Computational Elucidation of the Solvent-Dependent Addition of 4-Hydroxy-2-Nonenal (HNE) to Cysteine and Cysteinate Residues

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SUPPLEMENTARY INFORMATION

TABLE OF CONTENTS

Content	Page Number
Relative Energies	S2
Total Electronic Energies and Number of Imaginary Frequencies	S5
Cartesian Coordinates	S8

Table S1. Relative enthalpies (ΔHrel) and Gibbs free energies (ΔGrel) of the stationary points for the addition of HNE to Cys in conformer one, computed at the B3LYP/6-31G(d)//B3LYP/6-31G(d) level of theory in implicit cyclohexane, 1-octanol, and water. The respective energies are relative to the entrance level.

Solvent					
Cyclohexane			**1-Octanol**		
Stationary Point	**ΔH_{rel} / kcal/mol**	**ΔG_{rel} / kcal/mol**	**Stationary Point**	**ΔH_{rel} / kcal/mol**	**ΔG_{rel} / kcal/mol**
MIN_{1t}	-7.1	4.1	MIN_{1t}	-3.8	8.8
TS_{1t}	43.5	56.4	TS_{1t}	43.0	56.5
MIN_2	-9.9	4.6	MIN_2	-9.2	6.0
TS_2	-8.6	7.1	TS_2	-8.6	7.0
MIN_3	-8.1	6.1	MIN_3	-8.3	6.4
TS_3	-9.4	6.1	TS_3	-8.5	8.0
MIN_4	-9.1	4.7	MIN_4	-8.2	7.0
TS_4	22.5	38.7	TS_4	22.3	39.2
P(R)	-15.9	0.3	P(R)	-15.1	1.1
$MIN_{3'}$	-11.2	3.7	$MIN_{3'}$	-10.7	5.0
$TS_{3'}$	24.7	40.4	$TS_{3'}$	24.6	41.2
P(S)	-13.8	1.5	P(S)	-13.8	2.8
TS_{1c1}	39.8	54.1	TS_{1c1}	39.1	54.5
TS_{1c2}	46.6	58.8	TS_{1c2}	45.9	59.0
HNE_{c1} + Cys	3.7	4.2	HNE_{c1} + Cys	4.0	4.5
HNE_{c2} + Cys	3.3	3.4	HNE_{c2} + Cys	3.2	3.5
MIN_{1c2}	3.5	12.4	MIN_{1c2}	3.4	14.7
MIN_{1c1}	-1.9	8.8	MIN_{1c1}	0.1	11.7

Table S2. Relative enthalpies (ΔHrel) and Gibbs free energies (ΔGrel) of the stationary points for the addition of HNE to Cys in conformer one, computed at the B3LYP/6-31G(d)//B3LYP/6-31G(d) level of theory in implicit cyclohexane, 1-octanol, and water. The respective energies are relative to the entrance level, which included one explicit water molecule.

Solvent								
Cyclohexane			1-Octanol			Water		
Stationary Point	**ΔH_{rel} / kcal/mol**	**ΔG_{rel} / kcal/mol**	**Stationary Point**	**ΔH_{rel} / kcal/mol**	**ΔG_{rel} / kcal/mol**	**Stationary Point**	**ΔH_{rel} / kcal/mol**	**ΔG_{rel} / kcal/mol**
MIN_{1t}	-7.7	6.0	MIN_{1t}	-6.3	7.1	MIN_{1t}	-5.5	7.1
TS_{1t}	34.1	52.7	TS_{1t}	32.1	49.7	TS_{1t}	28.0	45.4
MIN_2	-7.4	9.0	MIN_2	-8.2	7.4	MIN_2	-9.0	6.7
TS_2	1.0	16.3	TS_2	-2.0	14.5	TS_2	-2.3	14.5
MIN_3	-3.3	11.8	MIN_3	-6.4	8.0	MIN_3	-7.6	6.6
TS_3	-3.7	12.3	TS_3	-6.7	8.4	TS_3	-7.9	7.6
MIN_4	-6.9	9.5	MIN_4	-7.4	8.5	MIN_4	-8.0	8.5
TS_4	10.4	29.4	TS_4	7.6	27.0	TS_4	6.5	25.1
P(R)	-10.4	5.5	P(R)	-12.6	2.1	P(R)	-13.4	2.4
TS_3'	-5.1	11.1	TS_3'	-7.2	7.7	TS_3'	-9.1	7.3
MIN_4'	-6.4	10.1	MIN_4'	-8.0	7.6	MIN_4'	-8.8	5.9
TS_4'	8.8	28.0	TS_4'	6.7	25.2	TS_4'	6.1	25.2
P(S)	-10.9	6.1	P(S)	-13.0	3.6	P(S)	-13.4	4.1

Table S3. Relative enthalpies (ΔHrel) and Gibbs free energies (ΔGrel) of the stationary points for the addition of HNE to Cys in conformer one, computed at the B3LYP/6-31G(d)//B3LYP/6-31G(d) level of theory in implicit cyclohexane, 1-octanol, and water. The respective energies are relative to the entrance level, which included two explicit water molecules.

Solvent								
Cyclohexane			**1-Octanol**			**Water**		
Stationary Point	**ΔH_{rel} / kcal/mol**	**ΔG_{rel} / kcal/mol**	**Stationary Point**	**ΔH_{rel} / kcal/mol**	**ΔG_{rel} / kcal/mol**	**Stationary Point**	**ΔH_{rel} / kcal/mol**	**ΔG_{rel} / kcal/mol**
MIN_{1t}	6.7	17.6	MIN_{1t}	5.8	17.3	MIN_{1t}	2.7	15.2
TS_{1t}	34.8	52.8	TS_{1t}	32.4	49.2	TS_{1t}	29.0	45.9
MIN_2	-2.1	12.0	MIN_2	-5.1	9.5	MIN_2	-5.8	8.6
TS_2	1.2	15.5	TS_2	-4.9	9.7	TS_2	-6.1	9.6
MIN_3	-7.5	6.1	MIN_3	-7.6	7.3	MIN_3	-7.6	6.7
TS_3	7.3	25.7	TS_3	6.5	25.6	TS_3	5.9	25.6
P(R)	-12.7	2.4	P(R)	-13.2	2.3	P(R)	-12.7	3.4
TS_2'	-4.4	11.4	TS_2'	-6.4	9.1	TS_2'	-7.0	8.2
MIN_3'	-2.1	11.1	MIN_3'	-4.7	8.6	MIN_3'	-6.8	7.5
TS_4'	10.5	27.7	TS_4'	8.1	25.2	TS_4'	7.7	24.9
P(S)	-13.4	1.6	P(S)	-14.5	1.9	P(S)	-14.4	2.3

Table S4. Electronic energies and number of imaginary frequencies of the stationary points for the addition of HNE to Cys in conformer one, computed at the B3LYP/6-31G(d)//B3LYP/6-31G(d) level of theory in implicit cyclohexane, 1-octanol, and water. The respective energies are relative to the entrance level.

Solvent					
Cyclohexane			1-Octanol		
Stationary Point	**Total Energy / Ha**	**No. of imaginary Freq.**	**Stationary Point**	**Total Energy / Ha**	**No. of imaginary Freq.**
MIN_{1t}	-1396.714179	0	MIN_{1t}	-1396.730756	0
TS_{1t}	-1396.601786	1	TS_{1t}	-1396.61883	1
MIN_2	-1396.627841	0	MIN_2	-1396.636635	0
TS_2	-1396.54713	1	TS_2	-1396.6	1
MIN_3	-1396.632257	0	MIN_3	-1396.645226	0
TS_3	-1396.632886	1	TS_3	-1396.6458	1
MIN_4	-1396.629369	0	MIN_4	-1396.643681	0
TS_4	-1396.580714	1	TS_4	-1396.594907	1
P(R)	-1396.641822	0	P(R)	-1396.654583	0
TS_{1c1}	-1396.634317	1	TS_{1c1}	-1396.568155	1
TS_{1c2}	-1396.634949	1	TS_{1c2}	-1396.557439	1
HNE_{c1} + Cys	-1396.595819	0	HNE_{c1} + Cys	-1396.612498	0
HNE_{c2} + Cys	-1396.596535	0	HNE_{c2} + Cys	-1396.613679	0
MIN_{1c2}	-1396.610976	0	MIN_{1c2}	-1396.625145	0
MIN_{1c1}	-1396.619537	0	MIN_{1c1}	-1396.630411	0

Table S5. Electronic energies and number of imaginary frequencies of the stationary points for the addition of HNE to Cys in conformer one, computed at the B3LYP/6-31G(d)//B3LYP/6-31G(d) level of theory in implicit cyclohexane, 1-octanol, and water. The respective energies are relative to the entrance level, which included one explicit water molecule.

Solvent								
Cyclohexane			1-Octanol			Water		
Stationary Point	**Total Energy / Ha**	**No. of imaginary Freq.**	**Stationary Point**	**Total Energy / Ha**	**No. of imaginary Freq.**	**Stationary Point**	**Total Energy / Ha**	**No. of imaginary Freq.**
MIN_{1t}	-1473.130179	0	MIN_{1t}	-1473.140974	0	MIN_{1t}	-1473.140837	0
TS_{1t}	-1473.010803	1	TS_{1t}	-1473.020997	1	TS_{1t}	-1473.020679	1
MIN_2	-1473.035055	0	MIN_2	-1473.046415	0	MIN_2	-1473.042425	0
TS_2	-1472.968516	1	TS_2	-1472.985225	1	TS_2	-1473.0000000	1
MIN_3	-1473.03465	0	MIN_3	-1473.049429	0	MIN_3	-1473.048036	0
TS_3	-1473.02112	1	TS_3	-1473.03951	1	TS_3	-1473.03731	1
P(R)	-1473.028053	0	P(R)	-1473.046519	0	P(R)	-1473.045833	0
TS_2'	-1473.028707	1	TS_2'	-1473.047059	1	TS_2'	-1473.046255	1
MIN_3'	-1473.033745	0	MIN_3'	-1473.048198	0	MIN_3'	-1473.046444	0
TS_4'	-1473.006182	1	TS_4'	-1473.02432	1	TS_4'	-1473.023239	1
P(S)	-1473.039301	0	P(S)	-1473.056381	0	P(S)	-1473.05508	0

Table S6. Electronic energies and number of imaginary frequencies of the stationary points for the addition of HNE to Cys in conformer one, computed at the B3LYP/6-31G(d)//B3LYP/6-31G(d) level of theory in implicit cyclohexane, 1-octanol, and water. The respective energies are relative to the entrance level, which included two explicit water molecules.

Solvent								
Cyclohexane			1-Octanol			Water		
Stationary Point	**Total Energy / Ha**	**No. of imaginary Freq.**	**Stationary Point**	**Total Energy / Ha**	**No. of imaginary Freq.**	**Stationary Point**	**Total Energy / Ha**	**No. of imaginary Freq.**
MIN_{1t}	-1549.426022	0	MIN_{1t}	-1549.555045	0	MIN_{1t}	-1549.555189	0
TS_{1t}	-1549.42939	1	TS_{1t}	-1549.42939	1	TS_{1t}	-1549.426826	1
MIN_2	-1549.414767	0	MIN_2	-1549.43462	0	MIN_2	-1549.43883	0
TS_2	-1549.369941	1	TS_2	-1549.392298	1	TS_2	-1549.396947	1
MIN_3	-1549.42877	0	MIN_3	-1549.452105	0	MIN_3	-1549.452395	0
TS_3	-1549.423455	1	TS_3	-1549.45168	1	TS_3	-1549.452847	1
P(R)	-1549.437259	0	P(R)	-1549.456038	0	P(R)	-1549.455214	0
TS_2'	-1549.413814	1	TS_2'	-1549.433569	1	TS_2'	-1549.433663	1
MIN_3'	-1549.445697	0	MIN_3'	-1549.464923	0	MIN_3'	-1549.463394	0
TS_4'	-1549.432317	1	TS_4'	-1549.454072	1	TS_4'	-1549.454301	1
P(S)	-1549.428707	0	P(S)	-1549.451357	0	P(S)	-1549.453869	0

CARTESIAN COORDINATES

Cysteine

Charge/multiplicity: 0 1
N -1.37565700 -0.61877300 0.20640900
H -1.28545300 -1.54423800 0.61289300
C -0.12099300 0.01096600 -0.14927900
H -0.17060600 0.34302700 -1.19321100
C 0.11787600 1.25513500 0.74562500
C 0.97162300 -1.06948400 0.01000300
H -0.82091600 1.80425800 0.82324100
H 0.42464000 0.95557800 1.75214900
S 1.41034400 2.42985400 0.14755900
O 0.71716400 -2.15575100 0.53397300
H 0.68523100 2.94529500 -0.86909200
N 2.19356000 -0.74760200 -0.46541600
H 2.35351000 0.20554100 -0.77083900
C 3.33298600 -1.63919900 -0.31457200
H 4.14738800 -1.27533200 -0.94487400
H 3.67981800 -1.68710500 0.72517100
H 3.05832700 -2.64889500 -0.63018800
C -2.57685900 -0.12352500 -0.20119900
C -3.78713600 -0.97045000 0.14994600
H -4.48245200 -0.36931600 0.74484700
H -4.30544800 -1.24857300 -0.77380800
H -3.53698500 -1.87944500 0.70510900
O -2.67502100 0.94393900 -0.80552700

MIN_{1t}

Charge/multiplicity: 0 1

N	3.55750400	-0.50822600	-0.51683900
H	3.31754800	-0.34385500	-1.48911600
C	3.06652900	0.48062300	0.43789700
H	3.82994800	0.57008500	1.22188400
C	2.92200500	1.85487000	-0.23248300
C	1.76319900	0.03172000	1.14960500
H	2.40938700	2.53595800	0.44782200
H	3.91930000	2.25794500	-0.42929700
O	0.72253300	0.70494000	1.11339000
N	1.87440500	-1.11261200	1.84238700
H	2.78117400	-1.58181100	1.83332500
C	0.75817000	-1.68455500	2.57749800
H	-0.02221500	-2.05059100	1.89958000
H	1.12752700	-2.52089200	3.17428900
H	0.31180400	-0.93802700	3.24166600
C	4.28535500	-1.59836800	-0.16937800
C	4.82219400	-2.43258200	-1.31390400
H	4.53328500	-3.47674900	-1.16032800
H	4.47219000	-2.10138400	-2.29585200
H	5.91678600	-2.39070900	-1.29682900
O	4.50756000	-1.89536000	1.01187300
C	-2.67323800	2.43242000	-0.25816400
H	-3.71051800	2.76775300	-0.24199300
C	-1.74441500	3.23343000	0.28633400
H	0.83456300	1.56710700	-1.48149400
C	-2.10330700	4.52930300	0.89069500
H	-1.24577700	5.10355200	1.30326200
C	-2.42806400	1.08735000	-0.88396700

H	-2.79121100	1.13675900	-1.92177000
C	-3.23900200	-0.00705900	-0.15252800
H	-4.28771000	0.31414900	-0.08799200
H	-2.87165000	-0.07311600	0.88208000
C	-3.15433000	-1.37915800	-0.83098400
H	-3.54347500	-1.29879500	-1.85682400
H	-2.09938700	-1.66516900	-0.92614800
C	-3.92366800	-2.47246700	-0.07893700
H	-4.98014600	-2.17954800	0.01463000
H	-3.53851700	-2.54783000	0.94923300
C	-3.83991500	-3.84949800	-0.75047300
H	-4.22594300	-3.77567300	-1.77712200
H	-2.78444700	-4.14307500	-0.84321800
O	-3.23330800	4.98644800	0.96045800
S	2.08986200	1.88779100	-1.87885600
O	-1.05402700	0.74263400	-0.99141400
H	-0.66126200	0.65057900	-0.09802400
H	-0.69576800	2.95046200	0.30193500
C	-4.60736600	-4.93812000	0.00488200
H	-4.52549100	-5.90868500	-0.49881800
H	-4.22374900	-5.06079000	1.02579600
H	-5.67433900	-4.69319600	0.08117700

TS_{1t}

Charge/multiplicity: 0 1

N	-4.09301000	-0.17717400	0.46849100
H	-4.12318400	0.37401500	1.31663200
C	-2.90225700	-0.06066100	-0.38253400
H	-3.23363500	-0.26057900	-1.40549200
C	-2.34621500	1.36104400	-0.28436100
C	-1.87253400	-1.14632200	0.02167500
H	-3.17099400	2.06417500	-0.43787700
H	-1.92012000	1.53638800	0.70795500
O	-0.88076700	-0.91326500	0.71604000
N	-2.18665700	-2.37950100	-0.43704100
H	-3.11058900	-2.49475700	-0.84864900
C	-1.41932800	-3.55447000	-0.06371700
H	-1.58551500	-3.84089400	0.98327500
H	-1.71174800	-4.38597800	-0.70926600
H	-0.35227700	-3.35711600	-0.19612500
C	-5.09848800	-1.05541900	0.20760800
C	-6.28567800	-1.00855600	1.14888300
H	-7.17978500	-0.74287300	0.57491800
H	-6.45018200	-2.00751700	1.56492400
H	-6.16737100	-0.29407700	1.96883300
O	-5.05811600	-1.83951200	-0.74599400
C	0.93942800	1.54238100	0.00946100
H	0.34658100	0.91739600	0.67454600
C	0.89622400	2.96071000	0.18159700
H	-0.16366400	2.88487700	-0.68867100
C	0.33024900	3.54367400	1.40592800
H	0.62770500	4.60009400	1.57987800
C	2.00861400	0.82889600	-0.76513300
H	1.56952300	-0.05468700	-1.23443100
C	3.08792100	0.35329000	0.24384200
H	2.59809000	-0.20630700	1.05041800
H	3.55052400	1.23574400	0.71128500
C	4.16209800	-0.52168600	-0.41830000
H	3.67821600	-1.40303900	-0.86232000
H	4.61801500	0.02938100	-1.25042100
C	5.24909600	-0.97457700	0.56468400
H	4.78296500	-1.51847800	1.39956100
H	5.73248300	-0.09158200	1.00896300
C	6.31923900	-1.86358300	-0.08229300

H	5.83643800	-2.74521100	-0.52714700
H	6.78717500	-1.31988900	-0.91529200
O	-0.43502800	2.98484600	2.18021800
S	-1.07192800	1.70681700	-1.57046500
O	2.55949200	1.59718500	-1.82504200
H	3.16151900	2.25464300	-1.43818300
H	1.64326800	3.56202900	-0.33535900
C	7.40071700	-2.31743600	0.90201700
H	8.14842700	-2.95048600	0.40969500
H	7.92810100	-1.45982100	1.33865100
H	6.96937500	-2.89554300	1.72905500

MIN_2

Charge/multiplicity: 0 1

N	-3.54241100	-0.87186300	-0.14017500
H	-4.12052800	-0.21128800	0.36333000
C	-2.15417100	-0.48952100	-0.42689000
H	-1.87570700	-1.01603200	-1.34419800
C	-2.08785900	1.02305600	-0.64844400
C	-1.23519700	-0.97472600	0.72183400
H	-2.90722500	1.31006100	-1.31513400
H	-2.19952800	1.57179100	0.28837200
O	-0.80495100	-0.21605000	1.59198800
N	-0.99038500	-2.30667000	0.67681600
H	-1.51335900	-2.84163500	-0.01366700
C	-0.27026700	-3.01799400	1.71692900
H	0.13323800	-2.28550000	2.41733000
H	-0.93393500	-3.70195000	2.26057000
H	0.55442000	-3.59864100	1.28844000
C	-4.04477000	-2.09971500	-0.44225900
C	-5.51135900	-2.31531000	-0.12513100
H	-5.60253000	-3.11461900	0.61800900
H	-6.01437100	-1.41977000	0.25153800
H	-6.02050600	-2.65466200	-1.03268500
O	-3.35229500	-2.98875600	-0.94733300
C	0.46688100	2.29306400	-0.06724400
H	0.05013900	1.84959200	0.84170300
C	0.36286900	3.82230400	-0.02064400
H	0.55698700	4.26768300	-1.00717800
C	-0.92670300	4.39733500	0.49641200
H	-0.99000200	5.50542000	0.41285300
C	1.95330500	1.85751300	-0.19829100
H	2.35283400	2.24711000	-1.14418500
C	2.19066300	0.34377800	-0.13354400
H	1.58040200	-0.14996300	-0.89715800
H	1.82081800	-0.02323700	0.83540100
C	3.66473500	-0.03858900	-0.32014600
H	4.00737700	0.31793800	-1.30315200
H	4.27473800	0.49007500	0.42330900
C	3.91740500	-1.54805100	-0.21435400
H	3.30721100	-2.07552300	-0.96280300
H	3.57142600	-1.90755800	0.76680300
C	5.39023100	-1.93420100	-0.40069500
H	5.73580200	-1.58025000	-1.38255300
H	5.99993600	-1.40433200	0.34506800
O	-1.84123600	3.77732700	1.00181700
S	-0.54903100	1.61029600	-1.47172100
O	2.72701700	2.52858500	0.80992200
H	2.50074800	2.11299400	1.66024100
H	1.15809700	4.21744400	0.63112400
C	5.64136100	-3.44041600	-0.28633200
H	6.70205800	-3.68167300	-0.42530800
H	5.34144300	-3.82081500	0.69858200

H	5.07304600	-3.99766100	-1.04197400

TS_2

Charge/multiplicity: 0 1

N	-3.84164900	0.05312500	-0.13007400
H	-4.30409000	0.77062900	0.41291500
C	-2.38255000	0.12885800	-0.27502700
H	-2.14645000	-0.34655500	-1.23107300
C	-1.94406800	1.59645200	-0.30398000
C	-1.70295700	-0.67649200	0.86096300
H	-2.64901600	2.15364700	-0.92888300
H	-1.97025100	2.02237000	0.70326100
O	-1.17527200	-0.13483200	1.83523000
N	-1.78425200	-2.01471200	0.69220400
H	-2.33254800	-2.34836700	-0.09730800
C	-1.29924200	-2.96270300	1.67999100
H	-0.27042300	-3.27810300	1.46457100
H	-1.31771000	-2.49905400	2.66895000
H	-1.94250600	-3.84703100	1.68110800
C	-4.57246100	-0.98824800	-0.61444200
C	-6.07382500	-0.89006500	-0.43207700
H	-6.55122200	-0.93318400	-1.41643500
H	-6.42188700	-1.75795100	0.13735900
H	-6.39405400	0.02372900	0.07721800
O	-4.04793500	-1.95390400	-1.17712300
C	0.81930600	2.02742500	0.44400500
H	0.28104600	1.50279800	1.23939500
C	1.00397700	3.49177100	0.86345900
H	1.59883500	3.53893900	1.78735100
C	1.68835000	4.40817600	-0.12076200
H	1.75289600	5.46585800	0.22315900
C	2.16990500	1.29322400	0.21644800
H	2.66042000	1.71500500	-0.66438300
C	2.03040300	-0.22531200	0.05975500
H	1.31687800	-0.43918200	-0.74388100
H	1.58411600	-0.63051100	0.98174300
C	3.36324700	-0.92689900	-0.23313300
H	3.77988600	-0.52747800	-1.16942800
H	4.08724800	-0.67610200	0.55276100
C	3.23095300	-2.45069700	-0.34705200
H	2.49810200	-2.69628700	-1.13029700
H	2.81818200	-2.85210900	0.59138300
C	4.55587500	-3.15962600	-0.65670800
H	4.96742200	-2.76191700	-1.59529000
H	5.28934800	-2.91432000	0.12465100
O	2.15479500	4.08922500	-1.19413500
S	-0.28753700	1.90147800	-1.04966900
O	3.05678800	1.60879000	1.30284300
H	2.73692400	1.11831600	2.07981000
H	0.03577700	3.94999000	1.11263700
C	4.41764700	-4.68063200	-0.76656000
H	5.37984900	-5.15529300	-0.99341800
H	4.04610300	-5.11623900	0.16988100
H	3.71466500	-4.95977000	-1.56177800

MIN_3

Charge/multiplicity: 0 1

N	3.81021400	-0.09845300	-0.12056900
H	4.27484500	-0.81161900	0.42626400
C	2.35164300	-0.17985700	-0.26644900
H	2.11358200	0.29650000	-1.22128600
C	1.91787600	-1.64856000	-0.29689200
C	1.67528900	0.62045500	0.87463700
H	2.62351200	-2.20263900	-0.92390300
H	1.94755500	-2.07563000	0.70976600
O	1.18361000	0.07181300	1.86342900
N	1.71367800	1.95920400	0.68099800
H	2.26619600	2.28881400	-0.10796100
C	1.25382100	2.91981500	1.66737100
H	0.76072100	2.37483200	2.47333800
H	2.09240600	3.49086600	2.08485800
H	0.54210300	3.62135500	1.21825400
C	4.53617700	0.94690600	-0.60455300
C	6.03773300	0.85689400	-0.41954400
H	6.51663500	0.90435500	-1.40295000
H	6.37995600	1.72574700	0.15197300
H	6.36201400	-0.05600500	0.08879700
O	4.00715300	1.90886300	-1.16897600
C	-0.85662800	-2.04529500	0.44315400
H	-0.30373400	-1.54423500	1.24368600
C	-1.10035800	-3.50287300	0.85611500
H	-1.70361600	-3.53254100	1.77515800
C	-1.80959900	-4.38729000	-0.13945500
H	-1.92830000	-5.44097600	0.20203400
C	-2.17623500	-1.25894300	0.20656800
H	-2.66834800	-1.65214400	-0.68653300
C	-1.97688600	0.25470600	0.07052600
H	-1.23563200	0.45160400	-0.71200500
H	-1.53984900	0.63303800	1.00812300
C	-3.27483900	1.00912000	-0.24692400
H	-3.68168200	0.63696200	-1.19857900
H	-4.02753600	0.77586300	0.51717500
C	-3.08326200	2.52822200	-0.33741300
H	-2.32441600	2.75591400	-1.10109100
H	-2.67671500	2.90215100	0.61489000
C	-4.37382100	3.28974900	-0.66704400
H	-4.77864700	2.91865400	-1.61930100
H	-5.13310100	3.06262500	0.09490500
O	-2.24115300	-4.04690700	-1.22087000
S	0.26353000	-1.96085000	-1.04401800
O	-3.09145100	-1.55241600	1.27536000
H	-2.76623000	-1.08258000	2.06272800
H	-0.15186500	-3.99850300	1.10926500
C	-4.17694400	4.80571700	-0.75450100
H	-5.11581600	5.31880600	-0.99502400
H	-3.80934100	5.21570100	0.19497900
H	-3.44748000	5.06801300	-1.53140800

TS_3

Charge/multiplicity: 0 1

N	-3.92892100	-0.48342900	0.38100400
H	-4.29191400	-0.20346000	1.28367300
C	-2.58808000	-0.02107500	0.00231300
H	-2.57507600	0.02019900	-1.08996700
C	-2.34222900	1.37714100	0.57856700
C	-1.53799700	-1.05357100	0.48398100
H	-3.26148800	1.96152000	0.46670600

