000	-2.79265600
C	7.23479500	-1.14945300	-2.02573300
C	6.79247300	-0.40010300	-0.95742900
C	6.22334400	-2.15269200	-2.24967100
N	5.57317600	-0.85245700	-0.50960200
C	5.20062300	-1.92656500	-1.28419500
C	6.06409400	-3.22518000	-3.15054300
C	4.04151200	-2.71002500	-1.20854900
C	4.92600200	-4.01998500	-3.06593200
C	3.92066200	-3.76340600	-2.10296200
C	2.29599800	5.23080300	-3.58904300
C	1.35047100	5.37906300	-2.39646200
N	0.51361700	4.18716100	-2.26404400
C	-0.81511100	4.13622100	-2.20750200
N	-1.53108700	5.27208100	-1.95806200
N	-1.47086700	3.01150200	-2.47949100
C	-2.59498700	3.25485600	4.16401600
C	-3.75689200	2.65758000	3.37886200
O	-4.61723700	3.74913600	3.04114200
C	-3.27804800	1.90734400	2.14668200
S	-2.12067700	0.61529400	2.40394000
C	-3.76071500	2.17090600	0.90583600
S	-3.16423000	1.30572100	-0.48565600
C	-4.89873400	3.15147800	0.71458200
C	-5.58042800	3.41316900	2.05723100
C	1.37411900	1.27715400	-4.42493200
C	2.13715900	1.00505400	-3.12848900
O	3.07332000	2.08067500	-2.97126200
C	1.23850000	0.91470100	-1.90050300
S	-0.24971200	-0.01341400	-2.03750800
C	1.57628000	1.53753300	-0.74701700
S	0.45600300	1.58425300	0.61931800
C	2.91948600	2.20052800	-0.53608100
C	3.81477800	1.95227800	-1.75273200
W	-1.22242500	-0.12168700	0.33605200
O	1.92330500	-4.26786000	1.00831700
C	-0.50881700	-1.43423100	1.72886100
C	-0.16887800	-1.85855400	0.54757900
C	-5.31633600	-4.05393900	-0.22021400
O	-6.27049600	-4.41271700	0.47623000
N	-4.35629800	-4.93618800	-0.59370100
N	-6.49902700	-1.97732000	-0.35763300
C	-7.38127800	-1.54849600	-1.31632200
O	-7.07206100	-1.29538700	-2.47421400
C	-4.42762400	-6.33024500	-0.13744000
C	-8.81986000	-1.41866800	-0.81155400
H	5.80288600	2.40663000	5.13006900
H	2.88405500	-0.57413300	4.15509200
H	2.77676500	-2.28650300	3.70626800
H	4.77239100	-1.87191800	5.18064800
H	5.36950600	0.11845100	3.13489300
H	8.31563200	-0.70840200	-3.85062600
H	9.15438700	-1.82204300	-2.77374300
H	7.27354100	0.44255300	-0.47719300
H	5.03218600	-0.49304800	0.29884900
H	6.82327400	-3.43304900	-3.90172200
H	4.80138800	-4.85085400	-3.75643600
H	3.28092000	-2.47749000	-0.47336100
H	3.03227400	-4.38926900	-2.07241600
H	2.86522400	4.30157400	-3.51606300
H	1.73071300	5.21149600	-4.52596300
H	1.91765400	5.52311900	-1.46903000
H	0.69949700	6.24785100	-2.52799600
H	0.99528000	3.28635000	-2.20284600
H	-2.53388900	5.16299000	-1.90883300
H	-1.14072000	5.92873600	-1.29836100

H	-2.33071800	2.80423300	-1.95875500
H	-0.94348300	2.13693800	-2.61019300
H	-3.82116200	-2.27426200	0.98329000
H	-4.40139100	-0.80022700	0.19439500
H	-2.00083600	3.90658300	3.51662300
H	-1.94452600	2.46884700	4.55271400