H	-2.10560800	1.31320200	1.64480800
O	-0.86900100	-0.88134600	1.50540100
N	-1.46666100	-2.15084200	-0.30543500
H	-2.17047100	-2.22961300	-1.03635600
C	-0.66105500	-3.31460700	0.01838600
H	-1.29071900	-4.16507200	0.30882100
H	-0.05133600	-3.60880000	-0.84266500
H	-0.00640500	-3.05924800	0.85247100
C	-4.64082900	-1.36866900	-0.37341500
C	-6.02509200	-1.70121300	0.15256000
H	-6.50504300	-2.40274500	-0.53116700
H	-5.96415100	-2.15764400	1.14782100
H	-6.64158100	-0.79876700	0.23519500
O	-4.18960100	-1.85461400	-1.41333100
C	0.52928600	1.86276100	0.53907900
H	0.20951400	1.22660600	1.36714000
C	1.24373000	3.09227800	1.12441000
H	2.23277700	2.81176600	1.51929400
C	1.46742700	4.27915400	0.22182500
H	1.90071300	5.16141800	0.74008900
C	1.41871700	0.98873200	-0.38520800
H	0.74394900	0.31331200	-0.93464300
C	2.39677000	0.12296200	0.41938900
H	1.81427100	-0.47339900	1.13263600
H	3.06295900	0.77323600	1.00384400
C	3.24613800	-0.80519500	-0.46004100
H	2.57956900	-1.45076700	-1.05145100
H	3.80874400	-0.20058100	-1.18133800
C	4.21182400	-1.67966100	0.34937100
H	3.64190400	-2.28281800	1.07269000
H	4.87259900	-1.03431000	0.94780000
C	5.07029500	-2.61014000	-0.51764400
H	4.41293300	-3.25570200	-1.11765900
H	5.64276700	-2.00745700	-1.23698800
O	1.21013000	4.34622700	-0.96473900
S	-1.06882500	2.39233800	-0.27690100
O	2.18896200	1.75749400	-1.30085600
H	1.62958200	2.47837100	-1.63970700
H	0.68815600	3.47477200	1.99293400
C	6.03175600	-3.47990600	0.29692800
H	6.63305400	-4.12889500	-0.35111100
H	6.72473900	-2.86407700	0.88436500
H	5.48795500	-4.12460100	0.99938300

MIN_4

Charge/multiplicity: 0 1

N	-3.92644500	-0.48322100	0.38289700
H	-4.29759700	-0.19590200	1.27918300
C	-2.58388400	-0.02090900	0.00981800
H	-2.56592600	0.01697700	-1.08256200
C	-2.34139900	1.37855700	0.58454700
C	-1.53584700	-1.05251300	0.49881500
H	-3.26157900	1.96130800	0.47151700
H	-2.10515200	1.31616700	1.65093800
O	-0.86738500	-0.87472800	1.51956200
N	-1.46515800	-2.15387300	-0.28456900
H	-2.16885900	-2.23564800	-1.01567400
C	-0.66044600	-3.31632600	0.04609000
H	-0.00268000	-3.05570100	0.87608500
H	-1.29048600	-4.16349900	0.34527300
H	-0.05410900	-3.61822900	-0.81464500
C	-4.63231200	-1.36637000	-0.37630400

C	-6.02491300	-1.70507500	0.11733300
H	-6.75032200	-1.41185200	-0.64873900
H	-6.10438600	-2.78947400	0.24362900
H	-6.28827300	-1.21462700	1.05933200
O	-4.17397800	-1.85505700	-1.41290900
C	0.52987100	1.86519200	0.54024900
H	0.21186000	1.23032800	1.36997600
C	1.24717500	3.09468600	1.12211500
H	2.23706300	2.81362100	1.51446500
C	1.46934300	4.28030800	0.21751300
H	1.90601800	5.16238500	0.73324200
C	1.41567200	0.98934700	-0.38573000
H	0.73870400	0.31312200	-0.93149500
C	2.39659300	0.12468300	0.41653600
H	1.81709600	-0.46884700	1.13457700
H	3.06652900	0.77593200	0.99555800
C	3.24027700	-0.80717800	-0.46448800
H	2.56985300	-1.45423300	-1.04988300
H	3.79927800	-0.20549300	-1.19102300
C	4.20980900	-1.67964400	0.34246000
H	3.64359300	-2.27911400	1.07172900
H	4.87509200	-1.03273600	0.93415900
C	5.06166000	-2.61481600	-0.52606600
H	4.39970900	-3.26211900	-1.11911200
H	5.63025000	-2.01590000	-1.25160800
O	1.20749800	4.34661800	-0.96809700
S	-1.07003900	2.39559900	-0.27170100
O	2.18269700	1.75629700	-1.30556900
H	1.62234400	2.47686300	-1.64345300
H	0.69450500	3.47871400	1.99181900
C	6.02725800	-3.48229200	0.28605500
H	6.62363400	-4.13475100	-0.36304500
H	6.72469600	-2.86480600	0.86643100
H	5.48718400	-4.12333700	0.99469400

TS_4

Charge/multiplicity: 0 1

N	-4.00356200	-0.35508200	0.49953000
H	-4.27106300	-0.12818700	1.44851900
C	-2.68524200	0.09043900	0.02991400
H	-2.77969800	0.24640900	-1.04826700
C	-2.31521100	1.40815900	0.71674200
C	-1.64356800	-1.02630400	0.28560800
H	-3.20088700	2.05215500	0.72202700
H	-2.01910100	1.22844300	1.75462300
O	-0.84168400	-0.98108400	1.22108700
N	-1.72154400	-2.05176500	-0.59280900
H	-2.52699000	-2.05829000	-1.21608100
C	-0.93812000	-3.26513200	-0.43398900
H	-1.00442200	-3.84936600	-1.35465600
H	0.10838400	-3.01172900	-0.24724000
H	-1.29469900	-3.87905500	0.40363700
C	-4.83072800	-1.12606800	-0.25797600
C	-6.18588700	-1.44080400	0.34311100
H	-6.96370500	-1.04703300	-0.31949700
H	-6.31403200	-2.52706200	0.38635000
H	-6.32982700	-1.02303400	1.34402900
O	-4.50435800	-1.53831800	-1.37526900
C	0.55205000	1.85459700	0.69776500

H	0.24986500	1.28463300	1.57646900
C	1.43952600	3.06159200	1.06254000
H	2.15605700	2.77143000	1.84026600
C	2.17637700	3.44866400	-0.21139900
H	3.22780700	3.75014600	-0.07885800
C	1.45541900	0.99104700	-0.21703400
H	0.86559000	0.44155300	-0.95486100
C	2.36083500	0.02681300	0.55133500
H	1.70554800	-0.63799900	1.12662800
H	2.96491900	0.59047200	1.27575100
C	3.28483300	-0.80058100	-0.35273700
H	2.67377700	-1.37880700	-1.06209300
H	3.90112800	-0.12443200	-0.95852200
C	4.18922200	-1.75640700	0.43514400
H	3.56802800	-2.42210200	1.05301500
H	4.80421400	-1.17584100	1.13925000
C	5.10838900	-2.60407400	-0.45428300
H	4.49565300	-3.19120400	-1.15333500
H	5.72529200	-1.93909200	-1.07517500
O	1.50351000	3.97214600	-1.21576400
S	-1.02288600	2.41379200	-0.12400400
O	2.28185300	1.93518600	-0.96082300
H	1.66484100	2.71536700	-1.60839900
H	0.85898000	3.91376400	1.42546500
C	6.01624200	-3.54605900	0.34105900
H	6.65558600	-4.14111000	-0.32193000
H	6.67227800	-2.98696800	1.02040700
H	5.42901400	-4.24453500	0.95086500

P(R)

Charge/multiplicity: 0 1

N	-4.36892400	0.26619400	0.22367100
H	-4.48615500	0.84322600	1.04637800
C	-3.00804500	0.04407200	-0.27718100
H	-3.10349700	-0.13472000	-1.35167900
C	-2.15891800	1.29271800	-0.02841100
C	-2.40287200	-1.21764200	0.38763700
H	-2.72239200	2.17571400	-0.34382300
H	-1.92610800	1.38918400	1.03553100
O	-1.59301200	-1.15232400	1.31358600
N	-2.87143600	-2.37727500	-0.12673400
H	-3.65402200	-2.31084600	-0.77389400
C	-2.52010100	-3.66894100	0.43715100
H	-1.45673800	-3.67913800	0.68718600
H	-3.08913800	-3.89058600	1.34998700
H	-2.72291100	-4.44683300	-0.30306100
C	-5.45244000	-0.37080600	-0.30142100
C	-6.79680200	0.00218700	0.29044600
H	-7.40977800	0.46425400	-0.49089000
H	-7.30987900	-0.90989000	0.61056500
H	-6.72772100	0.69130400	1.13743500
O	-5.35005700	-1.19259200	-1.21654400
C	0.69439900	0.88365700	0.31243800
H	0.39498800	-0.06125400	0.76574200
C	0.91165600	2.00105900	1.34153800
H	1.38479000	1.57283800	2.23369600
C	1.89419100	2.94572700	0.63590400
H	2.56082100	3.47291900	1.32397900
C	2.07567500	0.80840400	-0.38261600
H	1.97418800	0.66605100	-1.46741900
C	2.95948900	-0.31223700	0.17617200
H	2.44787500	-1.26867000	-0.00217900
H	3.04089700	-0.19446800	1.26596500

C	4.35947600	-0.34850300	-0.44851400
H	4.26473000	-0.47345500	-1.53762300
H	4.84444100	0.62283500	-0.29108600
C	5.24390100	-1.46751200	0.11585200
H	4.74630700	-2.43800600	-0.03194600
H	5.34264600	-1.33998700	1.20436000
C	6.64192400	-1.51699100	-0.51400900
H	6.54451300	-1.64602400	-1.60143300
H	7.13952000	-0.54796100	-0.36634800
O	1.27421600	3.95824900	-0.11424300
S	-0.58252400	1.29281000	-0.97889700
O	2.70183300	2.08945200	-0.16729400
H	0.00062300	2.51411100	1.65864900
H	0.62455800	3.52617300	-0.69974200
C	7.52238500	-2.63368800	0.05388300
H	8.51317600	-2.64056400	-0.41606100
H	7.66921700	-2.51462900	1.13496900
H	7.07059300	-3.62028300	-0.11069500

MIN_3’

Charge/multiplicity: 0 1

N	-4.37423500	0.28087100	0.35191200
H	-4.49092200	0.81375800	1.20374700
C	-3.01761600	0.13072400	-0.18922700
H	-3.12939900	0.02158100	-1.27132100
C	-2.19466200	1.38368700	0.12415200
C	-2.37441300	-1.15868800	0.37878200
H	-2.80550800	2.26482600	-0.09612300
H	-1.93374400	1.40498200	1.18656800
O	-1.56487300	-1.14290900	1.30869400
N	-2.81163800	-2.28970400	-0.21871800
H	-3.60179800	-2.19785000	-0.85341800
C	-2.42103600	-3.60907600	0.24617600
H	-1.35334500	-3.61239400	0.47750900
H	-2.96891100	-3.90815900	1.14983000
H	-2.61934800	-4.33672400	-0.54454200
C	-5.45228900	-0.35049300	-0.18935100
C	-6.79232400	-0.05143400	0.45331300
H	-7.45403600	0.38742100	-0.30076400
H	-7.24881100	-0.99139000	0.77951000
H	-6.72807300	0.63011100	1.30683400
O	-5.35113300	-1.11418500	-1.15366300
C	0.64749400	0.97608200	0.29715500
H	0.19770300	0.15318900	0.85955200
C	0.99208400	2.06878900	1.32641300
H	1.65741500	1.65435400	2.10381800
C	1.65639900	3.34679300	0.88513600
H	1.60065600	4.16394000	1.63462500
C	1.80600400	0.38236600	-0.54170600
H	1.40881900	-0.53667000	-0.98891500
C	3.02931600	0.01213400	0.31701900
H	2.69721200	-0.57156600	1.18837000
H	3.48756900	0.93226000	0.70738900
C	4.08579600	-0.77964000	-0.46400000
H	3.64234200	-1.72212700	-0.81787700
H	4.35558200	-0.21003600	-1.36171300
C	5.34433200	-1.08557600	0.35734600
H	5.06638300	-1.65107600	1.25994000
H	5.78382400	-0.14171500	0.71407200
C	6.40785700	-1.87095500	-0.42110300
H	5.97318200	-2.81655800	-0.77549300
H	6.68466200	-1.30673600	-1.32295600
O	2.25739400	3.54239400	-0.15567900
S	-0.66609500	1.54252100	-0.89276100

O	2.16294200	1.19688700	-1.65023500
H	2.34191000	2.09194600	-1.29617100
H	0.08688300	2.35716700	1.87799700
C	7.66547600	-2.16541400	0.40129000
H	8.40453300	-2.72599500	-0.18365500
H	8.14561700	-1.23861700	0.74044200
H	7.42909300	-2.75970800	1.29326400

TS_3’

Charge/multiplicity: 0 1

N	4.41688400	-0.32080700	0.28283500
H	4.51975000	-0.89996800	1.10601900
C	3.06904700	-0.12894000	-0.26463900
H	3.19832900	0.06060000	-1.33364800
C	2.24349600	-1.40142700	-0.05851600
C	2.41344700	1.11457900	0.38582400
H	2.84810000	-2.26532400	-0.35026900
H	1.96898500	-1.51200100	0.99459500
O	1.57667900	1.02884800	1.28659200
N	2.87193300	2.28693100	-0.10794700
H	3.67761500	2.24074300	-0.72826400
C	2.47795200	3.56727300	0.45375900
H	2.69066800	4.35472900	-0.27341300
H	1.40695400	3.55609800	0.66870300
H	3.01235800	3.79174200	1.38658500
C	5.50255500	0.34405400	-0.20142900
C	6.83467000	-0.00246300	0.43265100
H	7.49093400	-0.42450400	-0.33592900
H	7.30633100	0.91619800	0.79515600
H	6.75591400	-0.71532700	1.25894500
O	5.41240400	1.17058000	-1.11374500
C	-0.59964000	-1.05279700	0.17921200
H	-0.23403900	-0.18699000	0.73443500
C	-0.93702800	-2.23657600	1.10021500
H	-1.42459600	-1.87530600	2.01248100
C	-1.93669100	-3.13848800	0.37137400
H	-1.48231900	-3.93244900	-0.24036000
C	-1.91795500	-0.74033500	-0.56883700
H	-1.71962300	-0.31618600	-1.55914300
C	-2.84906100	0.19921200	0.20497900
H	-2.28999700	1.12078000	0.41459800
H	-3.09565700	-0.24862500	1.17674700
C	-4.13733000	0.54786400	-0.55431600
H	-3.87248900	0.99211900	-1.52499200
H	-4.69670600	-0.36987000	-0.78078800
C	-5.04387200	1.51437400	0.21861200
H	-4.48353700	2.43198100	0.45240500
H	-5.31181100	1.06597300	1.18668600
C	-6.32560200	1.88452400	-0.53886300
H	-6.05781200	2.33369900	-1.50596100
H	-6.88509400	0.96786100	-0.77314200
O	-3.12974200	-3.35060500	0.88202600
S	0.71120500	-1.45623400	-1.07683700
O	-2.52536000	-2.04345500	-0.78648600
H	-3.36225200	-2.40132800	-0.02185400
H	-0.04557700	-2.80034200	1.39250200
C	-7.22761900	2.84793900	0.23739200
H	-8.13170100	3.09554200	-0.33154100
H	-7.54598900	2.41276800	1.19312600
H	-6.70781400	3.78854800	0.45989700

P(S)

Charge/multiplicity: 0 1

N	3.85279600	-0.64328200	0.34989800
H	3.91135800	-1.21083400	1.18545600
C	2.53189000	-0.43786500	-0.25527800
H	2.70868800	-0.27037400	-1.32140500
C	1.67462500	-1.68996800	-0.06070600
C	1.87124500	0.82980300	0.34184400
H	2.26959000	-2.57090600	-0.31921900
H	1.36045100	-1.77723400	0.98321500
O	0.98742100	0.77968600	1.19937800
N	2.38475600	1.98304300	-0.14157500
H	3.21359600	1.90997200	-0.72735000
C	1.99172900	3.27932100	0.38276600
H	2.35801100	3.43731100	1.40554800
H	2.40094000	4.05797200	-0.26486300
H	0.90165200	3.36302900	0.39591400
C	4.97064500	-0.01026400	-0.10152500
C	6.26793100	-0.36980800	0.59471800
H	6.95311200	-0.80434000	-0.14082100
H	6.73444500	0.54487700	0.97381400
H	6.14207800	-1.07653500	1.42044000
O	4.93592100	0.80013000	-1.03202100
C	-1.17832100	-1.43661400	0.11662200
H	-0.86671000	-0.59140900	0.73109500
C	-1.50566700	-2.68638000	0.94027100
H	-1.96962700	-2.39135800	1.89224700
C	-2.55608600	-3.40759900	0.09044200
H	-2.09246800	-4.03515900	-0.68186800
C	-2.51466000	-1.15853600	-0.63321400
H	-2.33077700	-0.98173000	-1.70262700
C	-3.31346000	0.02069200	-0.06988500
H	-3.41461300	-0.10299300	1.01778700
H	-4.32720100	-0.04673200	-0.48650600
C	-2.71339500	1.39487400	-0.39379900
H	-1.70877000	1.47723000	0.04306000
H	-2.58358800	1.48474600	-1.48238200
C	-3.58049600	2.55758100	0.10800800
H	-3.70713500	2.47435600	1.19774300
H	-4.58915100	2.47113400	-0.32312400
C	-3.00606100	3.93938800	-0.22893400
H	-2.00166700	4.03058900	0.20894900
H	-2.87264700	4.02037400	-1.31716300
O	-3.41191300	-4.26086000	0.78537800
S	0.17227300	-1.69986800	-1.12607300
O	-3.30775600	-2.35323600	-0.50897300
H	-0.64168300	-3.31594400	1.16769100
C	-3.88157000	5.09518300	0.26338200
H	-3.44311500	6.06718400	0.00726200
H	-4.88264700	5.05488400	-0.18450300
H	-4.00642200	5.06448700	1.35325800
H	-3.91439400	-3.70764700	1.40888300

TS_{1c1}

Charge/multiplicity: 0 1

N	4.45282700	0.21079600	-0.40951100
H	4.54637700	0.71215800	-1.28330700
C	3.12822900	0.15712900	0.21770800
H	3.30184500	0.05032900	1.29216600
C	2.38148500	1.46136800	-0.06715300
C	2.36204900	-1.08889500	-0.29383400
H	3.05873800	2.30014900	0.12095400
H	2.06776700	1.49258800	-1.11672400
O	1.49516500	-1.02103100	-1.16857600
N	2.75910500	-2.24276200	0.28499900
H	3.59272500	-2.20111500	0.86778400
C	2.25258000	-3.53628000	-0.14099400
H	2.42705400	-4.26524700	0.65403800
H	1.17963100	-3.46139100	-0.33126100
H	2.74123500	-3.88784500	-1.05936100
C	5.51637200	-0.49130000	0.07278800
C	6.82894700	-0.29859100	-0.65945400
H	7.57829500	0.06042100	0.05338100
H	7.17410500	-1.26741400	-1.03495300
H	6.76700600	0.40667500	-1.49359800
O	5.42095500	-1.23323300	1.05409900
C	-0.82632100	1.04577000	-0.45476600
H	-0.21478100	0.31559000	-0.98276100
C	-0.90075100	2.36417400	-1.06663500
H	0.11158400	2.65972500	-0.03531400
C	-1.93084100	3.35389700	-0.87443500
H	-1.84913100	4.20740100	-1.57700200
C	-1.85240700	0.43963900	0.47505500
H	-1.40006000	-0.44948400	0.92675300
C	-3.05513300	-0.02181100	-0.39665500
H	-2.68893300	-0.63345400	-1.23274100
H	-3.53214300	0.86537500	-0.83066000
C	-4.08131700	-0.81903700	0.42031900
H	-3.60416400	-1.72822300	0.81475300
H	-4.37722500	-0.22139400	1.29068700
C	-5.32173900	-1.20423300	-0.39574500
H	-5.01643900	-1.79109900	-1.27530500
H	-5.79476000	-0.29174600	-0.78792100
C	-6.35674700	-2.00219000	0.40820000
H	-5.88811700	-2.91837800	0.79521200
H	-6.65759100	-1.41818900	1.28939700
O	-2.83349000	3.38000800	-0.02483800
S	0.91646900	1.71319100	1.01652200
O	-2.23563000	1.27104400	1.54413800
H	-2.60464100	2.09309200	1.13715600
H	-0.34248900	2.47697000	-1.99564400
C	-7.59942700	-2.37101200	-0.40702000
H	-8.31950000	-2.93814300	0.19501900
H	-8.11148300	-1.47446500	-0.77890300
H	-7.33779600	-2.98623400	-1.27746600

MIN_{1c1}

Charge/multiplicity: 0 1

N	4.40150200	0.00747400	-0.28894400
H	4.52845600	0.70149500	-1.01389900
C	3.16234800	0.04825900	0.49806700
H	3.40902600	-0.35014400	1.48558100
C	2.67487400	1.49235800	0.62699800
C	2.10118100	-0.86517700	-0.16254900
H	3.52539600	2.13188700	0.88075100
H	2.24788900	1.83616600	-0.31852100

O	1.19428400	-0.41878400	-0.86819400
N	2.28683900	-2.18114300	0.08031900
H	3.15711700	-2.44672500	0.53527600
C	1.46413300	-3.20148500	-0.54560000
H	1.75952500	-4.17681000	-0.15289400
H	0.40777800	-3.03302600	-0.31522500
H	1.57923200	-3.20610700	-1.63695900
C	5.32726400	-0.97942900	-0.14269900
C	6.57822500	-0.85137800	-0.98939500
H	7.44666500	-0.78224600	-0.32590400
H	6.69743500	-1.75969200	-1.58852300
H	6.57138400	0.01758200	-1.65425200
O	5.16836500	-1.91982000	0.64108700
C	-1.32643000	1.57602300	-1.57909100
H	-0.90505500	1.07775000	-2.45155000
C	-1.34436000	2.92830500	-1.62156700
H	0.33272000	1.33883400	1.32154000
C	-1.90903200	3.86384000	-0.64668300
H	-1.79777800	4.92905400	-0.92800100
C	-1.83247400	0.61357400	-0.53085100
H	-1.19986200	-0.27606000	-0.60721400
C	-3.29423400	0.21316100	-0.84998300
H	-3.36385200	-0.08646600	-1.90545500
H	-3.92916100	1.10245100	-0.73441800
C	-3.80363200	-0.92083500	0.04795800
H	-3.17739000	-1.81182700	-0.10839100
H	-3.66759800	-0.62902200	1.09632900
C	-5.27304200	-1.27913700	-0.20649900
H	-5.40760800	-1.55567100	-1.26332900
H	-5.89803500	-0.38840100	-0.04365300
C	-5.78336400	-2.42161400	0.68166000
H	-5.16224900	-3.31367800	0.51649900
H	-5.64649900	-2.14701200	1.73709500
O	-2.49805400	3.59317500	0.39788400
S	1.44884400	1.75710500	1.97233400
O	-1.67730200	1.05706600	0.80845000
H	-2.11126100	1.93822500	0.87251500
H	-0.91737600	3.41520900	-2.49657500
C	-7.25291400	-2.77164700	0.43195200
H	-7.58512200	-3.59142000	1.08017700
H	-7.90567400	-1.91094300	0.62534500
H	-7.41760100	-3.08341800	-0.60744500

TS_{1c2}

Charge/multiplicity: 0 1

N	4.02715400	-0.20252600	-0.55095700
H	4.36274100	-0.23984100	-1.50449100
C	2.62604700	0.18345200	-0.33362600
H	2.59133700	0.69548500	0.63231800
C	2.17562500	1.13090900	-1.44307200
C	1.73129200	-1.08129000	-0.25442400
H	2.90433600	1.94196900	-1.55473600
H	2.11321900	0.59618400	-2.39714000
O	0.98239200	-1.42568500	-1.16764600
N	1.87434100	-1.76873000	0.90441600
H	2.62700500	-1.47698400	1.52473800
C	1.22273900	-3.04748500	1.12255100
H	1.30706400	-3.31060000	2.17971100
H	0.16492100	-2.97698800	0.85529900
H	1.67160300	-3.84887700	0.52043800
C	4.86353900	-0.55759000	0.46013500
C	6.30022800	-0.84357000	0.06837800

H	6.95405900	-0.13225000	0.58410300
H	6.57178100	-1.84581400	0.41452200
H	6.48353400	-0.77462900	-1.00822900
O	4.48441700	-0.63359400	1.63356800
C	-2.07366800	2.42311700	-0.73610800
H	-2.37940700	2.37466800	-1.77996200
C	-1.45031500	3.61357800	-0.29416200
H	-0.18148000	3.28510300	-0.41820200
C	-1.52556100	4.02443500	1.14906500
H	-1.53819200	3.20930100	1.89586800
C	-2.55438200	1.30306600	0.15696100
H	-1.86258100	1.16042500	0.99094100
C	-2.73957200	-0.02307800	-0.58269600
H	-1.77445900	-0.30838500	-1.01671700
H	-3.43092400	0.13545800	-1.42656400
C	-3.26184400	-1.15100100	0.31551000
H	-2.55444200	-1.30345700	1.14360100
H	-4.21031200	-0.84629800	0.77666000
C	-3.45129600	-2.47273800	-0.43977000
H	-2.49915300	-2.76231900	-0.90760500
H	-4.16295700	-2.32236400	-1.26569700
C	-3.94918800	-3.61792700	0.45149500
H	-3.23479800	-3.77327900	1.27261900
H	-4.89711400	-3.32428200	0.92485900
O	-1.55121900	5.18866600	1.48704200
S	0.52973000	1.89413500	-1.14368700
O	-3.77347900	1.77168300	0.77317900
H	-4.46348200	1.78110800	0.08694900
H	-1.51110300	4.46704700	-0.97363600
C	-4.14489400	-4.93270600	-0.30856400
H	-4.49720400	-5.73093900	0.35567500
H	-4.88269200	-4.82132200	-1.11333000
H	-3.20682700	-5.27108100	-0.76639800

MIN_{1c2}

Charge/multiplicity: 0 1

N	-4.00962400	0.33910900	-0.82627200
H	-3.83633000	0.48206300	-1.81297700
C	-3.23557400	-0.69218500	-0.12772400
H	-3.86096700	-1.03172100	0.70252100
C	-2.93793300	-1.85064900	-1.07884900
C	-1.93288200	-0.07749100	0.44476700
H	-3.83524200	-2.11741000	-1.64296600
H	-2.15469800	-1.55822500	-1.78284100
O	-0.84287900	-0.21585000	-0.11321400
N	-2.12167700	0.63748000	1.57453900
H	-3.08460900	0.81799000	1.84899100
C	-1.04582800	1.38030600	2.20834400
H	-1.41113500	1.78327200	3.15535300
H	-0.19764900	0.71926400	2.40866500
H	-0.69469500	2.20909600	1.58038500
C	-4.84703100	1.18806000	-0.16735100
C	-5.60939400	2.17474000	-1.02823500
H	-6.68109800	2.04251500	-0.84819400
H	-5.35053500	3.19288000	-0.71950100
H	-5.41318800	2.06562800	-2.09892300
O	-4.98535000	1.15072800	1.05860700
C	2.25860100	-1.83560800	0.06378600
H	1.19961700	-1.60232900	-0.05139300
C	2.63276000	-3.10583600	-0.19055200
H	-3.47168000	-3.78464800	0.24374400
C	3.96693300	-3.71353200	-0.05646000

H	4.77052100	-3.07987200	0.35559600
C	3.06395800	-0.63506800	0.49804200
H	2.83078300	-0.45696400	1.55898800
C	2.63980700	0.61861000	-0.29572300
H	1.54746600	0.70558800	-0.25089600
H	2.89418800	0.45921300	-1.35575500
C	3.29747800	1.90702300	0.21211200
H	3.01132300	2.06531600	1.26283700
H	4.38787400	1.78436900	0.20974900
C	2.91412300	3.14392000	-0.61002800
H	1.81952200	3.25749000	-0.61175000
H	3.20347200	2.98734900	-1.66014700
C	3.55609400	4.44030000	-0.09898700
H	3.26438100	4.60043900	0.94888800
H	4.64936700	4.32555400	-0.09572200
O	4.18075700	-4.87939600	-0.36018300
S	-2.28483300	-3.34870500	-0.23328400
O	4.48080300	-0.81607900	0.47463100
H	4.74393700	-0.88368600	-0.45942200
H	1.86885600	-3.81081000	-0.51681100
C	3.17590200	5.67107800	-0.92680100
H	3.64962000	6.57919000	-0.53518100
H	3.48793300	5.55943700	-1.97301300
H	2.09066100	5.83493500	-0.92233000

In N-octanol implicit solvent

Cysteine

Charge/multiplicity: 0 1

N	1.14196900	-0.50468200	-0.29512000
H	0.92268700	-0.69339500	-1.26663700
C	0.01513500	-0.19874800	0.55836700
H	0.14189200	-0.73118800	1.50924400
C	-0.08637700	1.30127800	0.92086900
C	-1.25456900	-0.70967500	-0.13990900
H	-0.88749700	1.45931700	1.64828500
H	0.85249100	1.60194500	1.39229300
S	-0.30701100	2.46231400	-0.49023700
O	-1.25718500	-0.99941300	-1.34282600
H	-1.57856800	2.12301400	-0.79725900
N	-2.35352700	-0.78226700	0.63287600
H	-2.27372100	-0.58838200	1.62313600
C	-3.63706700	-1.22877100	0.10867600
H	-4.38521600	-1.13315100	0.89738600
H	-3.93858400	-0.61552100	-0.74623800
H	-3.59030900	-2.27477900	-0.21493500
C	2.40764500	-0.62370700	0.16958300
C	3.45725100	-0.99550200	-0.85607400
H	4.24210700	-0.23152400	-0.85303300
H	3.92084600	-1.94350600	-0.56129800
H	3.05702100	-1.09302300	-1.86900000
O	2.69441400	-0.44276500	1.36138600

MIN_{1t}

Charge/multiplicity: 0 1

N	3.63849800	-0.53963000	-0.46399000
H	3.46171000	-0.36624200	-1.44808300
C	3.07935800	0.42237900	0.48121200
H	3.77829500	0.48235900	1.32507700

C	3.00319400	1.81978600	-0.14428500
C	1.72567300	-0.03820500	1.07535100
H	2.49914900	2.49964300	0.54378000
H	4.01993100	2.18971500	-0.30186500
O	0.70385100	0.66991500	1.02018800
N	1.75369900	-1.22855600	1.68864700
H	2.64934200	-1.71255100	1.74453200
C	0.57732000	-1.80276800	2.32493600
H	-0.22108600	-1.97193300	1.59420700
H	0.85824400	-2.75897300	2.76961000
H	0.19301800	-1.14232900	3.11005100
C	4.36346800	-1.62060100	-0.09864400
C	4.96083800	-2.44002500	-1.21882200
H	4.56442300	-3.45976100	-1.16391600
H	4.75922400	-2.02837200	-2.21149600
H	6.04412600	-2.50066000	-1.06865800
O	4.52701600	-1.93166200	1.09446700
C	-2.68379100	2.46284800	-0.22941600
H	-3.72103600	2.78899800	-0.14972400
C	-1.72387200	3.26256200	0.26517800
H	0.94432300	1.64314800	-1.44352900
C	-2.04274100	4.54622300	0.90308000
H	-1.16653700	5.11757800	1.26946200
C	-2.47761200	1.12900100	-0.88787100
H	-2.90800200	1.19703600	-1.89842300
C	-3.23935000	0.02400600	-0.12257400
H	-4.27740600	0.35201800	0.02299500
H	-2.79583800	-0.06742400	0.87947500
C	-3.22007800	-1.33235900	-0.83654100
H	-3.67291200	-1.22027100	-1.83291900
H	-2.17939800	-1.63911100	-1.00378700
C	-3.96063100	-2.42894000	-0.06124500
H	-5.00088200	-2.11478300	0.11212500
H	-3.50614800	-2.54122900	0.93480800
C	-3.95641800	-3.78738100	-0.77368300
H	-4.41227100	-3.67582700	-1.76810000
H	-2.91726000	-4.10197700	-0.94787700
O	-3.17160000	5.00554300	1.04854800
S	2.21302700	1.93402700	-1.80866500
O	-1.10855900	0.79250500	-1.08892200
H	-0.67409700	0.65401300	-0.22036300
H	-0.67460600	2.98699000	0.21414800
C	-4.69525600	-4.87948400	0.00439500
H	-4.67697100	-5.83569000	-0.53290600
H	-4.24041300	-5.04380800	0.98991400
H	-5.74701200	-4.61034500	0.16683300

TS_{1t}

Charge/multiplicity: 0 1

N	-4.20956200	-0.11130000	0.44563600
H	-4.24930100	0.45527500	1.28466800
C	-2.99254800	-0.05003400	-0.37109600
H	-3.29528600	-0.28440300	-1.39481000
C	-2.39904900	1.35800600	-0.31982500
C	-2.00797900	-1.13908300	0.11390400
H	-3.20049000	2.07655100	-0.51816100
H	-1.99565100	1.56010000	0.67663500
O	-1.08031800	-0.91000400	0.90155700
N	-2.27589200	-2.37095600	-0.36466000
H	-3.15189400	-2.49387900	-0.86536200
C	-1.54773600	-3.54637700	0.08718000
H	-1.71762500	-3.74534800	1.15280600

H	-1.88354200	-4.40805600	-0.49305700
H	-0.47331200	-3.41041300	-0.06962100
C	-5.23502900	-0.95080900	0.16288400
C	-6.43902800	-0.87316900	1.07457300
H	-7.32102900	-0.62970300	0.47220500
H	-6.60905900	-1.85821400	1.52250900
H	-6.33458900	-0.13071100	1.87062600
O	-5.19787800	-1.73836500	-0.79626500
C	1.04181500	1.46533800	0.06418200
H	0.45848300	0.88162200	0.77291000
C	0.95710300	2.88731400	0.12046000
H	-0.07340300	2.78578200	-0.69513300
C	0.42565600	3.54294100	1.32921200
H	0.68654800	4.61595600	1.41464000
C	2.06868800	0.71682100	-0.71962300
H	1.62550300	-0.21719300	-1.07558100
C	3.22649300	0.35710400	0.25412700
H	2.80717300	-0.13567500	1.13995400
H	3.69730100	1.28864000	0.59859000
C	4.26767400	-0.55786500	-0.40647100
H	3.77045500	-1.47970100	-0.73971800
H	4.65985400	-0.07166500	-1.30862500
C	5.42624500	-0.91142600	0.53414100
H	5.02754900	-1.39050400	1.44060000
H	5.92207800	0.01235300	0.86773600
C	6.46486100	-1.83733900	-0.11212300
H	5.96837500	-2.75901900	-0.44784900
H	6.86447300	-1.35789000	-1.01726000
O	-0.27840800	3.00847900	2.17906400
S	-1.08574500	1.60275900	-1.59080700
O	2.52246100	1.40668100	-1.87418400
H	3.14290500	2.10131400	-1.59370200
H	1.69672500	3.45948500	-0.43933600
C	7.61967300	-2.19523200	0.82715200
H	8.34270300	-2.85809100	0.33616000
H	8.16087000	-1.29787300	1.15399200
H	7.25638200	-2.70856300	1.72682400

MIN_2

Charge/multiplicity: 0 1

N	-3.54469300	-0.86792700	-0.13948500
H	-4.13124900	-0.21363200	0.36518000
C	-2.15574900	-0.48154500	-0.41279000
H	-1.86699300	-0.99840000	-1.33185600
C	-2.08447100	1.03268100	-0.61812700
C	-1.25710000	-0.98056500	0.74153200
H	-2.90467800	1.33009300	-1.27839500
H	-2.19554800	1.56876000	0.32555600
O	-0.87338400	-0.24341400	1.65903300
N	-0.96514800	-2.29547100	0.68036100
H	-1.45623700	-2.84628500	-0.01955500
C	-0.27484100	-2.98126700	1.76244200
H	0.69667700	-2.51578800	1.95311500
H	-0.85635400	-2.95754000	2.69251100
H	-0.11649200	-4.02078200	1.46898700
C	-4.04679000	-2.08108100	-0.47535900
C	-5.50751700	-2.31261000	-0.16148800
H	-5.58968200	-3.12933100	0.56437100
H	-6.00952300	-1.42734100	0.23816900
H	-6.01740300	-2.63321600	-1.07602200
O	-3.34964100	-2.95760000	-1.01125900
C	0.49590600	2.30956900	-0.06115900

H	0.09658600	1.88672800	0.86495500
C	0.40012300	3.83899700	-0.03583600
H	0.59518500	4.27346500	-1.02654500
C	-0.87828500	4.42837000	0.48124900
H	-0.95106700	5.52951500	0.36163700
C	1.97224700	1.85225700	-0.22914200
H	2.32609700	2.17193000	-1.21829400
C	2.19281400	0.34250000	-0.07317100
H	1.51601300	-0.19390800	-0.74714300
H	1.90563900	0.05722200	0.94986100
C	3.64057600	-0.08221900	-0.35042100
H	3.90788000	0.20416100	-1.37884500
H	4.31664300	0.47726000	0.30924900
C	3.87813200	-1.58640500	-0.16766300
H	3.19727400	-2.14751400	-0.82536800
H	3.61502300	-1.87470200	0.86158500
C	5.32277500	-2.01399900	-0.45494900
H	5.58693700	-1.72901600	-1.48369400
H	6.00350400	-1.45281400	0.20145800
O	-1.78110900	3.81927400	1.02967100
S	-0.54481100	1.61614100	-1.44443200
O	2.80819200	2.57346300	0.69119300
H	2.59726300	2.25027100	1.58529100
H	1.19348100	4.24589400	0.61093100
C	5.55848600	-3.51517400	-0.26773000
H	6.59961300	-3.78692800	-0.48148500
H	5.33898900	-3.82783900	0.76153000
H	4.91798700	-4.10556000	-0.93584400

TS_2

Charge/multiplicity: 0 1

N	-3.86292000	0.00623200	-0.03763200
H	-4.27635800	0.66536300	0.61213200
C	-2.42010500	0.09342400	-0.28452400
H	-2.25095700	-0.32609000	-1.27941900
C	-1.98058200	1.55970400	-0.26417800
C	-1.68205100	-0.77682700	0.75702400
H	-2.69831500	2.14142600	-0.84985900
H	-1.98183400	1.95302700	0.75633700
O	-1.18024700	-0.30700300	1.78747400
N	-1.67642600	-2.09369600	0.47019000
H	-2.24810500	-2.40141300	-0.31182200
C	-1.17798400	-3.08490300	1.41218900
H	-1.76278600	-3.09034400	2.34035600
H	-1.24266100	-4.06954000	0.94544300
H	-0.13318000	-2.88153700	1.66515000
C	-4.63355200	-0.99178900	-0.54261400
C	-6.10633700	-0.91552800	-0.19979500
H	-6.54580800	0.01263000	-0.58270300
H	-6.62302300	-1.76872200	-0.64284200
H	-6.25139300	-0.93046200	0.88673600
O	-4.15800200	-1.89669100	-1.24400600
C	0.79040400	2.02209800	0.44469900
H	0.29231800	1.46678900	1.24461900
C	0.91729500	3.48360800	0.89130300
H	1.48316500	3.54362900	1.83241000
C	1.58159200	4.44437200	-0.05518500
H	1.63531300	5.48674000	0.32508100
C	2.15710000	1.33881300	0.15801900
H	2.55161200	1.71003800	-0.79207200
C	2.07048900	-0.19139300	0.12073900
H	1.28934300	-0.48901400	-0.58855800

H	1.73981500	-0.54060300	1.11112000
C	3.39426300	-0.86743500	-0.25737800
H	3.70436100	-0.52019500	-1.25427400
H	4.17974000	-0.54393300	0.43826000
C	3.31114600	-2.39882400	-0.25758500
H	2.52469900	-2.72184700	-0.95632600
H	2.99551900	-2.74599900	0.73828300
C	4.63146900	-3.08307900	-0.63316700
H	4.94672900	-2.74027500	-1.62933500
H	5.41802200	-2.75934600	0.06380400
O	2.04310000	4.17394000	-1.14959200
S	-0.33459200	1.86941300	-1.03187000
O	3.12379700	1.76721700	1.13124500
H	2.88021900	1.35529000	1.97895000
H	-0.07202300	3.90287000	1.12732900
C	4.54420900	-4.61163000	-0.62673500
H	5.50285600	-5.06856400	-0.90180900
H	4.26876900	-4.99117300	0.36588600
H	3.78954900	-4.97045700	-1.33870300

MIN_3

Charge/multiplicity: 0 1

N	3.85961800	-0.02678800	-0.04420100
H	4.27789800	-0.69570100	0.59151900
C	2.41425800	-0.10833600	-0.27995800
H	2.23914100	0.31862000	-1.27065700
C	1.97100500	-1.57360500	-0.26522500
C	1.68734100	0.75834800	0.77271000
H	2.68609600	-2.15462200	-0.85486900
H	1.97316200	-1.97141400	0.75354200
O	1.18444000	0.28279900	1.79990700
N	1.69141100	2.07754100	0.49758700
H	2.26319800	2.38751200	-0.28376700
C	1.20136600	3.06392100	1.44901200
H	0.15367400	2.86964400	1.69739600
H	1.78386400	3.05279400	2.37853000
H	1.27817800	4.05273200	0.99305600
C	4.62588400	0.97081300	-0.55138500
C	6.10219400	0.91198700	-0.23034100
H	6.66778200	0.94445200	-1.16745800
H	6.37467100	1.80111700	0.34908800
H	6.38802100	0.01804900	0.33066200
O	4.14622300	1.88278400	-1.24279900
C	-0.80288700	-2.02189000	0.44351300
H	-0.30042700	-1.47131200	1.24391700
C	-0.94131400	-3.48278500	0.88875700
H	-1.50763500	-3.53929500	1.82981100
C	-1.61308400	-4.43747700	-0.05860900
H	-1.67476700	-5.47977100	0.32061700
C	-2.16420700	-1.32765100	0.15793500
H	-2.56355300	-1.69727300	-0.79074800
C	-2.06525500	0.20171100	0.11772600
H	-1.28452800	0.49164300	-0.59521000
H	-1.72787200	0.55018000	1.10610100
C	-3.38481300	0.88801400	-0.25687400
H	-3.70331700	0.53857700	-1.25035000
H	-4.16971200	0.57548400	0.44441000
C	-3.28720300	2.41850400	-0.26567200
H	-2.50149200	2.73012500	-0.97038600
H	-2.96283200	2.76805100	0.72654500
C	-4.60290800	3.11342400	-0.63797900
H	-4.92732100	2.76737900	-1.63007600
H	-5.38860100	2.80204800	0.06555700

O	-2.07269000	-4.16243100	-1.15269300
S	0.32377300	-1.87706100	-1.03266700
O	-3.13243200	-1.74665000	1.13374000
H	-2.88276400	-1.33696200	1.98076100
H	0.04469400	-3.90994000	1.12439900
C	-4.50035600	4.64102100	-0.64196600
H	-5.45593200	5.10580000	-0.91457100
H	-4.21543500	5.02418600	0.34657900
H	-3.74621800	4.98760100	-1.36051400

TS_3

Charge/multiplicity: 0 1

N	-3.94694900	-0.46784000	0.45935800
H	-4.22915100	-0.23390100	1.40461900
C	-2.62804600	-0.01786900	0.00117200
H	-2.68933800	0.06153700	-1.08686400
C	-2.31360200	1.35465200	0.60328500
C	-1.58201300	-1.09420400	0.36898700
H	-3.21887300	1.96724500	0.54750400
H	-2.03436800	1.26321100	1.65698800
O	-0.86560300	-1.00981900	1.37582700
N	-1.55375600	-2.14594200	-0.47355800
H	-2.29078800	-2.19807600	-1.17193900
C	-0.75737300	-3.33276400	-0.19898700
H	0.29220400	-3.06126100	-0.05415300
H	-1.10554200	-3.85546000	0.70071100
H	-0.83337500	-4.00731800	-1.05392500
C	-4.73999300	-1.28401200	-0.28165800
C	-6.07954200	-1.62694300	0.33487100
H	-6.61671400	-2.30772000	-0.32781900
H	-5.94479900	-2.10537400	1.31189800
H	-6.67835500	-0.72140200	0.48591400
O	-4.38907200	-1.70708300	-1.39309700
C	0.56277500	1.83972600	0.53581200
H	0.24809100	1.20441000	1.36604700
C	1.25779100	3.07712100	1.12720400
H	2.24710300	2.81212800	1.53250100
C	1.47435500	4.26588500	0.23370600
H	1.88560400	5.15392400	0.75372800
C	1.46261100	0.97007400	-0.37985700
H	0.80010900	0.28155700	-0.92594000
C	2.45687400	0.12823500	0.43012900
H	1.88170300	-0.48514400	1.13509400
H	3.09892100	0.79113400	1.02659800
C	3.33644200	-0.78356100	-0.43690200
H	2.69271100	-1.41906000	-1.06346700
H	3.93016000	-0.17044800	-1.12669800
C	4.27301400	-1.67141400	0.39212200
H	3.67550800	-2.29107700	1.07806200
H	4.90710500	-1.03623400	1.02922600
C	5.16768200	-2.58123500	-0.45918100
H	4.53653800	-3.21498000	-1.09896300
H	5.76925400	-1.96256300	-1.14068200
O	1.23140800	4.32712900	-0.96110300
S	-1.04163000	2.34376800	-0.28589100
O	2.21908400	1.74498400	-1.31235200
H	1.65621800	2.47179100	-1.63555500
H	0.69198200	3.45167500	1.99234800
C	6.09583700	-3.46723100	0.37592100
H	6.72322100	-4.10305200	-0.26094300
H	6.76448800	-2.86342400	1.00326400

H	5.52399400	-4.12637200	1.04215000

MIN_4

Charge/multiplicity: 0 1

N	-3.94746700	-0.46207600	0.46420000
H	-4.23241300	-0.22059700	1.40614500
C	-2.62694900	-0.01536400	0.00661900
H	-2.68775500	0.06248000	-1.08158800
C	-2.31060300	1.35699900	0.60809800
C	-1.58351500	-1.09398500	0.37596100
H	-3.21534700	1.97050400	0.55359500
H	-2.02983000	1.26543300	1.66135800
O	-0.86254000	-1.00662900	1.37917400
N	-1.56219700	-2.14944400	-0.46179700
H	-2.30202200	-2.20193500	-1.15747600
C	-0.76634200	-3.33636900	-0.18618600
H	0.28488700	-3.06642400	-0.05045400
H	-1.10917300	-3.85306100	0.71898000
H	-0.85003100	-4.01560400	-1.03667900
C	-4.74039100	-1.27306500	-0.27900900
C	-6.08492600	-1.62665000	0.31525400
H	-6.87003300	-1.31411100	-0.38164300
H	-6.15186000	-2.71511900	0.41870700
H	-6.26601700	-1.16221900	1.28869500
O	-4.38863300	-1.69863200	-1.39052100
C	0.56588000	1.83943300	0.53600800
H	0.25175600	1.20450900	1.36673300
C	1.26280300	3.07633000	1.12619700
H	2.25248000	2.81054400	1.53007800
C	1.47903900	4.26473300	0.23214500
H	1.89185500	5.15252800	0.75133200
C	1.46359100	0.96880300	-0.38079000
H	0.79970300	0.28064000	-0.92565800
C	2.45834900	0.12644800	0.42804500
H	1.88368800	-0.48653700	1.13376200
H	3.10146300	0.78906900	1.02367000
C	3.33643400	-0.78593500	-0.43987500
H	2.69168000	-1.42144400	-1.06537300
H	3.92945700	-0.17324600	-1.13064400
C	4.27379600	-1.67374100	0.38829700
H	3.67696600	-2.29312600	1.07507600
H	4.90868700	-1.03848200	1.02452300
C	5.16741100	-2.58391600	-0.46373800
H	4.53550300	-3.21778900	-1.10263500
H	5.76829600	-1.96550500	-1.14608300
O	1.23429500	4.32591000	-0.96230200
S	-1.03931000	2.34481100	-0.28337900
O	2.21931300	1.74282300	-1.31462000
H	1.65666000	2.47014700	-1.63703100
H	0.69858300	3.45149300	1.99211300
C	6.09640400	-3.46973300	0.37062200
H	6.72312000	-4.10572800	-0.26672400
H	6.76570700	-2.86577700	0.99712600
H	5.52523000	-4.12868800	1.03760800

TS_4

Charge/multiplicity: 0 1

N	3.99879800	-0.36816900	-0.57034600
H	4.20066100	-0.20989800	-1.55060000
C	2.71082300	0.09918500	-0.04645800
H	2.86535100	0.30715600	1.01544600
C	2.29801500	1.38375800	-0.76933600
C	1.67026900	-1.03317700	-0.18919500
H	3.17373900	2.03729800	-0.83058200
H	1.96632300	1.16902500	-1.78926800
O	0.85597400	-1.07281600	-1.12103600
N	1.75563300	-1.98593200	0.76004400
H	2.56031200	-1.94847700	1.38101000
C	0.96950800	-3.20923900	0.69559900
H	1.18535100	-3.80674100	1.58329100
H	-0.09970100	-2.97728400	0.67675000
H	1.20962800	-3.79750100	-0.19869400
C	4.87607200	-1.08156700	0.17762600
C	6.17158200	-1.47105500	-0.49762000
H	7.00754400	-1.12541600	0.11948300
H	6.23045800	-2.56401700	-0.54845800
H	6.27614300	-1.06050500	-1.50579600
O	4.63348100	-1.39892700	1.35280400
C	-0.57310700	1.86297400	-0.71827000
H	-0.29226600	1.33125300	-1.62790500
C	-1.47017400	3.07897400	-1.02588600
H	-2.18487000	2.81305600	-1.81290600
C	-2.21205500	3.39358000	0.26474400
H	-3.26352100	3.69020500	0.13967000
C	-1.45974100	0.97220500	0.18310000
H	-0.87154600	0.41191400	0.91256700
C	-2.38616300	0.03281300	-0.58795400
H	-1.74580800	-0.62975500	-1.18267200
H	-2.99203100	0.61429000	-1.29588800
C	-3.30256800	-0.80781400	0.31155600
H	-2.68561400	-1.39721200	1.00608700
H	-3.91812300	-0.14342100	0.93197100
C	-4.21222600	-1.74951000	-0.48673600
H	-3.59397400	-2.40533300	-1.11796400
H	-4.83134100	-1.15645800	-1.17676000
C	-5.12538300	-2.61141600	0.39446000
H	-4.50803400	-3.21107500	1.07888900
H	-5.73912000	-1.95698000	1.03005800
O	-1.54034200	3.93958700	1.28229200
S	1.01909500	2.39127300	0.09026500
O	-2.27888800	1.91407500	0.96079200
H	-1.66870300	2.64355000	1.64914400
H	-0.90315500	3.95354700	-1.35447100
C	-6.03813800	-3.53921600	-0.41149400
H	-6.67379900	-4.14556100	0.24545300
H	-6.69824900	-2.96806600	-1.07725000
H	-5.45426800	-4.22756300	-1.03637200

P(R)

Charge/multiplicity: 0 1

N	-4.36107700	0.26471600	0.27576700
H	-4.44558500	0.82156900	1.11788000
C	-3.02078900	0.03515400	-0.27101600
H	-3.14782600	-0.11507900	-1.34645200
C	-2.14618400	1.26467700	-0.01908900
C	-2.42795600	-1.25375100	0.34270900
H	-2.69480000	2.15867400	-0.32747000
H	-1.90747100	1.35806700	1.04354500
O	-1.61852700	-1.23649100	1.27923600

N	-2.89856800	-2.39066600	-0.20554100
H	-3.67095400	-2.30677100	-0.86148800
C	-2.55736600	-3.70049000	0.32796600
H	-1.47088300	-3.82631300	0.35959200
H	-2.95000400	-3.84030600	1.34285900
H	-2.98350000	-4.46362900	-0.32608000
C	-5.47070300	-0.31252800	-0.24823100
C	-6.78620800	0.04777700	0.40372400
H	-7.44386300	0.48976400	-0.35263300
H	-7.26735900	-0.86866500	0.76199400
H	-6.68054700	0.74707700	1.23777500
O	-5.41402000	-1.08951300	-1.21424500
C	0.71144800	0.87421800	0.31428300
H	0.43468100	-0.06622400	0.79057100
C	0.91091200	2.01597000	1.31949900
H	1.38876800	1.61452200	2.22098900
C	1.88361400	2.95646700	0.60274300
H	2.54541500	3.50088000	1.28131300
C	2.09132500	0.79868300	-0.37941600
H	1.99564600	0.62998800	-1.46015900
C	2.99360800	-0.28957500	0.20927500
H	2.49260000	-1.25583500	0.05742400
H	3.07566500	-0.13999300	1.29496400
C	4.39119200	-0.33063800	-0.42078300
H	4.29182400	-0.46671200	-1.50813900
H	4.88308800	0.63986600	-0.27408700
C	5.27601700	-1.44515300	0.15138100
H	4.77638200	-2.41565100	0.01097400
H	5.37708600	-1.30839300	1.23860500
C	6.67204200	-1.50092700	-0.48155900
H	6.57164200	-1.63566800	-1.56824500
H	7.17332700	-0.53269400	-0.33903400
O	1.25487300	3.95791400	-0.17045700
S	-0.57594300	1.23203200	-0.98163700
O	2.69649900	2.10288000	-0.19934300
H	-0.00763700	2.52343500	1.62300700
H	0.58287800	3.52021600	-0.72794800
C	7.55035600	-2.61740400	0.08956500
H	8.54035400	-2.62895000	-0.38286600
H	7.70000600	-2.49365200	1.17003200
H	7.09521700	-3.60356800	-0.07013800

MIN_3
Charge/multiplicity: 0 1

N	4.35809700	0.26908000	-0.43187400
H	4.42165300	0.74296100	-1.32509400
C	3.03482500	0.13389300	0.18593500
H	3.20245400	0.07084700	1.26419600
C	2.18668200	1.36757200	-0.13300800
C	2.38460300	-1.18297700	-0.29437300
H	2.78621700	2.26079000	0.06531100
H	1.90642500	1.37660200	-1.19006900
O	1.56420200	-1.22403000	-1.22141300
N	2.82098700	-2.28251800	0.35022000
H	3.61205800	-2.16886400	0.97856000
C	2.42915100	-3.62136800	-0.06375500
H	1.33870600	-3.70952300	-0.07809200
H	2.80772400	-3.86366200	-1.06469800
H	2.83339600	-4.33913200	0.65258900
C	5.46771400	-0.31370600	0.08605500
C	6.76114100	-0.07589400	-0.65992100
H	7.49809700	0.33786300	0.03645100