H	-4.31564000	1.96103500	4.03180500
H	-5.61762500	2.74983400	-0.01037800
H	-6.15549400	2.52404000	2.36521300
H	0.78694700	2.19860800	-4.35983200
H	0.69663100	0.45176400	-4.65202800
H	2.69836400	0.06247300	-3.23634000
H	3.38866300	1.76460800	0.35510600
H	4.25655700	0.95090600	-1.69821300
H	2.12060200	-3.34576600	1.28304800
H	-2.97903900	3.84546700	5.00216600
H	-4.52639700	4.10161000	0.30355500
H	-6.27183300	4.26043400	1.99798600
H	2.08798100	1.38706600	-5.24693900
H	2.99019000	6.07699300	-3.62266400
H	4.62795000	2.68274600	-1.80986300
H	2.79774100	3.27946500	-0.34739900
H	7.48365100	1.88895200	5.25534400
H	6.65922600	1.86352800	3.67243900
H	9.07937700	-0.10173900	-2.37613900
H	5.27226400	-2.40778000	3.57120400
H	-5.07896900	-2.50032400	-1.77374500
H	2.71697800	-4.52004600	0.52039800
H	-0.44461200	-1.65199300	2.78644200
H	-9.32190800	-2.38841500	-0.90413500
H	-8.86614600	-1.11047800	0.23701900
H	-9.34938500	-0.69523000	-1.43311000
H	0.31851800	-2.66737900	0.02321600
H	-3.50748900	-4.58416100	-1.02061900
H	-6.91905000	-2.44254600	0.44183400
H	-5.42293200	-6.72790100	-0.34568400
H	-3.67781000	-6.91211100	-0.67663700
H	-4.24364900	-6.41372400	0.93944700

Int1-Displacement-0.2-Structure7 optimized

C	6.69682300	1.65951300	4.61175000
C	6.29298200	0.21448700	4.94209000
O	6.54394600	-0.27646800	6.04372600
N	5.66351100	-0.43308900	3.93292500
C	5.00434200	-1.73316700	4.04905900
C	3.53549200	-1.62430100	3.62218600
C	3.34960300	-1.12749300	2.17289700
O	4.10796400	-0.17498800	1.77624600
O	2.46757100	-1.68475600	1.48193300
C	-5.24370900	-2.48227400	-0.64732400
C	-3.95592300	-1.96856800	0.01670700
S	-2.67597300	-1.67365200	-1.26672900
C	8.39723500	-0.87473200	-2.95556600
C	7.16663700	-1.12789300	-2.11859800
C	6.82361600	-0.41391000	-0.98918800
C	6.10981700	-2.10490000	-2.29689900
N	5.63598100	-0.85991600	-0.46088800
C	5.17294700	-1.89154700	-1.24370600
C	5.82650100	-3.14466600	-3.20962800
C	3.99246400	-2.63449400	-1.09268000
C	4.66895000	-3.90398800	-3.05118200
C	3.74788800	-3.65452800	-2.00156200
C	2.38547000	5.22148800	-3.34499400
C	1.45545200	5.40036300	-2.14255000
N	0.54498300	4.26037600	-2.02422700
C	-0.78321500	4.29009200	-1.94037100
N	-1.42259200	5.45701500	-1.63747000
N	-1.50939000	3.21440100	-2.23364200
C	-2.33065100	2.96233400	4.27971100
C	-3.55936200	2.41895100	3.56246300
O	-4.42927800	3.53326300	3.34343300
C	-3.17467700	1.73225500	2.26423000
S	-2.01287800	0.42488200	2.37648200
C	-3.72760200	2.07291500	1.07298200
S	-3.21903500	1.29360200	-0.40256500
C	-4.86882900	3.06588100	1.01099500
C	-5.45804900	3.25748300	2.40831700
C	1.23471000	1.65359700	-4.46148000
C	2.02699200	1.12213600	-3.26582200