H	7.14784800	-1.03794600	-1.01404300
H	6.65335500	0.60104700	-1.51199900
O	5.42951200	-1.00412100	1.11653000
C	-0.66335300	0.98409200	-0.28620600
H	-0.23031600	0.16648900	-0.86828600
C	-1.00133400	2.10037500	-1.29045000
H	-1.67291200	1.70948200	-2.07412600
C	-1.65147900	3.37061400	-0.82394300
H	-1.63093900	4.18867100	-1.57002600
C	-1.82356200	0.38138200	0.54079900
H	-1.43573300	-0.54809100	0.97426500
C	-3.05032700	0.04052000	-0.32195000
H	-2.71867600	-0.52021700	-1.20768700
H	-3.50310200	0.97304600	-0.68751300
C	-4.10799100	-0.77377100	0.43452600
H	-3.66128700	-1.72054500	0.77286400
H	-4.39772600	-0.22731800	1.34147100
C	-5.35565000	-1.07118300	-0.40605700
H	-5.06260200	-1.61620300	-1.31629500
H	-5.79820800	-0.12307000	-0.74742200
C	-6.42061900	-1.88066700	0.34475800
H	-5.98234200	-2.83073400	0.68309800
H	-6.71200700	-1.33744600	1.25526200
O	-2.20663400	3.56278500	0.24805800
S	0.67015800	1.50166900	0.90611700
O	-2.17610200	1.18629400	1.66703800
H	-2.33092700	2.09280200	1.32472200
H	-0.09752000	2.39425900	-1.84149100
C	-7.66694800	-2.16703300	-0.49706900
H	-8.40698600	-2.74734000	0.06777700
H	-8.15191500	-1.23665700	-0.82009900
H	-7.41578800	-2.73927900	-1.39966100

TS_3’

Charge/multiplicity: 0 1

N	4.42417200	-0.35244200	0.29506700
H	4.49432300	-0.93214800	1.12304100
C	3.09453900	-0.11459500	-0.27390200
H	3.24515300	0.07315400	-1.34018100
C	2.22349800	-1.35831600	-0.08772300
C	2.47963900	1.14873400	0.36980400
H	2.79302100	-2.23718200	-0.40209100
H	1.95025100	-1.48728700	0.96314900
O	1.65412000	1.09544100	1.29112000
N	2.95016000	2.30678600	-0.13245900
H	3.73570400	2.25058700	-0.77559000
C	2.59002800	3.59559900	0.43868100
H	3.01796300	4.38331500	-0.18433600
H	1.50214900	3.71076500	0.45934400
H	2.96764400	3.70587900	1.46288400
C	5.54089600	0.24642100	-0.18801700
C	6.84438600	-0.12672400	0.48055800
H	7.52531700	-0.52969300	-0.27688200
H	7.30613400	0.77873000	0.88900300
H	6.72583700	-0.86145200	1.28185000
O	5.49960500	1.05212000	-1.13101300
C	-0.62226800	-0.98243500	0.17343300
H	-0.29222800	-0.10980800	0.73902200
C	-0.91348100	-2.18755000	1.08109400
H	-1.39578900	-1.84732500	2.00422600
C	-1.90294400	-3.08948900	0.34099800

H	-1.43606000	-3.86923200	-0.27694900
C	-1.95553300	-0.70639100	-0.55741300
H	-1.79414100	-0.30574500	-1.56289300
C	-2.90172700	0.21634200	0.21217600
H	-2.36931600	1.16418000	0.36592900
H	-3.09743200	-0.20508100	1.20682900
C	-4.22373800	0.48666200	-0.51912800
H	-4.00496800	0.86941000	-1.52670100
H	-4.77098600	-0.45585900	-0.65819100
C	-5.12088400	1.48682200	0.22081700
H	-4.57356600	2.43107300	0.36057500
H	-5.33732500	1.10568400	1.22990600
C	-6.44097000	1.77074600	-0.50667400
H	-6.22402000	2.14425200	-1.51789400
H	-6.99104200	0.82818600	-0.64032300
O	-3.08165500	-3.37482200	0.89799600
S	0.68705600	-1.31926000	-1.10288500
O	-2.53473700	-2.04205500	-0.74490000
H	-3.37408500	-2.39765000	-0.00285700
H	-0.00753900	-2.73697700	1.35261600
C	-7.32926900	2.77879400	0.22722000
H	-8.26531000	2.95703400	-0.31628300
H	-7.59157900	2.42168200	1.23151200
H	-6.82301600	3.74606000	0.34202300

P(S)

Charge/multiplicity: 0 1

N	3.89073800	-0.48389200	0.49583400
H	3.90771300	-0.94614600	1.39727500
C	2.60896600	-0.39126700	-0.20924900
H	2.84818900	-0.34002200	-1.27474900
C	1.77134600	-1.64104700	0.07037700
C	1.88873200	0.91540000	0.19615400
H	2.39722900	-2.52523900	-0.07875000
H	1.41476600	-1.64523000	1.10402300
O	0.97816700	0.94597100	1.03543700
N	2.36723000	2.01818900	-0.41106800
H	3.21027300	1.91330200	-0.96977700
C	1.90869300	3.35262100	-0.05607800
H	2.13408500	3.59202900	0.99039900
H	2.41057000	4.07519000	-0.70233200
H	0.82736300	3.43780400	-0.20264000
C	5.02132700	0.10396800	0.03210500
C	6.27363400	-0.10617500	0.85231700
H	7.04571700	-0.54152100	0.20898000
H	6.64152400	0.86757800	1.19390900
H	6.12188200	-0.75555500	1.71894600
O	5.03323600	0.77649800	-1.01112700
C	-1.09200500	-1.41752900	0.08361800
H	-0.81178900	-0.52429800	0.64175200
C	-1.47589800	-2.58888600	0.99141100
H	-2.02878300	-2.20971200	1.86218000
C	-2.42966300	-3.42185700	0.13170900
H	-1.90541100	-4.18236400	-0.45833000
C	-2.38152900	-1.20722500	-0.74456300
H	-2.15469200	-0.95353200	-1.78775100
C	-3.31344000	-0.13519200	-0.16674200
H	-3.44996900	-0.31563200	0.90905500
H	-4.29708600	-0.27309900	-0.63552200
C	-2.83059500	1.30150700	-0.40523000
H	-1.83549900	1.44389500	0.03927300

H	-2.71075000	1.46576700	-1.48633300
C	-3.79062900	2.35456700	0.16352300
H	-3.90765800	2.19260700	1.24563000
H	-4.78910400	2.21217100	-0.27659300
C	-3.33141200	3.79688600	-0.08319300
H	-2.33310800	3.93925200	0.35553500
H	-3.21654900	3.96077100	-1.16441700
O	-3.40107700	-4.13840200	0.84801100
S	0.32249900	-1.78887400	-1.05712500
O	-3.05424500	-2.48705900	-0.75518600
H	-0.62763300	-3.17146400	1.35919200
C	-4.29206200	4.84232900	0.48985500
H	-3.93587600	5.86182500	0.29707500
H	-5.29161800	4.75047100	0.04539300
H	-4.40187200	4.72919700	1.57623700
H	-3.88908200	-3.50079900	1.39981000

TS_{1C1}

Charge/multiplicity: 0 1

N	-4.31648600	0.18743500	0.67129200
H	-4.24723800	0.51189800	1.62875400
C	-3.09914500	0.16050600	-0.13923000
H	-3.41567600	0.27149100	-1.18077800
C	-2.22527700	1.34962000	0.26714500
C	-2.36835600	-1.19454500	0.00455000
H	-2.80291000	2.27010600	0.14749800
H	-1.89205500	1.27292200	1.30550200
O	-1.29270700	-1.30084200	0.60946700
N	-2.99997700	-2.23001800	-0.57314200
H	-3.91108200	-2.05689900	-0.99143600
C	-2.49124200	-3.59084700	-0.48528300
H	-1.46999000	-3.64517400	-0.87565000
H	-2.48409700	-3.94961700	0.55071300
H	-3.13500700	-4.23962300	-1.08180900
C	-5.50160800	-0.29978500	0.22295200
C	-6.68034500	-0.16211100	1.15775800
H	-7.46161900	0.41670400	0.65330500
H	-7.08894100	-1.15767800	1.36141000
H	-6.42982300	0.32450100	2.10427200
O	-5.61135100	-0.82582000	-0.89496000
C	0.74972400	1.13093500	0.39562300
H	0.30486600	0.46985900	1.13979900
C	1.01704100	2.51555400	0.94144500
H	-0.23670200	2.82236700	-0.16410500
C	1.96446000	3.43681300	0.47247100
H	1.99500100	4.37557700	1.05900000
C	1.79905400	0.36747900	-0.42396500
H	1.34303300	-0.58777100	-0.71182100
C	3.04239800	0.07549700	0.43634900
H	2.72030500	-0.38577700	1.38052400
H	3.52693400	1.02598100	0.69346600
C	4.04658200	-0.84542100	-0.26933300
H	3.55298200	-1.79734500	-0.51599400
H	4.33778900	-0.39132500	-1.22542600
C	5.29937500	-1.12474200	0.56955500
H	5.00371800	-1.57229800	1.53071100
H	5.79258500	-0.17229300	0.81523500
C	6.30658800	-2.04848600	-0.12728700
H	5.81501600	-3.00112600	-0.37258700
H	6.60276600	-1.60174900	-1.08732600

O	2.73185800	3.36209500	-0.53429600
S	-0.74189600	1.54865700	-0.80857600
O	2.11019000	1.03302000	-1.63919200
H	2.44708100	1.93470800	-1.36765300
H	0.57522200	2.73295700	1.91144100
C	7.55644300	-2.32316600	0.71317600
H	8.25442400	-2.98682900	0.18792100
H	8.09295100	-1.39384000	0.94459600
H	7.29795100	-2.80158400	1.66689900

MIN_{1C1}

Charge/multiplicity: 0 1

N	-4.48111700	0.01556600	0.30804200
H	-4.58061300	0.67633200	1.06958300
C	-3.25333300	0.06152700	-0.49259300
H	-3.51589000	-0.30018900	-1.48988800
C	-2.74668300	1.50086200	-0.58232800
C	-2.20217500	-0.88842700	0.12499800
H	-3.57667200	2.15279400	-0.86827900
H	-2.35944100	1.83639400	0.38282000
O	-1.28339600	-0.47635300	0.84521200
N	-2.39404300	-2.19035700	-0.16063100
H	-3.25646500	-2.43938900	-0.63804900
C	-1.57693800	-3.23867900	0.43091100
H	-0.52117600	-3.08521900	0.18612900
H	-1.67806300	-3.26200900	1.52295200
H	-1.89764700	-4.19944800	0.02390700
C	-5.43415300	-0.93093300	0.12428700
C	-6.65965000	-0.83200200	1.00425100
H	-7.54532000	-0.74798600	0.36523800
H	-6.75760600	-1.75826000	1.58073500
H	-6.63388000	0.01732100	1.69264500
O	-5.31463000	-1.82925800	-0.72398900
C	1.38324800	1.39704900	1.63910400
H	1.08765900	0.89669000	2.56107300
C	1.24329000	2.74318800	1.62763500
H	-0.39558600	1.24888700	-1.20102400
C	1.62723700	3.69433400	0.58588600
H	1.40666700	4.74859500	0.83243000
C	1.93511200	0.45117500	0.60078500
H	1.41659700	-0.50367200	0.74010000
C	3.44473300	0.22631600	0.85852500
H	3.58869400	-0.02954100	1.91745000
H	3.96778700	1.17771400	0.68969400
C	4.04424300	-0.87296700	-0.02674200
H	3.51211500	-1.81728100	0.16110900
H	3.86713900	-0.62187000	-1.08021700
C	5.54612000	-1.07773100	0.20685100
H	5.72104700	-1.33204600	1.26323000
H	6.07475600	-0.12912900	0.02941600
C	6.15674900	-2.16824900	-0.68266600
H	5.62840600	-3.11664300	-0.50787400
H	5.98417000	-1.91244000	-1.73796900
O	2.18062900	3.44794300	-0.48908800
S	-1.45877100	1.75948500	-1.87115100
O	1.66594500	0.82126000	-0.74668400
H	1.99871300	1.74208800	-0.86206800
H	0.81999600	3.21557500	2.51180100
C	7.65598200	-2.37018500	-0.44687400
H	8.06162300	-3.15385700	-1.09860200
H	8.21811000	-1.44869500	-0.64673300

H	7.86024300	-2.66335000	0.59114600

TS_{1C2}

Charge/multiplicity: 0 1

N	-4.05830400	0.28263700	-0.55222700
H	-4.39578900	0.34466000	-1.50526100
C	-2.66619700	-0.13501600	-0.34406400
H	-2.63518400	-0.65430900	0.61768500
C	-2.23865800	-1.08756600	-1.45788000
C	-1.75555500	1.11347400	-0.25437200
H	-2.97784700	-1.89076600	-1.55259800
H	-2.19645000	-0.55900400	-2.41656800
O	-1.02124100	1.47777000	-1.18141600
N	-1.85676700	1.78060300	0.91341300
H	-2.58340400	1.48152100	1.55947400
C	-1.17837400	3.04714400	1.13866800
H	-1.53175800	3.82452300	0.44978600
H	-1.37157800	3.36750200	2.16430300
H	-0.09830000	2.93376600	1.00076000
C	-4.88900800	0.61485300	0.46378100
C	-6.31195800	0.95897300	0.08464000
H	-6.99005100	0.27181700	0.60248600
H	-6.53809700	1.97103700	0.43718600
H	-6.50061400	0.90319300	-0.99110400
O	-4.51037700	0.63361700	1.64704000
C	2.05239300	-2.44804200	-0.71768600
H	2.37069500	-2.41549000	-1.75832200
C	1.37770500	-3.61536500	-0.28373400
H	0.13677200	-3.25379900	-0.41770900
C	1.42689500	-4.02936600	1.15505600
H	1.45149400	-3.22520400	1.91044900
C	2.57064800	-1.34281500	0.16941100
H	1.92147400	-1.20483300	1.03755300
C	2.75156100	-0.01043700	-0.55896500
H	1.77272500	0.30707500	-0.93711800
H	3.39350100	-0.17513600	-1.43811100
C	3.34849900	1.08926000	0.32734300
H	2.69151600	1.24836100	1.19502900
H	4.31425300	0.75456900	0.72840800
C	3.53403100	2.41543400	-0.42075800
H	2.56440900	2.74346800	-0.82385700
H	4.18782100	2.25329200	-1.29104000
C	4.12408800	3.53084200	0.45111300
H	3.46671700	3.70050600	1.31601000
H	5.08900200	3.19883100	0.86100700
O	1.41656300	-5.20051900	1.48793700
S	-0.59356400	-1.86134100	-1.17448900
O	3.81092000	-1.85069000	0.71190300
H	4.46706300	-1.85934400	-0.00868900
H	1.42628200	-4.46854100	-0.96506000
C	4.31921700	4.84720600	-0.30606400
H	4.74093000	5.62429600	0.34329800
H	5.00139100	4.71932200	-1.15660600
H	3.36689900	5.22455700	-0.70049500

MIN_{1C2}

Charge/multiplicity: 0 1

N	-4.16528500	-0.55422000	-0.54577000
H	-4.48624400	-0.33105800	-1.48048000
C	-2.72943000	-0.76288100	-0.33840400
H	-2.63704000	-1.43606900	0.51821300
C	-2.12056300	-1.41017100	-1.58081500
C	-2.05667300	0.58613800	0.01247500
H	-2.74345200	-2.24659400	-1.90689100
H	-2.06287800	-0.68332300	-2.39547700
O	-1.44702200	1.26222900	-0.82565800
N	-2.23103200	0.96461900	1.29374600
H	-2.87388800	0.41300600	1.85623100
C	-1.79912800	2.26490100	1.78274200
H	-2.30507400	3.08317100	1.25595100
H	-2.03257900	2.32946800	2.84718300
H	-0.71952800	2.38569000	1.64974500
C	-5.05511000	-0.55263700	0.47744800
C	-6.50628700	-0.35269500	0.10430000
H	-7.08583000	-1.20328000	0.47890200
H	-6.88089000	0.54640900	0.60560200
H	-6.66755900	-0.25623300	-0.97291900
O	-4.70190200	-0.71183200	1.65658600
C	4.60317700	-1.76705600	0.02044800
H	5.54863900	-1.77439600	-0.52392200
C	3.86964600	-2.89750500	0.01995200
H	-0.68139500	-3.05352400	-0.54205800
C	2.57003100	-3.04394100	0.67325800
H	2.22080400	-2.20144700	1.29798000
C	4.26432200	-0.43107500	0.63952200
H	3.64556500	-0.56415600	1.53217400
C	3.49974900	0.45664300	-0.36022200
H	2.59178400	-0.08220300	-0.65935600
H	4.10588700	0.57485700	-1.27098000
C	3.12210600	1.83101200	0.20728300
H	2.63368700	1.69392200	1.18339800
H	4.03138300	2.41615000	0.39778500
C	2.17977100	2.60836900	-0.72025700
H	1.26314800	2.02060100	-0.87097800
H	2.64364700	2.71545800	-1.71250500
C	1.79819900	3.99559000	-0.18896500
H	1.40311600	3.89562400	0.83260500
H	2.70015600	4.61947200	-0.10747600
O	1.86958200	-4.04677900	0.55605300
S	-0.39589900	-2.00042700	-1.33880000
O	5.45787300	0.19619800	1.12626300
H	5.99217600	0.45399500	0.35444200
H	4.22351100	-3.77606400	-0.51647200
C	0.75840500	4.70079800	-1.06442900
H	0.50094500	5.68994300	-0.66558900
H	1.12838000	4.84189700	-2.08843900
H	-0.16541500	4.11124100	-1.12366300

With one explicit water molecule

In cyclohexane implicit solvent

Cysteine(H_2O)

Charge/multiplicity: 0 1

N	-1.36117900	0.11210600	0.09351500
H	-1.54642900	-0.22152700	1.04367300

C	0.02021200	0.41722200	-0.24449300
H	0.01039100	0.72708300	-1.29239300
C	0.53664100	1.57029000	0.63544500
C	0.88233100	-0.84346500	-0.05735100
H	-0.16129300	2.40895800	0.57976400
H	0.59382200	1.24955400	1.67947700
S	2.23328000	2.15236700	0.21211000
O	0.99379300	-1.39948600	1.04515800
H	1.90576200	2.75030100	-0.95453700
N	1.48948600	-1.31938000	-1.15964100
H	1.41234400	-0.79569800	-2.02021300
C	2.35899500	-2.48585900	-1.12622600
H	2.59074600	-2.77886800	-2.15211500
H	3.29226700	-2.27085900	-0.59324100
H	1.85558700	-3.31373800	-0.61985400
C	-2.37438900	0.26222600	-0.80927200
C	-3.75742300	-0.08485200	-0.28597900
H	-4.40503600	0.79209100	-0.38910200
H	-4.18376100	-0.87822000	-0.90895300
H	-3.76129600	-0.40853000	0.75892400
O	-2.19626800	0.64917600	-1.96297800
O	-1.10467300	-0.91696700	2.78760800
H	-0.25464000	-1.14654100	2.34506700
H	-1.52012000	-1.77612700	2.96156200

MIN_{1t}

Charge/multiplicity: 0 1

N	-3.13716400	-0.75649800	-0.59771100
H	-2.85560800	-0.01605400	-1.24841800
C	-2.14259900	-1.78097500	-0.27369800
H	-2.68748000	-2.66339700	0.07360100
C	-1.34543700	-2.11909800	-1.53453700
C	-1.24016300	-1.27951500	0.87506500
H	-2.04481000	-2.39969500	-2.32704400
H	-0.77652900	-1.25030400	-1.87200600
O	-0.06686300	-0.91947100	0.67525900
N	-1.84076700	-1.24248600	2.07459200
H	-2.83615400	-1.46474200	2.09237900
C	-1.19136800	-0.71278900	3.26513000
H	-0.85315200	0.31723400	3.11138600
H	-1.90813400	-0.73737400	4.08815300
H	-0.32124200	-1.32101100	3.53491700
C	-4.29108200	-0.63071600	0.10531700
C	-5.23597300	0.45014500	-0.38222000
H	-4.78450800	1.09793900	-1.13872800
H	-6.12867100	-0.02315600	-0.80666000
H	-5.56027300	1.05455000	0.47024300
O	-4.57181400	-1.35753600	1.06808100
C	0.66379800	2.58171600	0.10607500
H	-0.03684700	1.89218100	-0.36556300
C	0.43826500	3.90735100	0.03949000
H	0.65393200	-2.94521100	-0.52073200
C	-0.71521300	4.50904100	-0.63092700
H	-0.77581300	5.61188800	-0.55302900
C	1.83748500	1.95075900	0.81169100
H	2.43813300	2.74136800	1.27883700
C	2.72207600	1.16451100	-0.17480400
H	3.02166500	1.83429000	-0.99339600
H	2.11468000	0.36711500	-0.62532500
C	3.96547300	0.56056200	0.49082600
H	4.58345000	1.37098600	0.90531600

H	3.64865600	-0.05108000	1.34436200
C	4.81188500	-0.28646100	-0.46782400
H	5.11700000	0.32695900	-1.32917100
H	4.19287400	-1.09839400	-0.87747000
C	6.06061900	-0.88757600	0.19055400
H	6.68379200	-0.07663400	0.59401200
H	5.75660000	-1.49615800	1.05400900
O	-1.59705900	3.91998000	-1.25190300
S	-0.21240300	-3.55705700	-1.35415400
O	1.36894400	1.14275400	1.88701500
H	0.90935900	0.35963600	1.50668900
H	1.12466400	4.60618800	0.51465600
C	6.89552200	-1.74301600	-0.76654800
H	7.78044300	-2.15537100	-0.26714300
H	6.31242400	-2.58621900	-1.15796200
H	7.24324100	-1.15555800	-1.62591800
O	-2.03603200	1.33408700	-2.19151000
H	-1.88388500	2.22279300	-1.79995200
H	-2.06097400	1.48088200	-3.14882700

TS_{1t}

Charge/multiplicity: 0 1

N	-2.05385700	-0.86583300	0.95323800
H	-1.40432400	-0.26127600	1.48443000
C	-2.56993100	-0.42540100	-0.34135900
H	-3.61252600	-0.76351800	-0.37727900
C	-2.63307300	1.10843900	-0.43959900
C	-1.82830800	-1.14638100	-1.49725900
H	-3.43448100	1.37894000	-1.13392300
H	-2.90121600	1.50600400	0.54287300
O	-0.93295000	-0.62387100	-2.16259900
N	-2.25610500	-2.41587300	-1.68390200
H	-2.84835000	-2.80493100	-0.94891800
C	-1.58640000	-3.31120100	-2.61149500
H	-2.19255200	-4.21258300	-2.72835700
H	-1.47666600	-2.82553200	-3.58476700
H	-0.58666400	-3.59757100	-2.25885600
C	-2.52541100	-1.99823000	1.53294100
C	-2.01203900	-2.28776200	2.92875500
H	-1.44667700	-3.22634100	2.91157800
H	-1.37952800	-1.48950800	3.32335200
H	-2.87002000	-2.43992500	3.59201100
O	-3.32409200	-2.75927400	0.96430500
C	0.38324500	1.55228200	-0.08010200
H	0.18888000	0.49181400	0.08329200
C	0.59326300	2.29271900	1.20095000
H	-1.42124000	3.35252300	-0.17498700
C	0.29634400	1.66311000	2.43184400
H	0.71781100	2.16720400	3.32681200
C	1.50448700	1.70591100	-1.11362600
H	1.21123500	1.14411900	-2.01064700
C	2.86612500	1.18291800	-0.63109800
H	3.18902600	1.76613900	0.23921300
H	3.59066200	1.39051900	-1.43390800
C	2.89443800	-0.31704800	-0.30549400
H	2.24906100	-0.51674100	0.56050600
H	2.46719100	-0.88416700	-1.14526200

C	4.30669500	-0.83741800	-0.00626800
H	4.73707800	-0.26309000	0.82760800
H	4.95656800	-0.64798500	-0.87387900
C	4.34583500	-2.33206800	0.33716900
H	3.69778500	-2.52089600	1.20467400
H	3.91474700	-2.90596200	-0.49563000
O	-0.41486600	0.64889000	2.62110200
S	-1.20355900	2.08404100	-1.10448200
O	1.56779100	3.10921800	-1.41742700
H	2.15881100	3.21709700	-2.17958200
H	1.41867400	3.00386300	1.21183300
C	5.75701800	-2.84701400	0.63376700
H	5.75064600	-3.91716400	0.87284000
H	6.42277200	-2.70339200	-0.22687800
H	6.20246300	-2.31947500	1.48679000
O	-1.30437100	4.13485900	0.83456800
H	-0.51715300	3.48284800	1.22764800
H	-0.84114100	4.93055600	0.50941200

MIN_2

Charge/multiplicity: 0 1

N	2.94980600	-0.07256400	0.25604400
H	2.33532400	-0.63457400	0.84270200
C	2.50691500	0.23941400	-1.09746100
H	3.41441000	0.48485100	-1.66098100
C	1.83704300	-0.95525600	-1.80612600
C	1.61780800	1.51133000	-1.13023800
H	1.20319900	-0.57595500	-2.60946300
H	2.61392100	-1.58081200	-2.25665700
O	0.42194100	1.48628600	-1.43199000
N	2.28768900	2.64165600	-0.81849000
H	3.26084200	2.54522100	-0.53148600
C	1.62778300	3.93239100	-0.72944800
H	2.38702400	4.71791200	-0.74322400
H	0.95577700	4.06715200	-1.58121300
H	1.03669400	4.02749500	0.19074600
C	4.04327400	0.51363500	0.80855800
C	4.41642500	0.03698700	2.19751800
H	4.64798000	0.90510900	2.82143700
H	3.63187100	-0.55715600	2.67261000
H	5.32708700	-0.56948100	2.12895000
O	4.71327400	1.36611300	0.20969800
C	-0.53693700	-1.26161900	-0.06379000
H	-0.19353900	-0.24876800	0.15218400
C	-0.91750500	-1.97493000	1.23698000
H	-2.28486100	-5.31533400	-0.20245400
C	0.07164200	-1.87393200	2.36420100
H	-0.22787000	-2.42353400	3.28066500
C	-1.68164200	-1.16728200	-1.10001500
H	-1.29704900	-0.56097700	-1.93001600
C	-2.97623300	-0.51863200	-0.59842500
H	-3.44865600	-1.17028900	0.14895900
H	-3.66343300	-0.49702600	-1.45398600
C	-2.81043200	0.90159500	-0.03878600
H	-2.22468400	0.87280100	0.89135100
H	-2.22476300	1.50874500	-0.74085300
C	-4.15507700	1.58552600	0.24247700
H	-4.74614500	0.96434400	0.93233800
H	-4.73593700	1.63870100	-0.69027700
C	-4.01173900	2.99567300	0.82892800
H	-3.43664000	2.94297400	1.76462500
H	-3.41766800	3.61418800	0.14136900