O	3.09533700	2.04737600	-3.03711700
C	1.17359300	0.96971900	-2.01340300
S	-0.36015200	0.12484000	-2.17554300
C	1.57972000	1.46827700	-0.82179500
S	0.49982200	1.45410200	0.57882900
C	2.97616100	2.00752800	-0.60219700
C	3.82323700	1.73101000	-1.84518400
W	-1.23725700	-0.16816300	0.21433600
O	1.84214200	-4.32997000	0.94881200
C	-0.51577700	-1.61850900	1.46000100
C	-0.22670800	-1.94088800	0.23396000
C	-5.53578500	-3.88921300	-0.31413400
O	-6.34623000	-4.25046300	0.53624500
N	-4.73257400	-4.72638900	-1.00239200
N	-6.42867000	-1.68036300	-0.22985900
C	-7.41334400	-1.30617500	-1.12190400
O	-7.25156900	-1.29343200	-2.33575300
C	-4.55625100	-5.95817000	-0.33379300
C	-8.76989600	-0.88126300	-0.50956100
H	6.16098400	2.33408600	5.28680700
H	3.01976200	-0.92221300	4.29073400
H	3.04142900	-2.59548400	3.71751300
H	5.09879500	-2.06166300	5.08773300
H	5.35249000	0.06336200	3.09528200
H	8.14415600	-0.59766300	-3.98768800
H	9.04764600	-1.75763500	-3.01567500
H	7.36076700	0.40034800	-0.51946400
H	5.13466200	-0.51690300	0.37386000
H	6.50567000	-3.35714500	-4.03273500
H	4.46248500	-4.70438300	-3.75808600
H	3.29773500	-2.39078900	-0.29618300
H	2.84337300	-4.24942700	-1.91279000
H	2.89812000	4.25820000	-3.30036800
H	1.81672900	5.26212000	-4.27916700
H	2.03648700	5.49050200	-1.21674600
H	0.85757200	6.30981300	-2.25096500
H	0.96481600	3.32581900	-1.99338800
H	-2.42989700	5.41673500	-1.58392700
H	-0.97859100	6.07411200	-0.97391800

H	-2.36575800	3.02200400	-1.70601000
H	-1.03590400	2.32402300	-2.44699300
H	-3.57793700	-2.66520100	0.77411400
H	-4.19628700	-1.02891000	0.51281600
H	-1.77623600	3.63307500	3.61661100
H	-1.66676000	2.14981400	4.58132200
H	-4.07571700	1.69569800	4.22105800
H	-5.63676000	2.70596000	0.31490200
H	-6.02007700	2.35622800	2.70518700
H	0.76229600	2.61374400	-4.23601300
H	0.45652100	0.94432300	-4.75064100
H	2.45715900	0.14151000	-3.52899300
H	3.41413800	1.49605600	0.26468400
H	4.12605500	0.67827700	-1.86896800
H	1.99299000	-3.41643500	1.27356100
H	-2.63591100	3.52070300	5.17098000
H	-4.51877800	4.03540900	0.62673500
H	-6.14391900	4.11068200	2.44110500
H	1.91244600	1.79948700	-5.30838400
H	3.12862000	6.02566100	-3.35973100
H	4.72723700	2.34691100	-1.86481300
H	2.95663200	3.08457300	-0.36952200
H	7.76559100	1.78081900	4.81005200
H	6.48474100	1.94736900	3.57860300
H	8.98957100	-0.05808000	-2.53038800
H	5.52239600	-2.46879800	3.41824300
H	-5.18235800	-2.35010100	-1.73090400
H	2.68771300	-4.55595600	0.54245500
H	-0.41710800	-1.93222500	2.48971700
H	-9.48061100	-1.70346300	-0.64014900
H	-8.70755800	-0.63495200	0.55427400
H	-9.13882200	-0.01970000	-1.06856600
H	0.22351200	-2.70825900	-0.37747300
H	-3.93541400	-4.31344700	-1.47484200
H	-6.76319300	-1.95077300	0.68837200
H	-5.51901500	-6.45695900	-0.20781000
H	-3.90547700	-6.61853000	-0.91546500
H	-4.11767200	-5.84147900	0.66726000

Int1-Displacement-0.2-Structure8 optimized

C	6.28485400	0.97342100	5.01544200
C	5.88312600	-0.57470300	5.05704100
O	6.18147000	-1.21002800	6.06810400
N	5.24109700	-1.13340600	3.98155500
C	4.70351600	-2.54776100	3.84034300
C	3.29764200	-2.49723600	3.26204000
C	3.30559800	-1.96346700	1.81885500
O	3.93030400	-0.87313900	1.59691600
O	2.70210800	-2.65841100	0.96735400
C	-5.11207300	-2.36714100	-1.08403300
C	-4.10322200	-1.71128800	-0.17345700
S	-2.43706000	-1.82119600	-0.91410100
C	8.67353000	-0.00966500	-2.94452200
C	7.47442500	-0.46980200	-2.15691300
C	7.08426200	-0.00271600	-0.91763200
C	6.49807600	-1.47040700	-2.52751100
N	5.93343900	-0.63355500	-0.49827500
C	5.55467600	-1.53406200	-1.46602400
C	6.30189300	-2.33470900	-3.62632000
C	4.44923500	-2.39133100	-1.46219200
C	5.21403800	-3.20317400	-3.62402500
C	4.28969500	-3.23365500	-2.54871300
C	2.35380800	5.78266500	-2.17338500
C	1.27360500	5.85428900	-1.09378400
N	0.32418400	4.75602200	-1.26534200
C	-1.00224000	4.82697700	-1.25445800
N	-1.62406400	5.95522500	-0.80812900
N	-1.73773800	3.83858700	-1.76459600
C	-2.86022400	2.05355700	4.40560200
C	-4.04705200	1.44945700	3.66399600
O	-5.06152400	2.45736900	3.62909500
C	-3.56990200	1.04407600	2.28514600
S	-2.23988300	-0.09653000	2.27757100
C	-4.02299600	1.65706000	1.16107600
S	-3.21711400	1.44628400	-0.36627000
C	-5.25342400	2.53624500	1.22519000
C	-5.97254200	2.30875300	2.55368800
C	1.36139300	2.49675100	-3.94164100
C	2.06191400	1.76468400	-2.79975500
O	3.16396300	2.57976500	-2.39321500
C	1.10193400	1.51965600	-1.64984800
S	-0.46149100	0.81594000	-2.08328100
C	1.40976800	1.89093600	-0.37819400
S	0.18016000	1.89465300	0.90194500
C	2.81936500	2.29605600	-0.00144300
C	3.75977300	2.08755600	-1.18973200
W	-1.19195900	-0.05119000	0.17446500
O	2.70230000	-5.19145600	-0.20333200
C	0.00163200	-1.37095800	1.17611300
C	0.45554900	-1.22717300	-0.03651300
C	-5.16636800	-3.98805100	-0.83354300
O	-5.95563400	-4.38502700	0.02517500
N	-4.39563300	-4.87226800	-1.55234600
N	-6.49296500	-1.94301100	-0.78580600
C	-7.35866500	-1.45463200	-1.73826700
O	-6.99839400	-1.06882700	-2.84420500
C	-4.39097400	-6.37370400	-1.37163500
C	-8.85278500	-1.40130100	-1.33967100
H	5.81948000	1.44827100	5.88171500
H	2.67237400	-1.85152600	3.89155500
H	2.86002400	-3.49934800	3.25692700
H	4.73380600	-2.99626000	4.83674100
H	4.95812100	-0.56933600	3.17933300
H	8.38761400	0.41767100	-3.91489800