O	1.11135300	-1.23997500	2.35854900
S	0.90858600	-2.18456900	-0.79783400
O	-2.04353900	-2.46652700	-1.60325400
H	-1.22167300	-2.84731200	-1.96636200
H	-1.85016200	-1.54838100	1.63981300
C	-5.35611000	3.67784600	1.09680100
H	-5.21936000	4.68179600	1.51616000
H	-5.94119500	3.78075800	0.17405800
H	-5.96112500	3.10092400	1.80783800
O	-2.72310300	-4.56266800	0.22353900
H	-1.17005000	-3.03458300	1.07971400
H	-2.63985800	-3.84163300	-0.43544200

TS_2

Charge/multiplicity: 0 1

N	-1.59086300	-1.35373200	1.30073900
H	-1.12410200	-0.69590800	1.91865500
C	-2.52828000	-0.83897400	0.32342000
H	-3.49599800	-1.33121200	0.49599100
C	-2.76144300	0.67520200	0.53484600
C	-2.07865900	-1.17913000	-1.11687200
H	-3.72860500	0.93894200	0.09518500
H	-2.83362300	0.86844300	1.60896800
O	-0.89956100	-1.20226000	-1.45617600
N	-3.10370300	-1.37485800	-1.98664800
H	-4.02512600	-1.54737200	-1.60809100
C	-2.86759100	-1.72233100	-3.37749700
H	-3.78277600	-1.54771200	-3.94915400
H	-2.07045700	-1.09046900	-3.77522900
H	-2.56667400	-2.77163700	-3.49392400
C	-1.45005000	-2.69705600	1.47400100
C	-0.44721800	-3.12182100	2.53189900
H	-0.87231400	-3.94208200	3.11709600
H	0.45299500	-3.50236300	2.03529900
H	-0.15645800	-2.30889900	3.20436400
O	-2.08351600	-3.50895400	0.80113900
C	0.09689700	1.43692900	0.20001900
H	0.08458400	0.37294500	0.43567300
C	0.60895900	2.26158600	1.38747600
H	-0.20774800	4.73561500	-0.46242200
C	0.08737000	1.86782600	2.73857300
H	0.32806700	2.58281500	3.55170500
C	0.94793400	1.59743500	-1.07058400
H	0.46016000	0.99129500	-1.84174200
C	2.41162400	1.14600600	-0.94278400
H	2.94541900	1.81266200	-0.25217800
H	2.87693800	1.30291800	-1.92759600
C	2.60133500	-0.32071400	-0.52915600
H	2.27396500	-0.45831100	0.51112100
H	1.94605500	-0.95958000	-1.13563200
C	4.05480000	-0.79631400	-0.65876300
H	4.71046400	-0.13885800	-0.06765500
H	4.38024800	-0.68879300	-1.70425900
C	4.26188900	-2.24931800	-0.21311500
H	3.94102100	-2.35633600	0.83316000
H	3.60423800	-2.90461800	-0.80121500
O	-0.51937100	0.84508000	3.00802300
S	-1.64747000	1.90461200	-0.26846500
O	0.89245900	2.99110400	-1.44448100
H	1.12614800	3.05368000	-2.38391300
H	1.70537500	2.16867700	1.48218700
C	5.71127300	-2.72363600	-0.35142900

H	5.82484400	-3.76352400	-0.02270200
H	6.05143900	-2.66674600	-1.39319300
H	6.39161800	-2.10897200	0.25185900
O	0.29203100	5.38638500	0.05809800
H	0.43284900	3.33575200	1.24330800
H	1.19953900	5.14100300	-0.18190100

MIN_3

Charge/multiplicity: 0 1

N	4.14563600	-0.47030400	-0.14205700
H	4.37038700	-1.34156900	0.32066300
C	2.73235600	-0.15901900	-0.38244500
H	2.70867400	0.49040900	-1.26180600
C	1.96673200	-1.45297400	-0.67014400
C	2.15218800	0.61948700	0.82454500
H	2.53963000	-2.04931900	-1.38620700
H	1.84550800	-2.03709700	0.24673000
O	1.43646300	0.08851400	1.67693100
N	2.53089700	1.91572100	0.86424200
H	3.24440000	2.20935000	0.20050600
C	2.19306100	2.78270800	1.98016000
H	1.13204400	2.67925700	2.22161200
H	2.77332300	2.54033200	2.88002700
H	2.39588000	3.81765700	1.69557300
C	5.14383200	0.41983500	-0.40204100
C	6.55479900	-0.06722200	-0.14165500
H	7.12590900	-0.00450900	-1.07364500
H	7.03529500	0.60064900	0.58051800
H	6.60125900	-1.09358900	0.23417600
O	4.91495600	1.55320300	-0.83369700
C	-0.82282400	-1.50258400	0.02259700
H	-0.28853500	-1.10554500	0.89137400
C	-1.05617000	-3.01593500	0.23956600
H	-1.61120400	-3.18979800	1.16513000
C	-1.78530100	-3.70679500	-0.88734600
H	-1.36747400	-3.55242400	-1.90235200
C	-2.14992800	-0.71245700	-0.13145200
H	-2.68658800	-1.06092700	-1.02316600
C	-1.97522100	0.80940600	-0.20520100
H	-1.32193300	1.05432800	-1.04951800
H	-1.44012000	1.14123900	0.69828900
C	-3.30133900	1.56983900	-0.34123300
H	-3.82009300	1.22963500	-1.24968300
H	-3.95926300	1.31321200	0.49818600
C	-3.11261200	3.09078700	-0.40413600
H	-2.45772900	3.34378700	-1.25132000
H	-2.58364000	3.42984400	0.49948800
C	-4.43065200	3.86508800	-0.53548800
H	-4.95968300	3.52896900	-1.43859900
H	-5.08435500	3.61267400	0.31150200
O	-2.76346900	-4.41886100	-0.74293100
S	0.30828500	-1.17848800	-1.42317400
O	-3.02637800	-1.05970800	0.95665800
H	-2.63648900	-0.69960400	1.77250800
H	-0.07702000	-3.50805600	0.33488300
C	-4.23610500	5.38269500	-0.59448000
H	-5.19535800	5.90603400	-0.68559300
H	-3.73938300	5.75594300	0.31024000
H	-3.61752100	5.67215400	-1.45350600
O	-3.85815300	-3.72075600	1.90764700
H	-3.80961600	-2.80165800	1.58778600

H	-3.64884900	-4.21978800	1.09734800

TS_3

Charge/multiplicity: 0 1

N	4.15065400	-0.44791300	-0.14648500
H	4.37506000	-1.31515800	0.32531600
C	2.73742900	-0.13890400	-0.38882600
H	2.71322900	0.50981400	-1.26862500
C	1.97410400	-1.43392300	-0.67738500
C	2.15422800	0.63812800	0.81723800
H	2.54663700	-2.02742300	-1.39604700
H	1.85665000	-2.02008600	0.23867700
O	1.44482900	0.10416700	1.67305900
N	2.52438100	1.93720100	0.85369400
H	3.23453600	2.23426900	0.18836900
C	2.18538600	2.80369500	1.96963600
H	2.77455700	2.57013900	2.86607600
H	2.37491200	3.84004700	1.68096300
H	1.12730500	2.68915700	2.21859600
C	5.15108400	0.44366100	-0.40315600
C	6.55487300	-0.06082700	-0.12689200
H	6.66976900	-0.33327600	0.92911400
H	6.77854200	-0.94941700	-0.72826600
H	7.26933500	0.72674300	-0.37022400
O	4.92185700	1.57485400	-0.83762600
C	-0.81218000	-1.49931500	0.02368800
H	-0.28029200	-1.09833600	0.89217600
C	-1.03025800	-3.01515400	0.23857400
H	-1.58215400	-3.19594600	1.16467900
C	-1.75404600	-3.71191500	-0.88818800
H	-1.34060400	-3.55042200	-1.90385100
C	-2.14729800	-0.72222800	-0.12774200
H	-2.68004600	-1.07369600	-1.02064200
C	-1.98812900	0.80152100	-0.19711900
H	-1.33286100	1.05532700	-1.03726700
H	-1.46146000	1.13676900	0.71008700
C	-3.32150300	1.54806000	-0.33866200
H	-3.83071300	1.20535700	-1.25155500
H	-3.98176900	1.28127600	0.49575700
C	-3.14902900	3.07119200	-0.39531600
H	-2.48988300	3.33393400	-1.23621900
H	-2.63148000	3.41333600	0.51372100
C	-4.47435200	3.83137000	-0.53568900
H	-4.99198700	3.49185400	-1.44409500
H	-5.13234700	3.56958600	0.30511900
O	-2.72335300	-4.43582300	-0.74287100
S	0.31239000	-1.16125100	-1.42393700
O	-3.02050300	-1.08134000	0.95911100
H	-2.63489600	-0.71889500	1.77594900
H	-0.04616300	-3.49777900	0.33191300
C	-4.29587600	5.35116200	-0.58907700
H	-5.25998900	5.86435900	-0.68639700
H	-3.81042400	5.72725800	0.32056800
H	-3.67367500	5.64971000	-1.44236300
O	-3.82245500	-3.75201500	1.90916800
H	-3.78439500	-2.83252400	1.58903700
H	-3.60847500	-4.24884200	1.09873800

MIN_4

Charge/multiplicity: 0 1

N	3.89166300	-0.69156100	-0.43727900
H	4.30085500	-0.53898400	-1.35008900
C	2.54177100	-0.16924900	-0.18933900
H	2.48134300	0.01872900	0.88585700
C	2.34768400	1.13612700	-0.96641300
C	1.49871300	-1.24845000	-0.57664800
H	3.28502300	1.70123500	-0.93320800
H	2.11404300	0.92228700	-2.01343700
O	0.86647500	-1.19969900	-1.63300600
N	1.38736700	-2.23606600	0.34338900
H	2.07330500	-2.23180800	1.09617800
C	0.59429900	-3.43384800	0.12808900
H	-0.11640400	-3.24058600	-0.67629900
H	1.22371100	-4.28719100	-0.15644200
H	0.04794700	-3.69145400	1.04088000
C	4.55348800	-1.46719600	0.46543700
C	5.95344700	-1.89543200	0.07331200
H	6.63203600	-1.67543200	0.90278800
H	5.96684400	-2.97997600	-0.08119300
H	6.32320400	-1.40351500	-0.83127400
O	4.04571300	-1.80371400	1.53902300
C	-0.52195600	1.70072200	-0.95740800
H	-0.25222200	1.07011300	-1.80778800
C	-1.37127400	2.88858400	-1.46096000
H	-2.25754000	2.49731900	-1.97220700
C	-1.81620900	3.84055900	-0.36563300
H	-2.90765400	3.99459300	-0.26497300
C	-1.32999000	0.85238500	0.06464800
H	-0.62499500	0.24018400	0.64421300
C	-2.31886700	-0.09226000	-0.63216900
H	-1.76046700	-0.70023000	-1.35421600
H	-3.04737100	0.50197700	-1.20081200
C	-3.06687500	-1.00199800	0.35088400
H	-2.33535600	-1.59635700	0.91922800
H	-3.59093300	-0.37743800	1.08399400
C	-4.06204400	-1.94703100	-0.33433300
H	-3.53104300	-2.56940700	-1.07062300
H	-4.79119300	-1.35535300	-0.90814300
C	-4.81375800	-2.85620800	0.64657800
H	-4.08670500	-3.44564000	1.22369000
H	-5.34832500	-2.23381800	1.37804600
O	-1.03975100	4.48688500	0.32108200
S	1.11445000	2.32933000	-0.30403000
O	-2.07477900	1.69102200	0.94223100
H	-1.47786000	2.04752700	1.64463600
H	-0.79290800	3.46755000	-2.19097900
C	-5.80436800	-3.80129700	-0.03941200
H	-6.32316400	-4.43614900	0.68893200
H	-6.56812300	-3.24275400	-0.59536500
H	-5.29558200	-4.46238300	-0.75267800
O	-0.34196600	3.02818700	2.65058700
H	-0.56107700	3.83632100	2.14807700
H	0.48630400	2.74085600	2.22579500

TS_4

Charge/multiplicity: 0 1

N	3.82709400	-1.08766400	0.37190400
H	3.84001000	-1.55686800	1.26815300
C	2.52368500	-0.72459000	-0.19795800

H	2.65301400	-0.73218800	-1.28405700
C	1.47837700	-1.76478200	0.21011700
C	2.13738700	0.71038400	0.23990300
H	1.89760900	-2.76416100	0.06031300
H	1.22726900	-1.65250000	1.26866500
O	1.29500600	0.94072100	1.11048500
N	2.83766500	1.67483400	-0.39677500
H	3.60211900	1.37377400	-0.99712100
C	2.71105000	3.07766600	-0.04178600
H	3.00971600	3.26156600	0.99762700
H	3.35059900	3.66393700	-0.70513600
H	1.67585100	3.41232500	-0.16130100
C	5.00673600	-0.74222400	-0.21208200
C	6.26143700	-1.25194200	0.46830500
H	6.80651000	-1.89212800	-0.23328400
H	6.90927400	-0.40214300	0.70561200
H	6.06391000	-1.81851300	1.38311200
O	5.05673100	-0.06268500	-1.24182500
C	-1.26424600	-1.00144300	0.48333000
H	-0.74699800	-0.16236300	0.95078200
C	-1.72246600	-2.01966800	1.54561600
H	-2.04486600	-1.47390800	2.44145100
C	-2.90096600	-2.79650100	0.97452800
H	-3.74490300	-2.92145700	1.67668800
C	-2.56156400	-0.52871100	-0.22528100
H	-2.43771100	-0.52529100	-1.31527400
C	-3.04916700	0.84928000	0.23429500
H	-3.10297100	0.85827600	1.33194200
H	-4.07837000	0.97034800	-0.12845800
C	-2.19041600	2.01962400	-0.26351000
H	-1.16105800	1.91457800	0.10372100
H	-2.13196900	1.98436800	-1.36138000
C	-2.74583000	3.38328900	0.17015500
H	-2.80675700	3.41823500	1.26806600
H	-3.77810600	3.49041200	-0.19570400
C	-1.91060400	4.57045400	-0.32548600
H	-0.88140100	4.46797800	0.04726400
H	-1.84371300	4.53406600	-1.42221400
O	-2.65164400	-3.78185200	0.16519200
S	-0.07311300	-1.66557300	-0.77306300
O	-3.59024000	-1.49998900	0.10414000
H	-3.98056600	-2.11943100	-0.82775800
H	-0.92628300	-2.71054800	1.83516400
C	-2.47396900	5.92753400	0.10543100
H	-1.85464700	6.75388200	-0.26357800
H	-3.49040100	6.07749500	-0.28042300
H	-2.52065500	6.01056900	1.19870600
O	-4.14244000	-3.10456600	-1.57652800
H	-3.47256100	-3.67079200	-0.83147900
H	-5.05144500	-3.43379600	-1.47216400

P(R)

Charge/multiplicity: 0 1

N	-4.54944000	0.35497600	0.24692900
H	-4.63701800	0.85527600	1.12187100
C	-3.20086900	0.07255000	-0.25566700
H	-3.29042900	-0.00257100	-1.34284500
C	-2.26702500	1.22768900	0.11333500
C	-2.70218000	-1.28563500	0.29815500
H	-2.75752300	2.17423000	-0.13103800
H	-2.04759300	1.21421700	1.18443600
O	-1.89449500	-1.36381400	1.22555500

N	-3.25706300	-2.35509800	-0.31467000
H	-4.02188400	-2.17097100	-0.96043000
C	-3.01217700	-3.71574300	0.13127100
H	-1.95883800	-3.82588900	0.39864500
H	-3.61854900	-3.97843500	1.00838600
H	-3.25098700	-4.40499900	-0.68239500
C	-5.66865900	-0.14602300	-0.34729600
C	-6.99095600	0.26818000	0.26570200
H	-7.60551100	0.73638700	-0.50983000
H	-7.52254700	-0.62642300	0.60645900
H	-6.88716600	0.96348700	1.10399800
O	-5.61084000	-0.88785700	-1.33177500
C	0.54074800	0.57650000	0.44852200
H	0.16119200	-0.37682900	0.81519900
C	0.82398400	1.58142800	1.57519300
H	1.25481100	1.04593900	2.42966000
C	1.88074200	2.50544000	0.96544200
H	2.57023700	2.93838300	1.69296800
C	1.92358000	0.44946500	-0.23364800
H	1.83621400	0.41432900	-1.32727200
C	2.71287000	-0.77395600	0.24154400
H	2.13749800	-1.67006500	-0.03005200
H	2.77405600	-0.75727900	1.33875300
C	4.12235800	-0.86099500	-0.35690700
H	4.04791500	-0.87814900	-1.45444400
H	4.67751100	0.04940000	-0.09892300
C	4.90370200	-2.09213900	0.11926000
H	4.34074500	-3.00355000	-0.13261100
H	4.97767000	-2.07424600	1.21694600
C	6.31337800	-2.18753100	-0.47868500
H	6.24053700	-2.20821200	-1.57538600
H	6.87472400	-1.27625600	-0.22826100
O	1.33402500	3.61442200	0.27894100
S	-0.67718300	1.19529600	-0.81452600
O	2.64035400	1.66285000	0.10331900
H	-0.05106400	2.13084200	1.92986400
H	0.64647700	3.27482100	-0.32723100
C	7.09248500	-3.41444500	0.00313000
H	8.09351800	-3.45290000	-0.44272900
H	7.21561600	-3.40542700	1.09363000
H	6.57499300	-4.34503300	-0.26270700
O	3.90229000	4.08609700	-1.04808700
H	3.89701300	3.11935100	-0.95784000
H	3.00626400	4.29439300	-0.72995800

TS_3’

Charge/multiplicity: 0 1

N	4.12308000	-0.60086700	0.61066700
H	4.11157600	-0.89599400	1.57840800
C	2.84545400	-0.54353200	-0.10954000
H	3.08269200	-0.69948200	-1.16512300
C	1.92340400	-1.66158100	0.38605900
C	2.22119400	0.86309400	0.06213300
H	2.50334400	-2.58690600	0.45503000
H	1.53953600	-1.42231000	1.38254600
O	1.32980600	1.09687800	0.88174300
N	2.77058500	1.80195200	-0.74011300
H	3.61290100	1.53762000	-1.24586600
C	2.41107300	3.20612900	-0.64185500

H	1.32613000	3.30061200	-0.55423700
H	2.86890200	3.68975800	0.23133200
H	2.74435900	3.72053000	-1.54636800
C	5.28743400	-0.14805600	0.06798600
C	6.52823800	-0.31006200	0.92348800
H	7.26246300	-0.90317200	0.36869600
H	6.97170900	0.67536500	1.09981000
H	6.33728000	-0.79338100	1.88629700
O	5.33494900	0.35623000	-1.05734100
C	-0.88592500	-1.10435500	0.09518000
H	-0.42717200	-0.19624200	0.49193900
C	-1.49035000	-1.91127400	1.26209600
H	-2.18467700	-1.29141000	1.84104200
C	-2.21142600	-3.17860400	0.86486500
H	-1.62824600	-3.89478300	0.25872500
C	-1.93745700	-0.73556500	-0.97532100
H	-1.40120100	-0.29220200	-1.82559200
C	-2.97330900	0.29431000	-0.49063700
H	-3.44271700	-0.05017100	0.44144900
H	-3.77155400	0.32258300	-1.24530500
C	-2.42115900	1.71464600	-0.30234900
H	-1.59344200	1.71196800	0.41905500
H	-1.99200200	2.05837300	-1.25474800
C	-3.48974400	2.71377500	0.16107600
H	-3.91136800	2.37705800	1.12008300
H	-4.32505400	2.71397600	-0.55497500
C	-2.95867200	4.14429500	0.31909000
H	-2.11830600	4.14203400	1.02786800
H	-2.54651900	4.48499900	-0.64153200
O	-3.33644900	-3.46147600	1.24894500
S	0.50819800	-2.02143000	-0.73564000
O	-2.54863000	-1.93880000	-1.43884100
H	-3.51050500	-1.93932600	-1.23468200
H	-0.67854500	-2.20321300	1.94436600
C	-4.02454000	5.13500300	0.79547600
H	-3.61436100	6.14699900	0.89589400
H	-4.86458100	5.18601900	0.09112800
H	-4.43061300	4.84340500	1.77241700
O	-5.18341000	-2.45232000	-0.59855600
H	-5.12431400	-2.10812700	0.30837700
H	-4.89795800	-3.37272600	-0.46375200

MIN_4’
Charge/multiplicity: 0 1

N	-3.99792700	-0.82027900	-0.55481200
H	-3.97767600	-1.21178700	-1.48747300
C	-2.72216800	-0.64279200	0.14883200
H	-2.95213500	-0.70214600	1.21603600
C	-1.75776800	-1.76700500	-0.23844700
C	-2.14932500	0.76254100	-0.16124500
H	-2.30259100	-2.71582400	-0.22684700
H	-1.37116900	-1.60374800	-1.24878900
O	-1.24325000	0.94382800	-0.97798300
N	-2.76256900	1.75878000	0.51441900
H	-3.59990500	1.51358200	1.03797000
C	-2.45904500	3.15800300	0.26654000
H	-2.81054000	3.48552400	-0.72050800
H	-2.94534200	3.76296800	1.03507600
H	-1.37922500	3.32134900	0.31454400
C	-5.17930500	-0.37073200	-0.04797600
C	-6.41632400	-0.67700400	-0.86805400
H	-7.09398700	-1.29090000	-0.26551300
H	-6.93706300	0.25934200	-1.09214200
H	-6.20304400	-1.20146000	-1.80424400

O	-5.24417200	0.23912200	1.02316900
C	1.05482600	-1.14815600	-0.00593100
H	0.59493100	-0.29176200	-0.50234500
C	1.66344600	-2.07694800	-1.07245200
H	2.43358700	-1.54812500	-1.64651300
C	2.24396200	-3.37421500	-0.56199700
H	1.60251300	-3.95168300	0.12604900
C	2.12978000	-0.65912900	1.00228400
H	1.61570200	-0.32457800	1.91180300
C	2.95856000	0.52361300	0.46797200
H	3.38630200	0.27182500	-0.51196800
H	3.81198300	0.64046100	1.14934000
C	2.19945600	1.85539200	0.38365700
H	1.32952800	1.76064000	-0.27919000
H	1.79927100	2.10392600	1.37788700
C	3.08356200	3.00995000	-0.10776600
H	3.49341700	2.75836100	-1.09731200
H	3.95012400	3.11618400	0.56163900
C	2.34503600	4.35169900	-0.19559700
H	1.48503600	4.24712200	-0.87234600
H	1.92955000	4.60181800	0.79132900
O	3.30435200	-3.84872800	-0.94713300
S	-0.34224800	-1.95909100	0.92471900
O	2.95886500	-1.75339000	1.39100100
H	3.79787100	-1.71914300	0.87455800
H	0.87624600	-2.35753200	-1.78905000
C	3.23540600	5.50071500	-0.67759900
H	2.67959100	6.44472500	-0.72881500
H	4.08744900	5.65342000	-0.00309200
H	3.63895500	5.29885400	-1.67797700
O	5.21147400	-1.96764500	-0.28440500
H	4.70898700	-2.64258600	-0.78991300
H	5.87230600	-2.48398000	0.20453500

TS_4’

Charge/multiplicity: 0 1

N	3.98521000	-0.97226600	0.51125900
H	3.91874600	-1.42978400	1.41122000
C	2.74121600	-0.67857200	-0.20873200
H	2.99934600	-0.66905500	-1.27137800
C	1.71329900	-1.77765600	0.06727900
C	2.22287100	0.72624200	0.18684800
H	2.19412800	-2.75264700	-0.05479500
H	1.34122000	-1.70085500	1.09303900
O	1.29902800	0.89479200	0.98545400
N	2.90530400	1.73722100	-0.39489800
H	3.74496700	1.49054400	-0.91352300
C	2.65617600	3.12747500	-0.05449700
H	2.91771700	3.34561500	0.98867900
H	3.25641400	3.76063800	-0.71152000
H	1.59889500	3.36888600	-0.19711500
C	5.20201200	-0.54644200	0.07201300
C	6.39599900	-0.97464100	0.90144000
H	6.96545400	-0.08637800	1.19225300
H	6.12551600	-1.53721500	1.79993300
H	7.05195700	-1.59416500	0.28075000
O	5.32994100	0.13544100	-0.94874700
C	-1.08291400	-1.14211900	0.04803100
H	-0.65908600	-0.32053600	0.62741400
C	-1.63633800	-2.25830300	0.93596200
H	-2.21443200	-1.83427300	1.76709100
C	-2.56667100	-3.11638800	0.08953500
H	-2.04911100	-3.66743100	-0.70633700
C	-2.29689300	-0.67464200	-0.80150500

H	-1.98882300	-0.45409800	-1.83037900
C	-3.00303400	0.55904200	-0.22110800
H	-3.21317500	0.39591700	0.84431300
H	-3.97822900	0.65021100	-0.71831300
C	-2.22069400	1.86586100	-0.41288000
H	-1.23917500	1.79623500	0.07450300
H	-2.02232900	2.01290000	-1.48482800
C	-2.97298500	3.08627400	0.13547100
H	-3.17317900	2.93830300	1.20693100
H	-3.95742200	3.15631300	-0.35099500
C	-2.21956100	4.40817700	-0.05811800
H	-1.24010400	4.34131400	0.43659000
H	-2.01301000	4.55477100	-1.12801600
O	-3.56936300	-3.73821900	0.62993700
S	0.27638000	-1.71492200	-1.08230000
O	-3.19820200	-1.80248500	-0.87122400
H	-4.21679000	-1.66738100	-0.25930300
H	-0.84698600	-2.88321200	1.36784300
C	-2.98059200	5.62132200	0.48413400
H	-2.41576200	6.54902400	0.33277700
H	-3.95084200	5.73880300	-0.01509000
H	-3.17320600	5.52205300	1.55991200
O	-5.08289600	-1.89462500	0.60264100
H	-4.46402900	-2.86329200	0.83854300
H	-5.89374100	-2.19015600	0.15435100

P(S)

Charge/multiplicity: 0 1

N	3.85226400	-1.31188300	0.33239500
H	3.77028500	-1.96391800	1.10169400
C	2.61722400	-0.79518300	-0.26718300
H	2.86571800	-0.53977700	-1.30119100
C	1.54129500	-1.88283800	-0.24317500
C	2.17234300	0.49371800	0.46859900
H	1.97768900	-2.81938500	-0.60260600
H	1.18052600	-2.03752900	0.77740000
O	1.25289500	0.50041500	1.28920200
N	2.91862300	1.57522600	0.14375900
H	3.72571400	1.41175300	-0.45418500
C	2.76959900	2.86632200	0.78949700
H	3.63868500	3.09985800	1.41742800
H	2.65589100	3.65907000	0.04178300
H	1.87847300	2.83375200	1.41777100
C	5.08556900	-0.85815100	-0.02434200
C	6.26195400	-1.52380300	0.66138000
H	6.94704800	-1.90146800	-0.10412100
H	6.80656700	-0.77451600	1.24570300
H	5.97424300	-2.34894000	1.31974800
O	5.23954000	0.03831600	-0.85864300
C	-1.23107100	-1.16395400	-0.07126200
H	-0.80085400	-0.47868000	0.66013900
C	-1.80385500	-2.43205300	0.57744700
H	-2.17577100	-2.20124000	1.58425900
C	-3.00158600	-2.78200500	-0.30908500
H	-2.68645000	-3.27972800	-1.23543200
C	-2.46285800	-0.53850600	-0.80279700
H	-2.25833600	-0.44386200	-1.87952600
C	-2.90961700	0.81988500	-0.26063200
H	-3.06749000	0.73475700	0.82366200
H	-3.88841300	1.04531200	-0.70618600
C	-1.93607000	1.96676900	-0.56250000
H	-0.96708700	1.76621300	-0.08708400
H	-1.74788200	2.00824900	-1.64520900
C	-2.46105900	3.32841700	-0.08724500