H	9.36854800	-0.83371500	-3.15400800
H	7.55893200	0.74728300	-0.29795700
H	5.39611400	-0.53071100	0.36639900
H	6.99412200	-2.32814300	-4.46580100
H	5.06798800	-3.87198600	-4.46932600
H	3.74742700	-2.39604800	-0.63444900
H	3.44882800	-3.92160700	-2.56883700
H	2.82793500	4.79814500	-2.19457300
H	1.92156000	5.97251900	-3.16062500
H	1.72060100	5.79333700	-0.09361400
H	0.72518600	6.79869800	-1.15958100
H	0.71688700	3.81031600	-1.32627600
H	-2.63302000	5.95514300	-0.82881200
H	-1.20356800	6.44856200	-0.03476700

H	-2.61327800	3.58945800	-1.30256400
H	-1.25706200	2.97211700	-2.06179500
H	-4.08304100	-2.18138900	0.81604000
H	-4.38564300	-0.66825800	-0.05791600
H	-2.41224300	2.84865000	3.80297800
H	-2.09758300	1.30038100	4.60855000
H	-4.43313200	0.57431300	4.21613800
H	-5.91766300	2.30770400	0.38198800
H	-6.43552200	1.30845700	2.56655800
H	0.90461300	3.42937100	-3.60062500
H	0.58480100	1.87003500	-4.38301300
H	2.45090500	0.80174200	-3.17090000
H	3.14924800	1.66562600	0.83358800
H	3.99756100	1.02287700	-1.30128500
H	2.58254700	-4.38468500	0.33549400
H	-3.19330400	2.48108800	5.35846900
H	-4.97622300	3.59682900	1.13691600
H	-6.76231000	3.05022100	2.71403800
H	2.09428100	2.74319700	-4.71698900
H	3.11967200	6.54179600	-1.98265400
H	4.69968900	2.63277100	-1.06434900
H	2.84777500	3.33918100	0.35105800
H	7.36974200	1.02857600	5.12958900
H	5.97987600	1.48885400	4.10006700
H	9.22986600	0.75866100	-2.39725800
H	5.37600300	-3.11716300	3.18770400
H	-4.91569500	-2.12485600	-2.13006400
H	3.56629700	-5.03832900	-0.60490900
H	0.18296000	-1.88752300	2.10772600
H	-9.38502700	-2.18239900	-1.89126900
H	-9.02423300	-1.54353800	-0.26904400
H	-9.25380100	-0.43527200	-1.65241200
H	1.24256000	-1.56662800	-0.69181800
H	-3.68073400	-4.47658300	-2.14920700
H	-6.89326700	-2.47740500	-0.02111500
H	-5.22242900	-6.61452200	-0.71023900
H	-4.52505400	-6.85215300	-2.34471000
H	-3.44896300	-6.69721300	-0.92066600

Int1-Displacement-0.2-Structure9 optimized

C	6.59735800	0.85345800	4.88611200
C	6.22031700	-0.68188100	5.00398300
O	6.56078500	-1.29068400	6.01900000
N	5.54327600	-1.25643300	3.96615100
C	4.99853500	-2.65684200	3.87250100
C	3.56483700	-2.60862100	3.34639300
C	3.45201500	-1.98884800	1.93616000
O	4.11777500	-0.92139900	1.71266900
O	2.70689600	-2.57264300	1.11937600
C	-5.11416900	-2.50675600	-1.23460700
C	-4.27038600	-1.42084400	-0.59514300
S	-2.52442400	-1.60378500	-1.11506100
C	8.47194600	-0.20479000	-2.97026700
C	7.22577900	-0.65696500	-2.24754000
C	6.86447100	-0.26994800	-0.97247500
C	6.17420300	-1.54778200	-2.69629500
N	5.67044400	-0.83961100	-0.59991400
C	5.22700000	-1.62856900	-1.63459300
C	5.90399100	-2.30230100	-3.85911100
C	4.05919100	-2.40253400	-1.69123500
C	4.74962200	-3.07995600	-3.92111400
C	3.82602900	-3.13579400	-2.84570600
C	2.11500400	5.83323600	-2.55720800
C	1.22179000	5.87181300	-1.31673900
N	0.30923200	4.72778000	-1.30733300
C	-1.01949800	4.76421200	-1.33394200
N	-1.67878800	5.90265200	-0.96807000
N	-1.72207100	3.72951800	-1.78954800
C	-2.64419100	2.04617200	4.79125800
C	-3.79991500	1.50370400	3.95602800
O	-4.80670600	2.52174800	3.97061000
C	-3.33147600	1.16687800	2.55020500
S	-2.06232200	-0.03699200	2.41960000
C	-3.84055900	1.78491600	1.45288200
S	-3.15333500	1.51799000	-0.12107400
C	-5.05562100	2.67971100	1.57617600
C	-5.74319600	2.41390400	2.91414200
C	1.36846200	2.52327600	-4.04153400
C	2.08240500	1.82396100	-2.88407500
O	3.16135900	2.68115600	-2.49602800
C	1.15834100	1.54287000	-1.70597400
S	-0.39096100	0.76640600	-2.06694400
C	1.51647900	1.87108000	-0.43939300
S	0.36748200	1.73389600	0.90464400
C	2.91796300	2.33409500	-0.09954600
C	3.82314300	2.19670700	-1.32486400
W	-1.17486100	-0.06746000	0.22955000
O	1.75449600	-4.60203600	-0.49272100
C	-0.09203600	-1.51620300	1.18137300
C	0.20008100	-1.54853000	-0.08562800
C	-4.91849500	-3.91792800	-0.70195500
O	-5.15474100	-4.18875500	0.47451000
N	-4.62247100	-4.83962700	-1.64903500
N	-6.56892800	-2.23195500	-0.90691300
C	-7.47960200	-1.55924400	-1.68638800
O	-7.20658100	-1.13207100	-2.80332900
C	-4.60545100	-6.24943200	-1.35238600
C	-8.92776800	-1.34374100	-1.11551800
H	6.16186300	1.36487900	5.74773700
H	2.95133200	-2.01562400	4.03718700
H	3.14511500	-3.61798700	3.30994700
H	5.05941000	-3.09706000	4.87132900
H	5.22204300	-0.70179500	3.16932200
H	8.23936300	0.33395900	-3.89874900
H	9.11844500	-1.04819800	-3.24786300
H	7.39298400	0.38838900	-0.29448700
H	5.16021000	-0.76732200	0.29651300
H	6.59034700	-2.28166700	-4.70333700
H	4.55052100	-3.65764500	-4.82113900
H	3.38346600	-2.42092300	-0.84223700
H	2.92593400	-3.73842900	-2.92619900
H	2.67239300	4.89440700	-2.60545100
H	1.51526100	5.93125400	-3.46723000
H	1.82662300	5.84786900	-0.40319800
H	0.62785600	6.78953400	-1.29843900
H	0.73058100	3.79140100	-1.34685700
H	-2.68669100	5.87246300	-1.00949600
H	-1.29064100	6.44296200	-0.20928400

H	-2.59988400	3.49399100	-1.32491100
H	-1.22180600	2.85798800	-2.04909900
H	-4.33350600	-1.49412700	0.49423100
H	-4.66559200	-0.45916300	-0.91506700
H	-2.19665600	2.90954300	4.29049600
H	-1.87246400	1.28583200	4.92820900
H	-4.20861400	0.59648000	4.43692800
H	-5.74440100	2.48728800	0.74374800
H	-6.21187600	1.41581500	2.90522800
H	0.86260500	3.43424000	-3.71251400
H	0.62491200	1.85941700	-4.48777900
H	2.50217800	0.87087500	-3.24689200