H	-2.64760100	3.28870400	0.99620300
H	-3.43590700	3.52752600	-0.55720300
C	-1.50829300	4.49117400	-0.39267300
H	-0.53512400	4.29450100	0.07897400
H	-1.31980500	4.53033100	-1.47507800
O	-3.97914200	-3.57771500	0.25218700
S	0.09845400	-1.49304200	-1.31912700
O	-3.54706000	-1.47593900	-0.63972300
H	-4.70454800	-1.16457600	0.87800100
H	-1.08834300	-3.25457400	0.65623600
C	-2.03904000	5.84718000	0.08105300
H	-1.33553500	6.65601500	-0.15026400
H	-2.99433800	6.09126800	-0.40081700
H	-2.20606700	5.85265800	1.16568000
O	-5.05816900	-1.47912800	1.73729700
H	-4.34655500	-3.08762900	1.02259300
H	-6.01792800	-1.52830000	1.59953600

In N-octanol implicit solvent

Cysteine(H_2O)

Charge/multiplicity: 0 1

N	1.34867500	-0.07226000	0.06444800
H	1.52172700	0.31756200	0.99566700
C	-0.02824400	-0.42589600	-0.25644400
H	-0.02931400	-0.76886800	-1.29289900
C	-0.50135000	-1.56253200	0.66705300
C	-0.91362500	0.82006800	-0.10056600
H	0.19855500	-2.39849600	0.59768500
H	-0.51955300	-1.21999000	1.70552600
S	-2.20885100	-2.16435500	0.32451900
O	-1.04337900	1.39115400	0.99844500
H	-1.94362900	-2.72840600	-0.87477000
N	-1.52206000	1.26533100	-1.20783500
H	-1.40015800	0.75540900	-2.07310600
C	-2.39081600	2.43474100	-1.20068700
H	-2.76257000	2.59482500	-2.21388900
H	-3.23982400	2.28481000	-0.52546800
H	-1.84089200	3.32394400	-0.87544500
C	2.38354600	-0.29400400	-0.78552100
C	3.74920000	0.10390300	-0.26419000
H	4.40021100	-0.77717500	-0.27012300
H	4.18820500	0.83983900	-0.94677000
H	3.72357200	0.52193700	0.74598200
O	2.24039700	-0.78376900	-1.91366700
O	1.13307300	1.11890900	2.72705800
H	0.26910300	1.27166700	2.27948400
H	1.55688700	1.99310200	2.70697700

MIN_{1t}

Charge/multiplicity: 0 1

N	-2.98941500	-0.60336600	-0.66252200
H	-2.58444700	0.02481300	-1.37133000
C	-2.19092300	-1.75183900	-0.22953100
H	-2.88541000	-2.51173200	0.13875200
C	-1.40430200	-2.30281600	-1.41912800
C	-1.27405600	-1.31769100	0.93369000

H	-2.10267500	-2.53790700	-2.22690600
H	-0.68859500	-1.56670500	-1.79068700
O	-0.06385300	-1.07617300	0.75697200
N	-1.89133200	-1.19791400	2.11687400
H	-2.90403200	-1.30329300	2.11775800
C	-1.22297400	-0.70375000	3.31338500
H	-0.89309000	0.33333100	3.19034800
H	-1.92507600	-0.76092800	4.14699500
H	-0.34778700	-1.31971500	3.54266700
C	-4.14504900	-0.26755300	-0.04598700
C	-4.87871300	0.92448400	-0.62087900
H	-4.26912900	1.49733200	-1.32447100
H	-5.78015100	0.57290000	-1.13684300
H	-5.19936700	1.57573900	0.19798800
O	-4.59889000	-0.90443100	0.92191800
C	0.57474700	2.43952100	0.18233700
H	-0.10293400	1.70575400	-0.25432800
C	0.27365000	3.74929100	0.11119200
H	0.41137800	-3.34780800	-0.24728400
C	-0.93842200	4.26536200	-0.52540200
H	-1.12577700	5.34410400	-0.37355200
C	1.80023000	1.87783000	0.85268900
H	2.36075000	2.69416700	1.32348000
C	2.70675300	1.16040600	-0.16378900
H	2.93905700	1.85845400	-0.97998700
H	2.13965600	0.33062200	-0.60926600
C	4.00619200	0.63365200	0.45833700
H	4.57874800	1.47946200	0.86720800
H	3.76059000	-0.01382600	1.30982500
C	4.87943000	-0.13987300	-0.53747900
H	5.11348200	0.50470200	-1.39825800
H	4.30603900	-0.98887500	-0.93875100
C	6.18657500	-0.65880300	0.07472100
H	6.76649300	0.19013400	0.46476500
H	5.95292800	-1.29339600	0.94178000
O	-1.74671500	3.61600100	-1.19131500
S	-0.52098600	-3.87903200	-1.06623600
O	1.40553900	1.01830800	1.92776300
H	0.93597100	0.24123100	1.54603400
H	0.92231000	4.49349700	0.56947300
C	7.04567700	-1.44889100	-0.91621700
H	7.97301000	-1.80250600	-0.44881100
H	6.50891700	-2.32828700	-1.29506900
H	7.32424700	-0.83367300	-1.78173500
O	-1.66953500	1.13960100	-2.51081000
H	-1.62323200	1.99852600	-2.03449300
H	-2.18612800	1.33493700	-3.30985800

TS_{1t}

Charge/multiplicity: 0 1

N	-2.00049900	-0.90621100	0.94834800
H	-1.36759800	-0.27552700	1.47384900
C	-2.53090100	-0.48494000	-0.35013600
H	-3.56906600	-0.83448400	-0.37797500
C	-2.62788500	1.04611300	-0.46148800
C	-1.78840800	-1.21463000	-1.49655200
H	-3.43562800	1.28661500	-1.15929500
H	-2.91352800	1.43976200	0.51772300
O	-0.88785900	-0.70070800	-2.17063600
N	-2.20549100	-2.48407800	-1.67906200
H	-2.81631100	-2.87393900	-0.96239900
C	-1.53043900	-3.37902300	-2.60621700
H	-2.06936900	-4.32830800	-2.62680600
H	-1.52623700	-2.95211700	-3.61379700

H	-0.49090900	-3.56482200	-2.30786100
C	-2.45803300	-2.02562100	1.55178700
C	-1.92458500	-2.30514100	2.93950900
H	-1.35047000	-3.23863100	2.91622700
H	-1.29188500	-1.50198300	3.32280100
H	-2.77157800	-2.45983800	3.61663700
O	-3.26835200	-2.80157600	1.00763400
C	0.37134100	1.57564500	-0.10435000
H	0.19921900	0.51211300	0.06240100
C	0.57517500	2.30850100	1.17429900
H	-1.53116200	3.37610400	-0.13816600
C	0.23576200	1.74582800	2.40491800
H	0.60517400	2.30191600	3.29081100
C	1.49776000	1.73770200	-1.13244600
H	1.22226500	1.16735200	-2.02950800
C	2.85895600	1.22967100	-0.63336600
H	3.16970900	1.82425000	0.23445500
H	3.58614300	1.43378400	-1.43376400
C	2.89292600	-0.26582900	-0.28963400
H	2.25141500	-0.45793200	0.58131500
H	2.46445400	-0.84376400	-1.12189100
C	4.30803100	-0.77712100	0.01038500
H	4.73939300	-0.18951000	0.83478500
H	4.95296800	-0.59755900	-0.86301700
C	4.35426700	-2.26622600	0.37490700
H	3.70901200	-2.44575800	1.24685000
H	3.92470400	-2.85417100	-0.44912800
O	-0.45749600	0.70450400	2.62661600
S	-1.23055200	2.06968100	-1.12265300
O	1.55798200	3.13646300	-1.45542600
H	2.16356700	3.23541400	-2.20891500
H	1.29227600	3.12702400	1.17665600
C	5.76821400	-2.77031700	0.67619400
H	5.76732100	-3.83756200	0.92994800
H	6.43190900	-2.63526800	-0.18780200
H	6.21236200	-2.22880500	1.52154300
O	-1.51448000	4.10404400	0.82651400
H	-0.72977300	3.59969700	1.27694900
H	-1.14905600	4.96357900	0.53034400

MIN_2

Charge/multiplicity: 0 1

N	2.97187800	-0.10540800	0.24649400
H	2.34576700	-0.64313800	0.84405700
C	2.51646600	0.21264800	-1.10202200
H	3.41784200	0.44322300	-1.68100800
C	1.83050200	-0.97707600	-1.80215200
C	1.65549200	1.50121300	-1.13211400
H	1.20586800	-0.59814100	-2.61274800
H	2.60305800	-1.61135100	-2.24758900
O	0.48070300	1.52023600	-1.52366200
N	2.30561500	2.60476500	-0.71936800
H	3.28108500	2.51142800	-0.44520300
C	1.66055200	3.90765300	-0.66958400
H	2.37506300	4.63290700	-0.27581300
H	1.34048900	4.22929000	-1.66730100
H	0.78001400	3.88565400	-0.01794800
C	4.09634100	0.42322700	0.78171000
C	4.46247000	-0.04969500	2.17050300
H	4.66772300	0.82177300	2.80041200
H	3.68594900	-0.66118700	2.63613800
H	5.38716100	-0.63539000	2.10828900
O	4.80540600	1.24023100	0.16686700

C	-0.55500100	-1.25864300	-0.06767400
H	-0.20861700	-0.24553000	0.14567000
C	-0.93994100	-1.95336700	1.24119800
H	-2.66359800	-3.86840800	-0.44366700
C	0.04450700	-1.84150800	2.36917000
H	-0.24650900	-2.39340700	3.28452800
C	-1.70431200	-1.17046000	-1.09847000
H	-1.32083000	-0.60035900	-1.95419700
C	-2.98271300	-0.48472500	-0.60196800
H	-3.45907100	-1.11133900	0.16437000
H	-3.67632400	-0.46658200	-1.45292500
C	-2.79120100	0.94196300	-0.07008800
H	-2.17686000	0.92268100	0.84099000
H	-2.22951100	1.53649600	-0.80299900
C	-4.12279700	1.63773900	0.24084100
H	-4.69153700	1.03255800	0.96309700
H	-4.73383800	1.67580300	-0.67333000
C	-3.95406100	3.05784900	0.79497900
H	-3.34734700	3.02044800	1.71138600
H	-3.38297700	3.66146300	0.07503900
O	1.07588900	-1.18909700	2.36214100
S	0.88969300	-2.19185600	-0.78855300
O	-2.10256900	-2.47446700	-1.56228700
H	-1.31453600	-2.88516100	-1.96528800
H	-1.86847300	-1.51581800	1.64155100
C	-5.28603100	3.74999500	1.09595000
H	-5.13124500	4.76186700	1.49023000
H	-5.90270900	3.83682300	0.19194500
H	-5.86731600	3.18957000	1.83976300
O	-2.85970200	-4.62197000	0.15460100
H	-1.18670600	-3.01490600	1.09990900
H	-3.63902300	-4.31741300	0.64665500

TS_2

Charge/multiplicity: 0 1

N	2.25193500	0.22323800	1.05175900
H	1.48925100	-0.13071800	1.62772000
C	2.65378400	-0.56980200	-0.11206600
H	3.74211100	-0.68352600	-0.04671400
C	2.11180800	-2.00773300	-0.02181500
C	2.35708100	0.20996800	-1.41357000
H	2.72255000	-2.63387300	-0.68069500
H	2.29224200	-2.34936600	1.00151900
O	1.26051700	0.20766800	-1.98156200
N	3.41259800	0.92023600	-1.87289700
H	4.16865000	1.08471100	-1.21546100
C	3.27316600	1.82757900	-3.00213900
H	4.25605800	2.23782400	-3.24263600
H	2.89146200	1.28769100	-3.87332300
H	2.58495300	2.65340500	-2.78049400
C	3.06251300	1.18796200	1.55268800
C	2.60216500	1.84244900	2.83668900
H	2.33408900	2.88468400	2.62792900
H	1.74422900	1.34035700	3.29139300
H	3.43504200	1.85298600	3.54701400
O	4.11261400	1.53381700	0.98856200
C	-0.81177700	-1.23551100	0.08309600
H	-0.24898200	-0.32355300	0.28608700
C	-1.54286400	-1.70960200	1.34180800
H	-2.57908000	-4.93780500	-0.14682600
C	-0.74336100	-1.73419600	2.60737000
H	-1.23330300	-2.24979000	3.45577000
C	-1.75530200	-0.92822200	-1.10395300

H	-1.12352900	-0.54285600	-1.90894000
C	-2.85668300	0.09522000	-0.81299000
H	-3.56960400	-0.31728100	-0.08634500
H	-3.41597600	0.22398900	-1.74892400
C	-2.34161000	1.45993300	-0.33538100
H	-1.86264200	1.35703000	0.64841700
H	-1.55856700	1.81338200	-1.02184400
C	-3.45283600	2.51358200	-0.24093900
H	-4.23999500	2.15218400	0.43782300
H	-3.92842700	2.62874200	-1.22622400
C	-2.95697300	3.88183900	0.24332100
H	-2.47950600	3.76724700	1.22727100
H	-2.17253300	4.24393400	-0.43670000
O	0.34807500	-1.21079800	2.77935300
S	0.40488300	-2.51353900	-0.51984600
O	-2.41269300	-2.12693300	-1.57885800
H	-1.81063300	-2.56721900	-2.20218700
H	-2.39046300	-1.04173400	1.57491700
C	-4.07104200	4.92782800	0.33788700
H	-3.68471700	5.89387700	0.68549200
H	-4.54648500	5.09231400	-0.63776400
H	-4.85506000	4.61221700	1.03840100
O	-3.33084100	-4.33589700	-0.02404000
H	-2.00414100	-2.69509900	1.20061200
H	-3.07663900	-3.55208500	-0.55746500

MIN_3

Charge/multiplicity: 0 1

N	4.13793500	-0.52855400	-0.00942800
H	4.30921300	-1.35439800	0.55215000
C	2.75164800	-0.20441100	-0.35681000
H	2.79219700	0.35670300	-1.29415800
C	1.96111500	-1.49756700	-0.56643400
C	2.14395300	0.70489700	0.73522100
H	2.53265600	-2.15353900	-1.22862100
H	1.80856600	-2.02015700	0.38191300
O	1.40742900	0.27392300	1.63312800
N	2.51708900	1.99573300	0.64599700
H	3.23874200	2.22728700	-0.03184300
C	2.15238500	2.97405100	1.65958300
H	1.06455500	3.02211800	1.76947100
H	2.58669300	2.72604800	2.63589000
H	2.51978100	3.95268600	1.34523500
C	5.17771000	0.28293700	-0.32616200
C	6.55194900	-0.20198900	0.07498700
H	7.18753300	-0.23540300	-0.81627800
H	6.99538100	0.52144900	0.76795600
H	6.54203800	-1.18887800	0.54550100
O	5.01347800	1.36248200	-0.91538200
C	-0.84165300	-1.52515600	0.05759900
H	-0.32625600	-1.13260000	0.93859800
C	-1.08918100	-3.03585800	0.27917400
H	-1.65806600	-3.19603700	1.19804400
C	-1.79490900	-3.72823600	-0.85507400
H	-1.34934800	-3.60070200	-1.85942000
C	-2.15690900	-0.72179400	-0.11970100
H	-2.68484500	-1.06638500	-1.01797300
C	-1.95620500	0.79675100	-0.19299800
H	-1.31342000	1.02943700	-1.04896100
H	-1.40343800	1.11639300	0.70355400
C	-3.26768300	1.58442700	-0.31077600
H	-3.81408200	1.24641400	-1.20398500

H	-3.91214900	1.35649000	0.54763200
C	-3.04461400	3.09959000	-0.39433600
H	-2.41209100	3.32885400	-1.26508000
H	-2.47881000	3.43227000	0.48924900
C	-4.34669700	3.90475100	-0.48961900
H	-4.91271000	3.57637600	-1.37336000
H	-4.97857100	3.67471100	0.38036500
O	-2.79187900	-4.42488200	-0.72889300
S	0.32285900	-1.21994100	-1.36376900
O	-3.05174300	-1.05281500	0.96016000
H	-2.66300900	-0.70837800	1.78434400
H	-0.11516200	-3.53358500	0.39485500
C	-4.11742800	5.41659300	-0.56597500
H	-5.06657900	5.96261800	-0.63183400
H	-3.58433200	5.78365900	0.32074700
H	-3.51866100	5.68496700	-1.44603200
O	-4.10323100	-3.63449300	1.74963900
H	-3.89393300	-2.71524100	1.48950800
H	-3.77610500	-4.13202100	0.97556200

TS_3

Charge/multiplicity: 0 1

N	4.13821100	-0.52096000	-0.01372100
H	4.31311000	-1.34582700	0.54903700
C	2.75064800	-0.20064300	-0.35820800
H	2.78720600	0.36211500	-1.29470200
C	1.96344900	-1.49556900	-0.56965900
C	2.14104700	0.70406900	0.73636500
H	2.53615200	-2.14847600	-1.23386300
H	1.81328900	-2.02073500	0.37767200
O	1.41117500	0.26800500	1.63738200
N	2.50567700	1.99747100	0.64701800
H	3.22280500	2.23443300	-0.03346600
C	2.14125400	2.97207200	1.66427900
H	2.58347800	2.72563700	2.63744100
H	2.50027300	3.95349500	1.34892100
H	1.05389200	3.01301200	1.78127100
C	5.17795600	0.29426200	-0.32906300
C	6.54671200	-0.20992500	0.07489400
H	6.60092700	-0.34785400	1.16117300
H	6.75901100	-1.17679500	-0.39547500
H	7.30231500	0.51510600	-0.23249200
O	5.00959300	1.37407700	-0.91428600
C	-0.83948400	-1.52624000	0.05719200
H	-0.32322500	-1.13425400	0.93796200
C	-1.08753900	-3.03689200	0.27851900
H	-1.65610800	-3.19715900	1.19757100
C	-1.79386600	-3.72879100	-0.85564600
H	-1.34873600	-3.60092700	-1.86013900
C	-2.15443000	-0.72218000	-0.11927200
H	-2.68223000	-1.06552000	-1.01811100
C	-1.95309300	0.79634100	-0.19071400
H	-1.30783400	1.02964200	-1.04463200
H	-1.40278200	1.11489600	0.70774600
C	-3.26400600	1.58450800	-0.31139600
H	-3.80798100	1.24742100	-1.20643300
H	-3.91093800	1.35602000	0.54502100
C	-3.04023000	3.09967100	-0.39312700
H	-2.40479200	3.32932200	-1.26164700
H	-2.47720200	3.43157100	0.49252200

C	-4.34172100	3.90533400	-0.49215800
H	-4.90495600	3.57766600	-1.37793300
H	-4.97651100	3.67502100	0.37562400
O	-2.79081000	-4.42544700	-0.72929500
S	0.32376500	-1.22128000	-1.36524600
O	-3.04982200	-1.05386400	0.95992400
H	-2.66132200	-0.71018000	1.78453000
H	-0.11359400	-3.53490200	0.39363200
C	-4.11163500	5.41713500	-0.56692500
H	-5.06034700	5.96357200	-0.63564000
H	-3.58132600	5.78351700	0.32175000
H	-3.50984300	5.68573500	-1.44485000
O	-4.10181900	-3.63532800	1.74923400
H	-3.89240100	-2.71614000	1.48897800
H	-3.77469200	-4.13297300	0.97523400

MIN_4

Charge/multiplicity: 0 1

N	3.92821600	-0.63519200	-0.42420700
H	4.33029700	-0.47169600	-1.33986400
C	2.56527600	-0.15111800	-0.17213100
H	2.49648600	0.03428700	0.90260300
C	2.33598400	1.15034300	-0.94682500
C	1.56541700	-1.26686000	-0.55648300
H	3.25868900	1.73815100	-0.90873600
H	2.11630100	0.93925700	-1.99727300
O	0.94473300	-1.26508800	-1.62767700
N	1.46600600	-2.25417100	0.35586500
H	2.13112000	-2.24089600	1.12548100
C	0.71152900	-3.47120100	0.09452800
H	1.14046900	-4.04151300	-0.73882600
H	0.72790600	-4.08944700	0.99405100
H	-0.32700100	-3.23181500	-0.15190300
C	4.62240700	-1.37229100	0.47719900
C	6.02026500	-1.78164100	0.07163900
H	6.70850600	-1.54130100	0.88805800
H	6.04458200	-2.86812100	-0.07135200
H	6.36359100	-1.29489100	-0.84527500
O	4.13918300	-1.70011500	1.57273000
C	-0.54449300	1.65975600	-0.95845300
H	-0.25579600	1.01868800	-1.79443700
C	-1.39525100	2.82568400	-1.51216400
H	-2.26273300	2.41026800	-2.03562900
C	-1.88292900	3.80099900	-0.46114300
H	-2.97865300	3.90613800	-0.35810000
C	-1.35539000	0.82244800	0.06582500
H	-0.65308600	0.21434800	0.65185400
C	-2.35320900	-0.12085700	-0.61876200
H	-1.80254400	-0.73243900	-1.34431300
H	-3.08325100	0.47224900	-1.18620200
C	-3.09377100	-1.03380500	0.36735800
H	-2.35757900	-1.61447100	0.94362400
H	-3.63499500	-0.41573400	1.09490900
C	-4.07224400	-1.99544000	-0.31846600
H	-3.52620900	-2.61594100	-1.04526600
H	-4.80424100	-1.41642500	-0.90163000
C	-4.81915000	-2.90766900	0.66270200
H	-4.08877400	-3.48373500	1.24927600
H	-5.36956200	-2.28793500	1.38512600

O	-1.13693900	4.51706800	0.19591700
S	1.07122000	2.30650800	-0.27817200
O	-2.09490500	1.67353900	0.94282400
H	-1.49023300	2.07342800	1.61418500
H	-0.80355900	3.39113200	-2.24181500
C	-5.79044800	-3.87054400	-0.02569200
H	-6.30629800	-4.50820500	0.70284500
H	-6.55759400	-3.32607100	-0.59146500
H	-5.26587300	-4.52909700	-0.73022600
O	-0.52866300	3.18053000	2.68003400
H	-0.69942400	3.93902900	2.08834900
H	0.37916200	2.91986700	2.44568900

TS_4

Charge/multiplicity: 0 1

N	3.81949200	-1.14724700	0.39099000
H	3.80489600	-1.58676900	1.30378900
C	2.54009100	-0.75233200	-0.20586100
H	2.68762600	-0.77320200	-1.28913500
C	1.45542100	-1.75477100	0.19000800
C	2.19730600	0.69543500	0.21357700
H	1.83324600	-2.76740700	0.02471500
H	1.20793400	-1.65118600	1.24989300
O	1.38799100	0.96007600	1.11336200
N	2.88688100	1.63751000	-0.45815100
H	3.62831100	1.31994400	-1.07737400
C	2.80312200	3.04811500	-0.11230700
H	3.13865400	3.23171800	0.91566900
H	3.43713500	3.61167100	-0.79938300
H	1.77312800	3.40664200	-0.20662900
C	5.01271200	-0.86874600	-0.18895600
C	6.24237500	-1.37840500	0.52743700
H	6.79622700	-2.03683600	-0.15058100
H	6.89253100	-0.52967600	0.76555600
H	6.01267300	-1.92397600	1.44671600
O	5.09531800	-0.23606800	-1.25374500
C	-1.29023800	-1.01968400	0.50999700
H	-0.79399900	-0.20873100	1.04484200
C	-1.72672000	-2.12519500	1.49102800
H	-1.99896700	-1.65891300	2.44574200
C	-2.95410400	-2.80595100	0.89868400
H	-3.74741100	-3.01241400	1.63829800
C	-2.59669300	-0.51264700	-0.15894900
H	-2.52086700	-0.53450100	-1.25273200
C	-3.03601500	0.87998700	0.29816100
H	-3.05824900	0.89882500	1.39669700
H	-4.06974000	1.02808000	-0.04176800
C	-2.15986700	2.02186200	-0.23345700
H	-1.12380500	1.89229100	0.10693100
H	-2.13358400	1.97748500	-1.33213900
C	-2.66541900	3.40233700	0.20696800
H	-2.69827900	3.44274900	1.30604700
H	-3.70253700	3.53668100	-0.13544400
C	-1.80853000	4.56255600	-0.31403900
H	-0.77330900	4.43172900	0.03283500
H	-1.77143400	4.52180700	-1.41223700
O	-2.76599700	-3.72108700	-0.02405900
S	-0.08771100	-1.55612700	-0.79501400
O	-3.64048400	-1.45562200	0.22899200

H	-4.17647800	-1.96741800	-0.71308800
H	-0.93925100	-2.85882100	1.68351800
C	-2.32130900	5.93622300	0.12685500
H	-1.68755900	6.74335100	-0.26082500
H	-3.34282500	6.11437400	-0.23354900
H	-2.33690300	6.02316800	1.22103800
O	-4.44543500	-2.85979300	-1.52765700
H	-3.73722900	-3.49815000	-0.94605000
H	-5.34510200	-3.17907500	-1.33101100

P(R)

Charge/multiplicity: 0 1

N	-4.51723300	-0.24588200	-0.25432800
H	-4.63854600	-0.72933200	-1.13633200
C	-3.15198500	-0.02698100	0.23174200
H	-3.21720400	0.02206900	1.32176300
C	-2.26636700	-1.20438600	-0.18207100
C	-2.62495200	1.32795000	-0.29325500
H	-2.78541400	-2.13701900	0.05514400
H	-2.07143800	-1.18346900	-1.25750000
O	-1.85600000	1.41467200	-1.25991600
N	-3.10184200	2.39894300	0.36936800
H	-3.83815900	2.23560400	1.05165300
C	-2.81950300	3.75904500	-0.06379600
H	-1.73923100	3.91978700	-0.13074600
H	-3.26098300	3.97154500	-1.04541200
H	-3.23601300	4.45120000	0.67047200
C	-5.60586800	0.24864100	0.38591600
C	-6.94998200	-0.09121600	-0.21591900
H	-7.58454500	-0.52431700	0.56417300
H	-7.43141300	0.83247500	-0.55628700
H	-6.88397000	-0.78967300	-1.05441600
O	-5.50739500	0.94274200	1.41003700
C	0.56152100	-0.65017600	-0.55115300
H	0.22952400	0.33519100	-0.87588700
C	0.76369800	-1.62010800	-1.72490300
H	1.18179700	-1.06756200	-2.57426400
C	1.80965900	-2.60268700	-1.19964600
H	2.44811000	-3.03230400	-1.97432700
C	1.96387300	-0.60537900	0.10136200
H	1.91159900	-0.67043500	1.19505800
C	2.76478600	0.63512500	-0.29523900
H	2.21118000	1.51309400	0.06531600
H	2.79406600	0.70517000	-1.39165100
C	4.19061700	0.65735100	0.26935900
H	4.14678000	0.57514300	1.36547300
H	4.73511800	-0.22694000	-0.08656100
C	4.96492300	1.92348500	-0.11723800
H	4.41547000	2.80907400	0.23610400
H	5.00319000	2.00550100	-1.21399300
C	6.39337600	1.96069800	0.44051500
H	6.35655000	1.88113700	1.53656600
H	6.94292000	1.07582100	0.08836300
O	1.27029900	-3.70747000	-0.50651100
S	-0.65983700	-1.24879900	0.71754200
O	2.65162600	-1.80395500	-0.35979100
H	-0.14515200	-2.12311800	-2.06364000
H	0.57551400	-3.37529100	0.09572800
C	7.16120600	3.22568000	0.04785400
H	8.17754800	3.22127000	0.46065000
H	7.24657800	3.31745500	-1.04275900