H	3.30634800	1.70598500	0.71171000
H	4.10895300	1.14725200	-1.46763900
H	1.99743000	-3.97384400	0.21621500
H	-3.01157100	2.35970600	5.77417400
H	-4.76774700	3.73926300	1.51844200
H	-6.52445400	3.15402500	3.11792800
H	2.10323000	2.79447400	-4.80585000
H	2.82706500	6.66527300	-2.52499900
H	4.73816100	2.78732700	-1.22020200
H	2.91167100	3.37057700	0.27355500
H	7.68510800	0.93260000	4.95446900
H	6.24928600	1.32471000	3.96257200
H	9.06140900	0.46716900	-2.33790700
H	5.63806800	-3.24414700	3.20140800
H	-5.02893200	-2.45772100	-2.32299000
H	2.60276700	-4.77225200	-0.91985200
H	0.13158500	-1.98017000	2.13101900
H	-9.63179000	-1.78054200	-1.82724500
H	-9.08642400	-1.78094700	-0.12556400
H	-9.10896900	-0.26728600	-1.07259000
H	0.77711400	-2.09642800	-0.81617700
H	-4.35615700	-4.51802500	-2.56698100
H	-6.83631100	-2.55572800	0.01386500
H	-4.98675300	-6.37447600	-0.33848000
H	-5.24251000	-6.80225700	-2.05256100
H	-3.59189600	-6.66510000	-1.39628000

Int1-Displacement-0.2-Structure10 optimized

C	6.35694100	0.29696700	4.83703500
C	6.07480700	-1.17865200	4.98881300
O	6.15234400	-1.76702000	6.06660700
N	5.69959600	-1.73903400	3.81327600
C	4.93685900	-2.96340900	3.77612600
C	3.50076400	-2.69647900	3.28983300
C	3.49050800	-2.06510600	1.88362900
O	4.13630800	-0.96612000	1.75232700
O	2.87976100	-2.66851600	0.97687100
C	-5.23677800	-2.14564200	-1.18785500
C	-4.11949400	-1.70920400	-0.25008500
S	-2.48511000	-1.73181700	-1.07456600
C	8.49187800	0.01989100	-2.85684800
C	7.31597000	-0.36988900	-2.05571400
C	6.91727900	-0.07158100	-0.77256700
C	6.32968300	-1.23132200	-2.60608200
N	5.71933400	-0.70024500	-0.49657400
C	5.34608500	-1.42035400	-1.60565800
C	6.22755200	-1.85154500	-3.86092200
C	4.23824200	-2.23436600	-1.83011600
C	5.13144100	-2.66218100	-4.09020300
C	4.17181400	-2.83356700	-3.07496300
C	2.27490300	6.08448500	-1.73451600
C	1.22047300	5.92528200	-0.64009200
N	0.31708500	4.82513300	-0.97304600
C	-1.01011300	4.82494800	-0.89425900
N	-1.65813500	5.84727200	-0.26555600
N	-1.72799800	3.88435600	-1.50861400
C	-2.83767600	1.53367500	4.79377700
C	-3.94445800	1.04040400	3.86941400
O	-4.97852300	2.02692000	3.92943000
C	-3.40345000	0.84414700	2.46285700
S	-2.06020100	-0.27231600	2.30863300
C	-3.89723100	1.53445100	1.39982500
S	-3.14906400	1.43468500	-0.16616400
C	-5.15008300	2.37190800	1.54872200
C	-5.87495000	1.97706100	2.83349200
C	1.32909800	2.76573400	-3.91072100
C	2.05405900	1.99206600	-2.81144100
O	3.12691200	2.82761500	-2.36482100
C	1.12772000	1.63171400	-1.65811400
S	-0.43955600	0.91990800	-2.08104900
C	1.47874600	1.89345300	-0.37105100
S	0.30939000	1.73918600	0.95376800
C	2.88628700	2.31400900	-0.00152300
C	3.79144800	2.25906200	-1.23298900
W	-1.12203500	-0.10785700	0.14952800
O	1.83196000	-4.43559700	-0.88184400
C	0.08017500	-1.52759400	0.99846400
C	0.41502500	-1.38598900	-0.25208900
C	-5.34365700	-3.74005000	-1.27841200
O	-6.24646100	-4.30384200	-0.65347300
N	-4.45789500	-4.44881500	-2.03614300
N	-6.54235700	-1.73081000	-0.68576200
C	-7.46111900	-1.12141100	-1.50700900
O	-7.17182600	-0.51534100	-2.53083400
C	-4.47940700	-5.93222600	-2.11767200
C	-8.90093800	-1.28093400	-1.03038100
H	5.42001600	0.85525600	4.95767600
H	3.01382300	-2.01093800	3.99501800
H	2.93334500	-3.63091200	3.26436300
H	4.94212300	-3.39148200	4.78364400
H	5.42533100	-1.11571500	3.04763300
H	8.20043700	0.54068000	-3.77924200
H	9.07997000	-0.85523600	-3.16559100
H	7.40095600	0.54443500	-0.02567000
H	5.17055000	-0.71127800	0.38227900
H	6.98984500	-1.69832400	-4.62097300
H	5.00142600	-3.16792000	-5.04350600
H	3.49687800	-2.39956700	-1.05764500
H	3.31253000	-3.47183900	-3.27882200
H	2.78400500	5.13577400	-1.92593600
H	1.81162700	6.41574000	-2.66893900
H	1.69449600	5.72402200	0.32876000
H	0.62919200	6.84034400	-0.54174900
H	0.74875000	3.91861900	-1.18119000
H	-2.66495600	5.78364400	-0.22808100
H	-1.22180000	6.23868800	0.55616500

H	-2.57824800	3.55313900	-1.04755800
H	-1.23056700	3.06937400	-1.90690600
H	-4.06489600	-2.35595700	0.63368900
H	-4.34904500	-0.69963200	0.07964600
H	-2.38860700	2.44289700	4.38374900
H	-2.05528700	0.78041600	4.90426200
H	-4.34654400	0.08370800	4.24965900
H	-5.79996800	2.22423300	0.67745600
H	-6.30908200	0.96939000	2.72724800
H	0.85488700	3.67003900	-3.51581200
H	0.56045500	2.14681800	-4.37708000
H	2.47845800	1.06938400	-3.24134600
H	3.26632200	1.62485800	0.76311100
H	4.07477400	1.22182900	-1.45032200
H	2.09372000	-3.90019300	-0.10762700
H	-3.25249100	1.76075300	5.78166400
H	-4.89831100	3.44172400	1.58638800
H	-6.68683700	2.67399200	3.06657100
H	2.05055500	3.06803900	-4.67583100
H	3.01716100	6.83101200	-1.43320000
H	4.70843900	2.83742800	-1.08794600
H	2.88976500	3.31939900	0.44855100
H	7.04956800	0.62876400	5.61305400
H	6.76580000	0.54275500	3.85246900
H	9.17291200	0.68702900	-2.31423100
H	5.41757000	-3.69114100	3.10618800
H	-5.10015900	-1.69977500	-2.17604700
H	2.68194900	-4.65058000	-1.28487600
H	0.32374700	-2.07620900	1.89672300
H	-9.27098100	-2.26735500	-1.33281400
H	-8.98418900	-1.21096900	0.05848300
H	-9.52148400	-0.51560900	-1.49817400
H	1.07700800	-1.77680700	-1.01022600
H	-3.64417300	-3.95844800	-2.38850700
H	-6.92953500	-2.43915100	-0.06773800
H	-5.49269400	-6.26037800	-1.88833000
H	-4.20240000	-6.23697700	-3.12943200
H	-3.78449700	-6.38099500	-1.39956700