H	6.65719300	4.12839000	0.41684200
O	3.08256500	-3.22877400	2.07759000
H	3.09975100	-2.78441400	1.20562900
H	2.53133800	-4.00665800	1.89645800

TS_3'

Charge/multiplicity: 0 1

N	4.09086800	-0.60116100	0.63576500
H	4.05099400	-0.88538500	1.60742300
C	2.83736800	-0.54801800	-0.12246500
H	3.10519500	-0.70112300	-1.17074300
C	1.90406800	-1.67092400	0.33811900
C	2.21422700	0.85712700	0.03256500
H	2.47597500	-2.60214300	0.38159000
H	1.51481000	-1.46575100	1.33967300
O	1.34298600	1.11076300	0.87641000
N	2.73086300	1.78578500	-0.79466300
H	3.55458900	1.52458100	-1.32944500
C	2.36447200	3.19093400	-0.69921700
H	1.27889000	3.30428200	-0.77270900
H	2.69408800	3.63295300	0.24933700
H	2.83424900	3.72910900	-1.52464300
C	5.27036000	-0.17460400	0.11834000
C	6.48179000	-0.30127200	1.01439900
H	7.25310900	-0.87008500	0.48460100
H	6.88567500	0.69879300	1.20757200
H	6.26749300	-0.79039400	1.96877400
O	5.35512200	0.29184700	-1.02808200
C	-0.91445600	-1.11965900	0.06767300
H	-0.47097300	-0.21903400	0.49566000
C	-1.49197800	-1.97332800	1.21198400
H	-2.21617900	-1.39420100	1.79642800
C	-2.14402400	-3.26820800	0.79957200
H	-1.55828800	-3.91585900	0.12329700
C	-1.98095200	-0.71845800	-0.97728100
H	-1.45618400	-0.27935000	-1.83586600
C	-2.98229500	0.32802200	-0.45916000
H	-3.42127800	-0.00633400	0.49074200
H	-3.80563500	0.36431900	-1.18579700
C	-2.40101500	1.73982500	-0.29886500
H	-1.54892100	1.72743800	0.39397300
H	-2.00166900	2.07333200	-1.26789500
C	-3.43730000	2.75614900	0.19831200
H	-3.83236200	2.42644500	1.17104300
H	-4.29480800	2.76952100	-0.49116900
C	-2.87863800	4.17774800	0.33718400
H	-2.01886700	4.16377000	1.02253500
H	-2.48869600	4.51015100	-0.63574600
O	-3.21808700	-3.65247500	1.24296800
S	0.49341800	-1.97385100	-0.80727100
O	-2.63787700	-1.89587000	-1.45816200
H	-3.56308900	-1.93085200	-1.11955200
H	-0.67409800	-2.24185300	1.89751000
C	-3.91434500	5.18643600	0.84106200
H	-3.48436700	6.19179600	0.92905100
H	-4.77212400	5.25102000	0.15903000
H	-4.29864900	4.90232600	1.82933600
O	-5.22041200	-2.36004700	-0.46458400
H	-5.14219900	-2.08574000	0.46501800
H	-5.05103000	-3.31684300	-0.41214100

MIN$_4$'

Charge/multiplicity: 0 1

N	-4.00360200	-0.76841100	-0.58395000
H	-3.95603500	-1.14535400	-1.52313600
C	-2.75109100	-0.59892000	0.15866500
H	-3.01049600	-0.66639000	1.21824600
C	-1.77637000	-1.72086700	-0.20530600
C	-2.17772800	0.80823800	-0.12326300
H	-2.31290900	-2.67338100	-0.17878200
H	-1.38356600	-1.57982300	-1.21614800
O	-1.28765800	1.01024000	-0.96120900
N	-2.76072700	1.79403600	0.58476000
H	-3.58364200	1.55196100	1.13013700
C	-2.45040500	3.19666300	0.35235300
H	-2.72761500	3.50928800	-0.66193600
H	-3.00516200	3.79874300	1.07438500
H	-1.37980200	3.37831900	0.48745100
C	-5.19916000	-0.35128300	-0.09768700
C	-6.40784400	-0.62126300	-0.96457300
H	-7.13306100	-1.20229100	-0.38487500
H	-6.88128400	0.33280200	-1.22094300
H	-6.16993200	-1.16194900	-1.88483500
O	-5.30040000	0.21688100	1.00074300
C	1.04830700	-1.13683800	0.00634100
H	0.62477200	-0.26820500	-0.50033700
C	1.60028700	-2.10197900	-1.05872400
H	2.38239800	-1.61018200	-1.64873300
C	2.12932300	-3.41476000	-0.54624500
H	1.48373300	-3.95610600	0.16652400
C	2.15443500	-0.67169100	0.99045500
H	1.67079200	-0.31164400	1.90684900
C	3.00649000	0.47895300	0.42538900
H	3.36331600	0.22291800	-0.58160300
H	3.89941300	0.55370800	1.06067500
C	2.29658300	1.83966100	0.40022100
H	1.37248900	1.77922900	-0.19045200
H	1.98920500	2.10182800	1.42337100
C	3.17961500	2.95956300	-0.16597700
H	3.48175200	2.70016200	-1.19174900
H	4.10909500	3.02227400	0.41967700
C	2.49430200	4.33163400	-0.17430600
H	1.56374100	4.26847200	-0.75683300
H	2.19633300	4.59400000	0.85120500
O	3.15954600	-3.94428900	-0.94999200
S	-0.36765000	-1.86423000	0.97481200
O	2.96010900	-1.78748400	1.38318200
H	3.77622400	-1.80692000	0.82656200
H	0.78992600	-2.35782800	-1.75875900
C	3.37729500	5.44382300	-0.74688100
H	2.85926100	6.41079600	-0.73833300
H	4.30173500	5.55730100	-0.16587100
H	3.66357500	5.23008400	-1.78487600
O	5.17609200	-2.10288900	-0.31041200
H	4.65935800	-2.77050700	-0.80884900
H	5.78334200	-2.63826200	0.22804400

TS_4'

Charge/multiplicity: 0 1

N	3.99756700	-0.94628000	0.53017900
H	3.91732500	-1.38207100	1.44131000
C	2.76565200	-0.65401800	-0.20761100
H	3.03534000	-0.65178200	-1.26701700
C	1.72963300	-1.74718200	0.05902600
C	2.25925100	0.75569700	0.17341200
H	2.20275700	-2.72333500	-0.07815700
H	1.35979200	-1.68768700	1.08635700
O	1.35664700	0.94250800	1.00089300
N	2.91594300	1.75927800	-0.43961900
H	3.73584600	1.51387500	-0.98811000
C	2.67478800	3.15464000	-0.10554600
H	1.62420500	3.41223300	-0.27267800
H	2.91865900	3.36648000	0.94264900
H	3.29819900	3.77825100	-0.74902100
C	5.21980600	-0.55675300	0.08967800
C	6.39938400	-0.95195900	0.94859000
H	6.95323400	-0.04919800	1.22740600
H	6.11333800	-1.49254100	1.85498300
H	7.07254400	-1.58032800	0.35509800
O	5.36671900	0.08146500	-0.96430500
C	-1.07669800	-1.13481400	0.05127600
H	-0.68020600	-0.30987400	0.64399000
C	-1.60277200	-2.27405700	0.92568400
H	-2.17638900	-1.86652700	1.76824400
C	-2.54182500	-3.11116700	0.06774600
H	-2.02036200	-3.65236200	-0.73439000
C	-2.30429100	-0.68708500	-0.78653000
H	-2.01787400	-0.46558900	-1.82116000
C	-3.02779300	0.53145300	-0.20025100
H	-3.20919000	0.36948400	0.87080700
H	-4.01302300	0.59968000	-0.68108500
C	-2.27580400	1.85192000	-0.41592300
H	-1.27828900	1.79925200	0.04098200
H	-2.11430500	2.00207500	-1.49348300
C	-3.03042500	3.05823700	0.15835400
H	-3.18976500	2.90679000	1.23637800
H	-4.03189900	3.11029200	-0.29454900
C	-2.30739900	4.39266100	-0.06152400
H	-1.30716200	4.34128400	0.39225500
H	-2.14790700	4.54571500	-1.13867500
O	-3.52282500	-3.77415000	0.62744500
S	0.29395900	-1.65049800	-1.09155600
O	-3.18973600	-1.83607000	-0.84174400
H	-4.24775700	-1.71077900	-0.23914300
H	-0.80311100	-2.89974000	1.33592900
C	-3.06570500	5.59096400	0.51571600
H	-2.52391000	6.52889400	0.34214300
H	-4.05861900	5.69209000	0.05850800
H	-3.20985700	5.48665300	1.59893700
O	-5.10965300	-1.96532400	0.57894600
H	-4.50951300	-2.88631300	0.81956200
H	-5.89405000	-2.27658800	0.09045000

P(S)

Charge/multiplicity: 0 1

N	3.89803200	-1.19133800	0.40452400
H	3.79436600	-1.80140400	1.20663400
C	2.68116400	-0.71665300	-0.26159900

H	2.95351100	-0.53229900	-1.30470000
C	1.60335100	-1.79957400	-0.18980100
C	2.23111100	0.62025600	0.37138500
H	2.04145000	-2.75290200	-0.49739900
H	1.23394300	-1.90655500	0.83353700
O	1.30348700	0.69789500	1.18808500
N	2.96494100	1.68245800	-0.01282000
H	3.79107600	1.49963200	-0.57703300
C	2.78243100	2.99920800	0.57818500
H	2.98048000	2.98805800	1.65695100
H	3.47330800	3.69394200	0.09690800
H	1.75836400	3.35269800	0.42105100
C	5.13880000	-0.78570100	0.03954500
C	6.29445400	-1.39857000	0.79719900
H	6.96855800	-1.88021200	0.08081400
H	6.85755100	-0.60028300	1.29285300
H	5.98125200	-2.13355300	1.54380600
O	5.32077100	0.04077200	-0.86867900
C	-1.19264200	-1.17692200	-0.07190200
H	-0.81070000	-0.46713800	0.66259300
C	-1.71169700	-2.46358800	0.58301800
H	-2.11828400	-2.23536500	1.57653800
C	-2.86726900	-2.88559800	-0.32309800
H	-2.51323400	-3.40211000	-1.22451800
C	-2.44132200	-0.61500500	-0.82106700
H	-2.22261800	-0.48454100	-1.89068600
C	-2.98350500	0.70024700	-0.26122100
H	-3.14055600	0.58795500	0.82062400
H	-3.97228200	0.86622300	-0.71079800
C	-2.08849800	1.91325900	-0.54499000
H	-1.10079700	1.76406400	-0.08804500
H	-1.92031200	1.99263100	-1.62907100
C	-2.69064500	3.22640000	-0.02800000
H	-2.85116100	3.15038900	1.05787500
H	-3.68581500	3.37126500	-0.47500200
C	-1.82194800	4.45489600	-0.32480200
H	-0.82804300	4.31223500	0.12369900
H	-1.65995100	4.53068900	-1.40975700
O	-3.83049300	-3.71228800	0.24611300
S	0.17176000	-1.44973300	-1.29572700
O	-3.47016800	-1.62459100	-0.70224000
H	-4.68644900	-1.30680400	0.87037200
H	-0.95587100	-3.24558500	0.69176300
C	-2.42873500	5.76218100	0.19162700
H	-1.78450900	6.62027800	-0.03652200
H	-3.40923700	5.95319500	-0.26373300
H	-2.56988400	5.73319000	1.27986900
O	-4.98122100	-1.64345500	1.74143600
H	-4.22290800	-3.21941400	1.00467500
H	-5.93952200	-1.76609100	1.63180500

In water implicit solvent

Cysteine(H_2O)

Charge/multiplicity: 0 1

N	-1.34627700	-0.01679700	0.03028200
H	-1.50041100	-0.47280200	0.93309000
C	0.01497800	0.42042200	-0.25997700
H	0.01334900	0.80658900	-1.28072000
C	0.41972600	1.53788500	0.71654000
C	0.96056000	-0.78248700	-0.14795800

H	-0.30374300	2.35317900	0.64975800
H	0.41440500	1.15767600	1.74162000
S	2.11716000	2.20190100	0.45335700
O	1.13171400	-1.37592000	0.93748300
H	1.88772600	2.75671800	-0.75720300
N	1.57473700	-1.16857600	-1.27190200
H	1.42062800	-0.63883400	-2.12010300
C	2.49818700	-2.29626600	-1.30391900
H	2.84747900	-2.42614000	-2.32832500
H	3.35821800	-2.11485400	-0.65171100
H	1.99927300	-3.21284500	-0.97565500
C	-2.40506200	0.29933000	-0.75432300
C	-3.75362300	-0.16878600	-0.25346000
H	-4.41505400	0.69866300	-0.15808400
H	-4.19470600	-0.83854900	-0.99940100
H	-3.70070800	-0.68748600	0.70705700
O	-2.29330200	0.92123700	-1.82406800
O	-1.08744700	-1.38404600	2.64720900
H	-0.22271000	-1.42442100	2.17767600
H	-1.49383900	-2.24045600	2.43322300

MIN_{1t}

Charge/multiplicity: 0 1

N	-2.84649300	-0.58572400	-0.77173500
H	-2.35438100	-0.00924600	-1.46823200
C	-2.15336500	-1.75938800	-0.23679900
H	-2.91815000	-2.45475000	0.11685300
C	-1.33271200	-2.41770100	-1.34556000
C	-1.28504900	-1.33319300	0.96466100
H	-1.99357800	-2.65741000	-2.18208300
H	-0.55251700	-1.74561800	-1.70877100
O	-0.05511700	-1.14863100	0.85120100
N	-1.95689200	-1.16109700	2.11044500
H	-2.97181600	-1.20229800	2.05390000
C	-1.32926500	-0.65578900	3.32563900
H	-0.96832300	0.36893000	3.19444800
H	-2.06790600	-0.67702500	4.12763500
H	-0.48223300	-1.28864800	3.60456200
C	-4.01151100	-0.14454500	-0.24837000
C	-4.59966400	1.09297700	-0.88604300
H	-4.02690700	1.43675000	-1.74994600
H	-5.62891100	0.87893700	-1.19157000
H	-4.63596800	1.89334600	-0.13888100
O	-4.57848600	-0.71596800	0.70473000
C	0.48272400	2.37525900	0.27775000
H	-0.19517300	1.62130700	-0.12161900
C	0.15561700	3.67707600	0.18585800
H	0.33697000	-3.50476000	-0.00263600
C	-1.08547800	4.14399200	-0.43165800
H	-1.32407300	5.20933500	-0.26686100
C	1.73656100	1.84846600	0.92028800
H	2.29193600	2.67865900	1.37084900
C	2.62851900	1.14507400	-0.11765600
H	2.82825600	1.84981000	-0.93599900
H	2.06429900	0.30721300	-0.55086500
C	3.95352900	0.63983900	0.46617300
H	4.50089500	1.48748800	0.90369900
H	3.74615000	-0.05444700	1.29046200
C	4.83853200	-0.05404100	-0.57607400
H	5.04085200	0.64172100	-1.40380700
H	4.28905700	-0.90007500	-1.01483300
C	6.16912100	-0.55867300	-0.00494100
H	6.71776600	0.28665100	0.43411500
H	5.96715600	-1.25496500	0.82128500
O	-1.86656800	3.45769200	-1.09682800

S	-0.57242900	-4.02085000	-0.85606100
O	1.39056500	0.98314100	2.01281300
H	0.90779600	0.20782000	1.64438600
H	0.79591700	4.44518100	0.61425900
C	7.04883800	-1.24879500	-1.05071400
H	7.99316600	-1.59571700	-0.61443800
H	6.54177300	-2.12082000	-1.48290100
H	7.29370300	-0.56685000	-1.87488900
O	-1.40678900	1.12367700	-2.62599000
H	-1.48913000	1.92447000	-2.06135200
H	-2.09128900	1.25372800	-3.30349100

TS_{1t}

Charge/multiplicity: 0 1

N	-1.38252800	-1.24870700	1.35088600
H	-0.84031600	-0.51997300	1.84823300
C	-2.47849700	-0.85243500	0.48399900
H	-3.40894100	-1.28460700	0.87299800
C	-2.67692100	0.67677900	0.51365100
C	-2.27832500	-1.37490000	-0.95409300
H	-3.70635200	0.90304900	0.22514100
H	-2.52275100	1.04895300	1.52945000
O	-1.15448700	-1.46528400	-1.47144000
N	-3.40851600	-1.66651700	-1.61953100
H	-4.29467100	-1.61052700	-1.13372100
C	-3.39319300	-2.10927600	-3.00715100
H	-4.42311000	-2.24411400	-3.33883300
H	-2.90650500	-1.36622100	-3.64634500
H	-2.85822500	-3.05903600	-3.11088700
C	-1.12119400	-2.55343500	1.57271400
C	0.02129600	-2.85759700	2.51633100
H	0.77090600	-3.45304100	1.98406100
H	0.49427000	-1.95733200	2.91505300
H	-0.35455000	-3.46709000	3.34505000
O	-1.78233600	-3.46210100	1.03473300
C	0.21951000	1.45974200	-0.02438000
H	0.21787700	0.39158900	0.18741100
C	0.57554200	2.26845100	1.15287400
H	-1.86924900	3.06103600	0.17788800
C	0.50444300	1.78638200	2.45147900
H	0.91648800	2.46574000	3.22328900
C	1.03422300	1.71492500	-1.29499800
H	0.65625100	1.04876200	-2.08321000
C	2.53402600	1.44090300	-1.10936700
H	2.93511500	2.13602700	-0.36173400
H	3.02090600	1.68439100	-2.06507000
C	2.87251900	-0.00442500	-0.72132300
H	2.47688100	-0.21864000	0.28073300
H	2.36603700	-0.69755100	-1.40877700
C	4.38003300	-0.28637700	-0.73450900
H	4.88763700	0.41974700	-0.06069200
H	4.77779300	-0.08954700	-1.74096200
C	4.73390100	-1.72001900	-0.32130900
H	4.33561100	-1.91454900	0.68453300
H	4.22589700	-2.42591900	-0.99362400
O	0.02660400	0.67018900	2.86538400
S	-1.66303800	1.68953000	-0.65663800
O	0.80481200	3.08113100	-1.67507900
H	1.26115400	3.22280300	-2.52171900
H	1.05925000	3.22873400	0.99021500

C	6.23966100	-1.99619500	-0.33556300
H	6.46069800	-3.02770800	-0.03637200
H	6.66158900	-1.84232100	-1.33678800
H	6.77183100	-1.32849800	0.35383500
O	-1.82023900	3.95958400	1.04758000
H	-0.97374300	3.65545300	1.48381500
H	-1.58883800	4.79118500	0.58419900

MIN_2

Charge/multiplicity: 0 1

N	2.95148900	-0.10039200	0.26108400
H	2.32144200	-0.63451800	0.85827500
C	2.50930300	0.19882300	-1.09640100
H	3.41434500	0.43472900	-1.66668100
C	1.85476000	-1.00821700	-1.79601800
C	1.63845300	1.47851300	-1.16587900
H	1.24033300	-0.64732400	-2.62178600
H	2.64512400	-1.63444000	-2.21944400
O	0.50129900	1.49569300	-1.66505400
N	2.23048900	2.58288300	-0.68047400
H	3.18917700	2.50865400	-0.35090000
C	1.56841800	3.87985200	-0.69441400
H	2.23074200	4.61094900	-0.22944200
H	1.34709000	4.20041300	-1.71809500
H	0.62905200	3.84452500	-0.13380700
C	4.07048900	0.43010200	0.80216400
C	4.41677600	-0.01520100	2.20328400
H	4.58672900	0.86961100	2.82461400
H	3.64436700	-0.63777900	2.65955400
H	5.35575400	-0.57898900	2.16842900
O	4.79283800	1.23585900	0.18126800
C	-0.53301600	-1.29148400	-0.06769900
H	-0.18320100	-0.28564400	0.17434700
C	-0.93309200	-2.00556000	1.22557400
H	-2.77663600	-3.72558600	-0.44157100
C	0.02928300	-1.88759400	2.37043200
H	-0.26953000	-2.44595500	3.27750400
C	-1.66814700	-1.17308000	-1.11024900
H	-1.26558900	-0.59706100	-1.95294400
C	-2.94057200	-0.47618800	-0.61618400
H	-3.43497100	-1.10842200	0.13340800
H	-3.62415800	-0.42712500	-1.47377700
C	-2.72754600	0.93584700	-0.05488500
H	-2.13099500	0.88533400	0.86632500
H	-2.14154900	1.53189000	-0.76763700
C	-4.04941900	1.65354200	0.24401300
H	-4.64227100	1.04821700	0.94571200
H	-4.64248700	1.71968200	-0.68003000
C	-3.86084500	3.05990700	0.82507800
H	-3.27415500	2.99325700	1.75225600
H	-3.26262400	3.66223600	0.12673200
O	1.05505400	-1.22284000	2.38167300
S	0.91353600	-2.22355900	-0.78400800
O	-2.07707500	-2.46480700	-1.60087400
H	-1.27292600	-2.90585100	-1.93512400
H	-1.87738200	-1.59096800	1.61172300
C	-5.18425600	3.77454100	1.11014100
H	-5.01789000	4.77621000	1.52403200
H	-5.77901100	3.88696300	0.19475800
H	-5.79089500	3.21275900	1.83171300
O	-3.09848400	-4.43087700	0.16346500
H	-1.15408600	-3.07011100	1.07028100
H	-3.48680700	-3.92317800	0.89386900

TS_2

Charge/multiplicity: 0 1

N	2.20301000	0.34004900	1.04783700
H	1.41816200	0.00386400	1.60503400
C	2.66450200	-0.50809600	-0.05557100
H	3.74832400	-0.61021000	0.06805000
C	2.13329400	-1.94572900	0.07946400
C	2.43499200	0.19756600	-1.40943100
H	2.76967800	-2.58955100	-0.53586700
H	2.28874700	-2.24252600	1.11999000
O	1.37978900	0.12995000	-2.05434800
N	3.49448000	0.91976900	-1.83350600
H	4.20384700	1.13139500	-1.13860400
C	3.39692500	1.77649500	-3.00776600
H	4.36763900	2.24399000	-3.17817200
H	3.13051400	1.18428600	-3.88717000
H	2.64059900	2.55964300	-2.87733400
C	2.99334800	1.31333800	1.56033200
C	2.47873800	2.00660900	2.80070400
H	2.23010700	3.04404900	2.55038300
H	1.59611700	1.52276600	3.22554500
H	3.27696000	2.02948300	3.54896800
O	4.07517100	1.63944200	1.03787900
C	-0.80914000	-1.22994800	0.09513900
H	-0.27201500	-0.29733300	0.27197700
C	-1.54651800	-1.66884300	1.36265000
H	-2.20664500	-4.93645600	0.02766600
C	-0.76687800	-1.62327200	2.63895300
H	-1.25838300	-2.11358100	3.49973500
C	-1.74689500	-0.98669100	-1.11181300
H	-1.12211800	-0.60420000	-1.92421800
C	-2.88085900	0.01001200	-0.85805400
H	-3.58897500	-0.40787700	-0.13054700
H	-3.43137200	0.10556600	-1.80284700
C	-2.41084300	1.39674200	-0.40071700
H	-1.93135100	1.32278000	0.58485500
H	-1.63943200	1.76559100	-1.09209900
C	-3.55662700	2.41341100	-0.32417500
H	-4.33251900	2.03467700	0.35749900
H	-4.03228700	2.49988400	-1.31215100
C	-3.10801100	3.80266700	0.14396800
H	-2.63113700	3.71540100	1.13049000
H	-2.33401100	4.18184400	-0.53820700
O	0.31134400	-1.06791900	2.80439000
S	0.44729100	-2.49915500	-0.44124000
O	-2.36411900	-2.21613200	-1.56339500
H	-1.72009300	-2.67804400	-2.12705800
H	-2.41008200	-1.01014800	1.55711400
C	-4.25787300	4.81045700	0.22166200
H	-3.90753900	5.79314100	0.55920100
H	-4.73414400	4.94526600	-0.75779600
H	-5.03247700	4.47422300	0.92248600
O	-3.07405700	-4.50235000	-0.01434300
H	-1.98036400	-2.67015700	1.25695600
H	-2.87879400	-3.68223600	-0.51788300

MIN_3

Charge/multiplicity: 0 1

N	2.20301000	0.34004900	1.04783700
H	1.41816200	0.00386400	1.60503400
C	2.66450200	-0.50809600	-0.05557100
H	3.74832400	-0.61021000	0.06805000
C	2.13329400	-1.94572900	0.07946400
C	2.43499200	0.19756600	-1.40943100
H	2.76967800	-2.58955100	-0.53586700
H	2.28874700	-2.24252600	1.11999000
O	1.37978900	0.12995000	-2.05434800
N	3.49448000	0.91976900	-1.83350600
H	4.20384700	1.13139500	-1.13860400
C	3.39692500	1.77649500	-3.00776600
H	4.36763900	2.24399000	-3.17817200
H	3.13051400	1.18428600	-3.88717000
H	2.64059900	2.55964300	-2.87733400
C	2.99334800	1.31333800	1.56033200
C	2.47873800	2.00660900	2.80070400
H	2.23010700	3.04404900	2.55038300
H	1.59611700	1.52276600	3.22554500
H	3.27696000	2.02948300	3.54896800
O	4.07517100	1.63944200	1.03787900
C	-0.80914000	-1.22994800	0.09513900
H	-0.27201500	-0.29733300	0.27197700
C	-1.54651800	-1.66884300	1.36265000
H	-2.20664500	-4.93645600	0.02766600
C	-0.76687800	-1.62327200	2.63895300
H	-1.25838300	-2.11358100	3.49973500
C	-1.74689500	-0.98669100	-1.11181300
H	-1.12211800	-0.60420000	-1.92421800
C	-2.88085900	0.01001200	-0.85805400
H	-3.58897500	-0.40787700	-0.13054700
H	-3.43137200	0.10556600	-1.80284700
C	-2.41084300	1.39674200	-0.40071700
H	-1.93135100	1.32278000	0.58485500
H	-1.63943200	1.76559100	-1.09209900
C	-3.55662700	2.41341100	-0.32417500
H	-4.33251900	2.03467700	0.35749900
H	-4.03228700	2.49988400	-1.31215100
C	-3.10801100	3.80266700	0.14396800
H	-2.63113700	3.71540100	1.13049000
H	-2.33401100	4.18184400	-0.53820700
O	0.31134400	-1.06791900	2.80439000
S	0.44729100	-2.49915500	-0.44124000
O	-2.36411900	-2.21613200	-1.56339500
H	-1.72009300	-2.67804400	-2.12705800
H	-2.41008200	-1.01014800	1.55711400
C	-4.25787300	4.81045700	0.22166200
H	-3.90753900	5.79314100	0.55920100
H	-4.73414400	4.94526600	-0.75779600
H	-5.03247700	4.47422300	0.92248600
O	-3.07405700	-4.50235000	-0.01434300
H	-1.98036400	-2.67015700	1.25695600
H	-2.87879400	-3.68223600	-0.51788300

TS_3

Charge/multiplicity: 0 1

N	4.12460100	-0.54388100	0.02999800
H	4.27982400	-1.35958200	0.61177500
C	2.74979900	-0.22342000	-0.35969600
H	2.81253000	0.31143600	-1.31031000
C	1.95659000	-1.51658400	-0.55458900

C	2.12089500	0.71512600	0.69164800
H	2.52451700	-2.18201700	-1.20901100
H	1.80044900	-2.02909700	0.39830400
O	1.42430900	0.29830400	1.63164900
N	2.42324800	2.01644300	0.52834000
H	3.13970200	2.24189000	-0.15554900
C	2.04832500	3.01890400	1.51689200
H	2.51305600	2.81960700	2.48927800
H	2.37470800	3.99642000	1.16005100
H	0.96294300	3.03475500	1.64957300
C	5.17774600	0.25289700	-0.27881400
C	6.52881900	-0.24279000	0.18546500
H	6.54360000	-0.34578200	1.27622200
H	6.74815000	-1.22589500	-0.24496700
H	7.29879600	0.46716200	-0.12026000
O	5.03571500	1.31601700	-0.90756600
C	-0.84375400	-1.53880100	0.06736300
H	-0.32680800	-1.15835600	0.95224100
C	-1.09901600	-3.04876300	0.28206300
H	-1.66561000	-3.20926700	1.20173100
C	-1.80247700	-3.73482000	-0.85459500
H	-1.36039900	-3.59789200	-1.85787800
C	-2.14973100	-0.72051200	-0.10252800
H	-2.68134200	-1.04947900	-1.00394800
C	-1.92733500	0.79546800	-0.16045600
H	-1.28145500	1.02592300	-1.01435800
H	-1.37219800	1.09765500	0.74041200
C	-3.22584900	1.60404900	-0.27330000
H	-3.78623500	1.26748600	-1.15806000
H	-3.86538900	1.39846500	0.59415100
C	-2.97642400	3.11359200	-0.37453900
H	-2.35037600	3.32225900	-1.25468500
H	-2.39543500	3.44473700	0.49931600
C	-4.26525900	3.93953100	-0.46393600
H	-4.84682100	3.60997500	-1.33669900
H	-4.88945600	3.73070200	0.41641600
O	-2.79654600	-4.44072600	-0.73205200
S	0.32034100	-1.23325200	-1.35324200
O	-3.04984900	-1.04686400	0.97691000
H	-2.64229500	-0.73143700	1.80363300
H	-0.12619800	-3.54907200	0.39480800
C	-4.00924900	5.44569500	-0.56195600
H	-4.94816000	6.00868600	-0.62438600
H	-3.45899600	5.81209700	0.31398700
H	-3.41505700	5.68994000	-1.45162100
O	-4.18340000	-3.60015600	1.66353700
H	-3.88611700	-2.69037000	1.45567100
H	-3.80063700	-4.09688400	0.91371400

MIN_4

Charge/multiplicity: 0 1

N	3.78578700	-0.82818700	-0.39687600
H	4.28154400	-0.65245000	-1.26288100
C	2.43863200	-0.26368800	-0.24429100
H	2.30597700	-0.06397100	0.82165100
C	2.33599300	1.04170800	-1.04341600
C	1.39885900	-1.32101000	-0.68489600
H	3.30740900	1.54352500	-1.01022300
H	2.10261100	0.83371500	-2.09076400
O	0.81395000	-1.26687000	-1.77884900
N	1.21063700	-2.31893600	0.19736200

H	1.83954300	-2.35676400	0.99620700
C	0.38246300	-3.47504500	-0.11951400
H	0.77843900	-4.02863000	-0.97856600
H	0.36236300	-4.13424000	0.74917500
H	-0.63998500	-3.16305600	-0.35142300
C	4.37656600	-1.58124700	0.55849800
C	5.78891400	-2.03573300	0.27993700
H	6.44150700	-1.66184900	1.07592000
H	5.82149600	-3.12972000	0.31271100
H	6.16789000	-1.69274300	-0.68575500
O	3.79216800	-1.88371400	1.61662200
C	-0.49718200	1.76607000	-0.98154600
H	-0.29924300	1.15563700	-1.86557100
C	-1.34121100	2.98235700	-1.42228800
H	-2.26520400	2.61830600	-1.88202500
C	-1.69713000	3.94078700	-0.30788300
H	-2.77408000	4.09943600	-0.12073200
C	-1.25845800	0.91106000	0.06534900
H	-0.53666200	0.26049500	0.57550900
C	-2.33035100	0.02553300	-0.58196700
H	-1.85576200	-0.55009200	-1.38588000
H	-3.09373500	0.66138900	-1.05000000
C	-2.99837900	-0.93876400	0.40661400
H	-2.22390500	-1.55881500	0.88222000
H	-3.47507100	-0.36622300	1.21241500
C	-4.03881500	-1.84985200	-0.25593800
H	-3.55967400	-2.42211100	-1.06437000
H	-4.81195500	-1.23145500	-0.73587600
C	-4.70729800	-2.82320500	0.72211500
H	-3.93473900	-3.44153000	1.20094000
H	-5.18657500	-2.25223100	1.52987900
O	-0.86698200	4.59135800	0.31915400
S	1.18835300	2.32958500	-0.40689100
O	-1.90233700	1.74468800	1.03463800
H	-1.22574500	2.10138900	1.65942400
H	-0.79116500	3.54934900	-2.18272100
C	-5.74392400	-3.73057900	0.05403400
H	-6.19875200	-4.41951500	0.77580100
H	-6.55199800	-3.14282500	-0.39960200
H	-5.28792700	-4.33439500	-0.74080300
O	-0.05726600	3.06634800	2.66991700
H	-0.30613400	3.87062300	2.17542800
H	0.73257300	2.76044000	2.18606500

TS_4

Charge/multiplicity: 0 1

N	3.77100800	-1.25455000	0.41789200
H	3.75026700	-1.67365200	1.34027300
C	2.49908900	-0.84530600	-0.18411700
H	2.63858500	-0.90281600	-1.26665300
C	1.38697400	-1.80268400	0.24444200
C	2.19812000	0.62150300	0.19246100
H	1.72824200	-2.83067600	0.10182300
H	1.14752400	-1.66562900	1.30208200
O	1.43964200	0.93320000	1.12554300
N	2.85772400	1.53087100	-0.54841300
H	3.58147000	1.18082100	-1.16988000
C	2.82314800	2.95165600	-0.22812400
H	3.23024400	3.14917000	0.77012100
H	3.41892300	3.48778600	-0.96782100
H	1.79601300	3.32671900	-0.26225700
C	4.96508000	-1.03026000	-0.17919400
C	6.18678600	-1.53783600	0.54857800

H	6.72661900	-2.22657300	-0.10969300
H	6.85064400	-0.69254600	0.75806800
H	5.94803300	-2.04843400	1.48475100
O	5.05582300	-0.44245100	-1.27311600
C	-1.35054600	-1.01924300	0.55743000
H	-0.83312100	-0.25144000	1.13403800
C	-1.86141300	-2.13708600	1.48621100
H	-2.12552400	-1.69450400	2.45370300
C	-3.11499700	-2.71581800	0.84278900
H	-3.92103700	-2.93438500	1.56249000
C	-2.61664000	-0.42853200	-0.12001600
H	-2.53167700	-0.44735700	-1.21270500
C	-2.97519500	0.98414700	0.34058600
H	-2.99666700	1.00369300	1.43874800
H	-3.99523500	1.19911000	-0.00340500
C	-2.02491900	2.06432200	-0.19172400
H	-1.00043500	1.86673600	0.15045300
H	-2.00142500	2.01500200	-1.28993900
C	-2.43532100	3.47687900	0.24315600
H	-2.45736700	3.52678900	1.34182100
H	-3.46295100	3.67731000	-0.09402800
C	-1.50514900	4.57119800	-0.29373700
H	-0.47750700	4.36901000	0.04144000
H	-1.48481100	4.52162000	-1.39169000
O	-2.95553100	-3.59715900	-0.13084500
S	-0.14913600	-1.56460400	-0.74365800
O	-3.71833200	-1.31659300	0.24738700
H	-4.28423500	-1.74588800	-0.72420900
H	-1.11815200	-2.91921900	1.66015100
C	-1.91686700	5.97890700	0.14516000
H	-1.23500100	6.73884000	-0.25476700
H	-2.92839800	6.22241400	-0.20370200
H	-1.91295900	6.07052000	1.23867700
O	-4.59401100	-2.56477600	-1.59241000
H	-3.92936500	-3.26290200	-1.05838600
H	-5.50526200	-2.84895300	-1.39319800

P(R)

Charge/multiplicity: 0 1

N	-4.47238700	-0.16954400	-0.43740200
H	-4.51954800	-0.55019200	-1.37521200
C	-3.15202500	-0.00623500	0.17517700
H	-3.30086000	-0.07084000	1.25560600
C	-2.22842500	-1.13435000	-0.28735700
C	-2.59786600	1.39312400	-0.16606900
H	-2.73988500	-2.08996100	-0.15043400
H	-1.98413800	-1.02503100	-1.34684600
O	-1.81661700	1.58829000	-1.11116000
N	-3.05947300	2.38305300	0.62021800
H	-3.82168400	2.15499900	1.25186900
C	-2.76419900	3.78236200	0.34189400
H	-1.68308900	3.94380700	0.31737800
H	-3.18353900	4.09990600	-0.61973700
H	-3.19513900	4.39239500	1.13665400
C	-5.61264500	0.24617400	0.16343100
C	-6.89697400	-0.00970600	-0.58876300
H	-7.56336700	-0.60424500	0.04477800
H	-7.39166800	0.94825200	-0.78084000
H	-6.74242500	-0.53104100	-1.53676300
O	-5.60761500	0.80346900	1.27611200
C	0.60258000	-0.59793800	-0.53999000
H	0.28581100	0.39310700	-0.86281300

C	0.84207200	-1.56077400	-1.71078900
H	1.32805600	-1.01298700	-2.52566800
C	1.81927500	-2.58701000	-1.13615000
H	2.51016300	-3.00121000	-1.87258900
C	1.98309800	-0.56905100	0.14480300
H	1.90746200	-0.52737200	1.23669900
C	2.86081400	0.58364900	-0.34616100
H	2.34679100	1.51919300	-0.08729400
H	2.92402900	0.54770200	-1.44220900
C	4.26930300	0.58907200	0.25948000
H	4.19097500	0.62573200	1.35586900
H	4.77562100	-0.35385400	0.01504700
C	5.12114700	1.76571700	-0.23124400
H	4.60922500	2.70998600	0.00671300
H	5.19669300	1.72660700	-1.32804800
C	6.53142000	1.79135500	0.36997400
H	6.45674000	1.83340400	1.46583800
H	7.04273500	0.84732000	0.13380600
O	1.19959800	-3.70619100	-0.53652200
S	-0.66274700	-1.21001700	0.68013000
O	2.59986100	-1.85198100	-0.17776100
H	-0.06004200	-2.03027000	-2.10883200
H	0.48257200	-3.37066500	0.03779200
C	7.37578900	2.96680400	-0.12904600
H	8.37726300	2.95884600	0.31747200
H	7.49740100	2.93322100	-1.21916900
H	6.90707900	3.92678900	0.12195200
O	2.32792400	-3.08280100	2.39462100
H	2.54580900	-2.77161300	1.49176700
H	1.58254700	-3.68171100	2.22796600

TS_3’

Charge/multiplicity: 0 1

N	-3.98216500	-0.74606600	-0.63550500
H	-3.89933500	-1.07752300	-1.58989300
C	-2.75977000	-0.61478400	0.16066600
H	-3.05571100	-0.73388700	1.20532400
C	-1.76949900	-1.71733000	-0.21771600
C	-2.17602000	0.80006600	-0.03226500
H	-2.29218800	-2.67679300	-0.21666200
H	-1.36646200	-1.55120800	-1.22030800
O	-1.31320200	1.05281600	-0.88989900
N	-2.70691700	1.74051900	0.77057700
H	-3.53070200	1.47900400	1.30366700
C	-2.38963000	3.15358600	0.61006100
H	-1.31186100	3.31283100	0.70175800
H	-2.71371400	3.53174900	-0.36636100
H	-2.89794100	3.71405800	1.39549600
C	-5.19487400	-0.34163300	-0.18183100
C	-6.35245600	-0.55857400	-1.13056300
H	-6.45258700	-1.62006200	-1.38176400
H	-7.27356700	-0.20780200	-0.66267300
H	-6.18859600	-0.00902900	-2.06427900
O	-5.33973800	0.16678200	0.94336400
C	1.04935000	-1.13698900	0.00853200
H	0.62877500	-0.27291800	-0.50771000
C	1.60189400	-2.10691800	-1.05246500
H	2.39554300	-1.62260400	-1.63204600
C	2.10600500	-3.42719100	-0.54204000
H	1.44419300	-3.96740400	0.15566700
C	2.14799200	-0.65253200	0.99035300
H	1.65695900	-0.27594600	1.89558800
C	2.99855200	0.48927900	0.40669600

H	3.34661800	0.22074100	-0.59979500
H	3.89484300	0.57269800	1.03544500
C	2.28785600	1.84891000	0.37038500
H	1.35398800	1.77840900	-0.20353500
H	1.99832300	2.12833000	1.39382400
C	3.16095300	2.95772900	-0.23031100
H	3.44371900	2.68080700	-1.25668700
H	4.10038800	3.02950500	0.33757800
C	2.47572800	4.32924100	-0.24866500
H	1.53394800	4.25572500	-0.81102900
H	2.19889300	4.60890000	0.77777200
O	3.14250100	-3.96294300	-0.92634800
S	-0.37152400	-1.85428200	0.97655200
O	2.95977700	-1.75482500	1.41642700
H	3.76058600	-1.79830900	0.83987500
H	0.79349900	-2.35084400	-1.75863700
C	3.34813800	5.42937500	-0.85899000
H	2.83220100	6.39695700	-0.85754900
H	4.28395100	5.55009900	-0.29872800
H	3.61253200	5.19479500	-1.89788700
O	5.16871500	-2.11018600	-0.30342000
H	4.60707100	-2.75273900	-0.78640600
H	5.71485100	-2.67677100	0.26754400

MIN_4’

Charge/multiplicity: 0 1

N	-3.98197200	-0.74531400	-0.63881000
H	-3.90097400	-1.09324800	-1.58686100
C	-2.75899200	-0.61107600	0.15681800
H	-3.05486200	-0.72816200	1.20179600
C	-1.76822100	-1.71334600	-0.22087200
C	-2.17798100	0.80478500	-0.03881800
H	-2.29090500	-2.67283100	-0.22109600
H	-1.36394700	-1.54659100	-1.22282800
O	-1.30806500	1.05569500	-0.88954900
N	-2.71921000	1.74692700	0.75490100
H	-3.54799600	1.48463700	1.28031500
C	-2.40413900	3.16012300	0.59135300
H	-2.72101000	3.53364300	-0.38922100
H	-2.92033800	3.72243400	1.37031300
H	-1.32757200	3.32240600	0.69136300
C	-5.19286900	-0.34543200	-0.18259700
C	-6.36528800	-0.56619600	-1.10858000
H	-7.10574300	-1.18903500	-0.59587100
H	-6.83602200	0.39959300	-1.32021700
H	-6.08504700	-1.04376500	-2.05080400
O	-5.33744800	0.17053200	0.94061400
C	1.05086200	-1.13630600	0.00838600
H	0.63222500	-0.27119300	-0.50768600
C	1.60226800	-2.10679400	-1.05268800
H	2.39712600	-1.62360300	-1.63154800
C	2.10378300	-3.42820600	-0.54261000
H	1.44066200	-3.96763500	0.15446000
C	2.14974200	-0.65445700	0.99123500
H	1.65886700	-0.27776200	1.89651300
C	3.00247700	0.48636500	0.40887600
H	3.35083200	0.21784800	-0.59752200
H	3.89845100	0.56795100	1.03831800
C	2.29401900	1.84715900	0.37285700
H	1.36068300	1.77862100	-0.20216700
H	2.00379000	2.12626100	1.39617900
C	3.16971600	2.95495700	-0.22593800

H	3.45328100	2.67833500	-1.25217500
H	4.10857100	3.02465800	0.34317100
C	2.48696900	4.32770100	-0.24406900
H	1.54595000	4.25645000	-0.80799100
H	2.20902300	4.60689300	0.78219200
O	3.13953400	-3.96558600	-0.92664100
S	-0.37200200	-1.85123400	0.97523200
O	2.95952600	-1.75838200	1.41685800
H	3.76047700	-1.80275900	0.84057200
H	0.79391700	-2.34894500	-1.75951500
C	3.36239400	5.42680400	-0.85193400
H	2.84822600	6.39532600	-0.85048000
H	4.29747400	5.54530200	-0.28997400
H	3.62812400	5.19268400	-1.89059400
O	5.16880000	-2.11645000	-0.30215400
H	4.60633700	-2.75790000	-0.78564000
H	5.71350800	-2.68411400	0.26910400

TS_4’

Charge/multiplicity: 0 1

N	3.93991600	-1.04064700	0.53814500
H	3.83687500	-1.47993900	1.44539800
C	2.72583400	-0.73063800	-0.22096700
H	3.01229800	-0.72917500	-1.27520900
C	1.66991800	-1.80979800	0.02283000
C	2.23414700	0.68287400	0.15586100
H	2.12292400	-2.79092600	-0.13788700
H	1.30205600	-1.76837800	1.05143000
O	1.35617000	0.87979800	1.01228400
N	2.86471400	1.68229200	-0.48816800
H	3.68369700	1.43352800	-1.03545800
C	2.64357100	3.07921600	-0.13775400
H	2.92425100	3.28225100	0.90198800
H	3.24833400	3.70188700	-0.79802100
H	1.59013200	3.34357400	-0.26874400
C	5.17305100	-0.66469300	0.12313600
C	6.32879200	-1.05816800	1.01168900
H	7.01917100	-1.68370400	0.43608200
H	6.87089400	-0.15383700	1.30706000
H	6.01621100	-1.59942300	1.90802900
O	5.34957100	-0.03534100	-0.93609300
C	-1.11798100	-1.13838800	0.03801600
H	-0.69832100	-0.34124800	0.65168200
C	-1.67150600	-2.28275200	0.88746900
H	-2.21234200	-1.87577600	1.75135500
C	-2.66419400	-3.04603400	0.02079500
H	-2.17925200	-3.57919300	-0.80940600
C	-2.33694100	-0.63289000	-0.77921900
H	-2.06096600	-0.43066000	-1.82018500
C	-2.98482400	0.62123900	-0.18326700
H	-3.14530000	0.47057700	0.89252000
H	-3.97576500	0.74029700	-0.64097200
C	-2.16712600	1.89691500	-0.42433700
H	-1.16017900	1.78729700	0.00068600
H	-2.03335800	2.03831100	-1.50650600
C	-2.82864700	3.14435600	0.17423900
H	-2.95228400	3.00438300	1.25822600
H	-3.84236600	3.25374100	-0.23862400
C	-2.03733400	4.43236400	-0.08176500
H	-1.02015100	4.31803800	0.32015800
H	-1.92408500	4.57768100	-1.16542500
O	-3.65340100	-3.70410700	0.58988900
S	0.23504900	-1.65638400	-1.12298700

O	-3.28473500	-1.73544500	-0.81199300
H	-4.31294400	-1.56289500	-0.14675600
H	-0.89015100	-2.95192100	1.26146600
C	-2.69208100	5.67194600	0.53330100
H	-2.10720600	6.57686200	0.32993100
H	-3.70014100	5.82922000	0.12911500
H	-2.78411400	5.57266200	1.62228300
O	-5.15375800	-1.80123800	0.68260000
H	-4.61668100	-2.74743600	0.86274300
H	-5.96329100	-2.04780200	0.19732500

P(S)

Charge/multiplicity: 0 1

N	3.82672000	-1.31254900	0.41906400
H	3.70491800	-1.91842100	1.22204100
C	2.62701600	-0.80638300	-0.25326300
H	2.90935100	-0.62757500	-1.29367000
C	1.51659200	-1.85604000	-0.19638200
C	2.21043800	0.53794300	0.38137400
H	1.92102100	-2.81780300	-0.52031300
H	1.14159600	-1.96867500	0.82392900
O	1.33741900	0.62174300	1.26107500
N	2.90181900	1.60233100	-0.06575500
H	3.70670300	1.41609200	-0.65684600
C	2.75547500	2.92056500	0.53734700
H	3.01185400	2.90548700	1.60267100
H	3.42118900	3.61287400	0.02068000
H	1.72613400	3.27736000	0.43496800
C	5.07705800	-0.94367800	0.05298200
C	6.21507000	-1.56964100	0.82319900
H	6.87018500	-2.09304300	0.11899200
H	6.80338800	-0.77473600	1.29339800
H	5.87967700	-2.27108200	1.59104100
O	5.28333200	-0.13618100	-0.87164200
C	-1.26519000	-1.16796300	-0.08102500
H	-0.87582000	-0.50398000	0.69092300
C	-1.83567100	-2.46195300	0.51628900
H	-2.20873600	-2.26755600	1.52902500
C	-3.03054100	-2.77461700	-0.38178200
H	-2.72885500	-3.26958400	-1.31302000
C	-2.48190200	-0.52648900	-0.81906400
H	-2.26417000	-0.41552500	-1.89094400
C	-2.93105400	0.82163600	-0.25870400
H	-3.10455600	0.71557800	0.82104600
H	-3.89910200	1.06579100	-0.71626400
C	-1.94110700	1.96238800	-0.52623500
H	-0.98110600	1.74631800	-0.03797100
H	-1.73646700	2.01927000	-1.60501700
C	-2.45785500	3.32137100	-0.03761200
H	-2.66958700	3.26461400	1.04033700
H	-3.41736100	3.54275500	-0.52778600
C	-1.47976500	4.47268100	-0.30000300
H	-0.52207700	4.25356900	0.19415100
H	-1.26402200	4.52536100	-1.37656900
O	-4.03325000	-3.57372700	0.17916000
S	0.10317100	-1.42985900	-1.29994500
O	-3.57194400	-1.46871700	-0.68752700
H	-4.62556600	-1.14866800	1.00877800
H	-1.11763300	-3.28391800	0.56341800
C	-2.00315600	5.82832500	0.18158200
H	-1.28218000	6.63009400	-0.01781800

H	-2.94174500	6.09201500	-0.32212500
H	-2.19870400	5.81739200	1.26131600
O	-4.96295800	-1.51033300	1.85402300
H	-4.36264500	-3.09541800	0.97602000
H	-5.91942200	-1.59045200	1.69863000

Anionic case

In cyclohexane implicit solvent

Cysteinate($2H_2O$)$^-$

Charge/multiplicity: -1 1

N	1.70796200	-0.13039000	0.13450000
H	1.86425100	0.67872700	0.72988200
C	0.34584700	-0.42862800	-0.28582300
H	0.41791000	-1.01520900	-1.20622600
C	-0.39042400	-1.31290500	0.76812200
C	-0.39796600	0.88764300	-0.58158800
H	0.31839100	-2.10630300	1.02843200
H	-0.54190200	-0.71366400	1.67755400
S	-1.97227300	-2.09246600	0.21047300
O	0.08853700	2.01220300	-0.34600400
N	-1.61811400	0.71387400	-1.11589500
H	-1.98919400	-0.25050900	-1.02836000
C	-2.57262000	1.79658600	-1.28310000
H	-2.09311900	2.73854300	-1.00996200
H	-2.90939300	1.85865000	-2.32577000
H	-3.43820500	1.61499900	-0.63583400
C	2.78476900	-0.84098600	-0.28736600
C	4.12096600	-0.37112800	0.27851700
H	4.04027000	0.51904700	0.90990400
H	4.56113400	-1.18260100	0.86868700
H	4.80560300	-0.16621800	-0.55171900
O	2.72251000	-1.79755700	-1.06030400
O	2.13090800	2.61640100	1.36686600
H	2.79615900	2.90610900	0.72287200
H	1.32043300	2.52432100	0.80861300
O	-4.22605700	0.12229800	1.18218500
H	-3.68013500	0.57869900	1.84089300
H	-3.61537500	-0.59977500	0.87872700

HNE_t

Charge/multiplicity: 0 1

C	-4.39235900	-0.67803900	0.29644000
O	-5.33851500	-1.18044300	-0.28495000
H	-4.42184400	-0.51325300	1.39670100
C	-3.15109500	-0.24506500	-0.35762600
H	-3.09205500	-0.38020000	-1.43653100
C	-2.14118100	0.28848900	0.34804400
H	-2.24786000	0.41195200	1.42764200
C	-0.83212100	0.76365700	-0.22084200
H	-0.86667800	0.69971900	-1.31992600
C	0.34643200	-0.07535900	0.28916600
H	0.14656900	-1.12789600	0.04902000

H	0.37644000	0.00222100	1.38464700
C	1.69665600	0.35133700	-0.30229800
H	1.65099300	0.27463600	-1.39885000
H	1.86946300	1.40931300	-0.07250700
C	2.86917700	-0.49034600	0.21722800
H	2.68874600	-1.55169600	-0.01071000
H	2.91121600	-0.41782500	1.31421100
C	4.22462200	-0.07199500	-0.36744100
H	4.18400100	-0.14468900	-1.46370400
H	4.40487500	0.98805800	-0.13911000
C	5.39337000	-0.91183200	0.15525400
H	5.26097400	-1.97389000	-0.08736200
H	6.34554200	-0.58832600	-0.28191500
H	5.48512000	-0.83163000	1.24585500
O	-0.59623700	2.11695400	0.18993000
H	-1.29849300	2.66634200	-0.19483500

MIN_{1t}

Charge/multiplicity: -1 1

N	3.23909400	-0.01650400	0.04198700
H	2.58918600	-0.27149300	0.80134400
C	2.85737300	1.03427500	-0.88537400
H	3.61394700	1.00932200	-1.67974800
C	1.49899300	0.79232100	-1.57293100
C	2.93312300	2.45282300	-0.28649500
H	1.38384200	1.52707700	-2.37272500
H	1.50287100	-0.21388700	-2.00155700
O	2.54008600	3.42783700	-0.92663100
N	3.48927700	2.53437500	0.94895300
H	3.76568800	1.66393100	1.38375600
C	3.64358700	3.77981700	1.66826600
H	3.27792600	4.58235200	1.02491700
H	3.06241900	3.77571400	2.59907900
H	4.69628400	3.96910400	1.91425000
C	4.23831400	-0.90461000	-0.25823100
C	4.38138700	-2.04154800	0.74197900
H	3.44294600	-2.60153200	0.83433800
H	5.18192400	-2.70588300	0.40963500
H	4.62616600	-1.65313200	1.73806300
O	4.97394400	-0.79052800	-1.23858400
C	-0.72805400	-0.87697900	-0.43343000
H	-0.70135900	-1.09972500	0.63591200
C	0.07174300	-1.89758400	-1.14627000
H	0.00657900	-1.94769600	-2.23141100
C	0.81989100	-2.83723100	-0.49465200
H	1.34930200	-3.56791900	-1.13601500
C	-2.21583600	-0.83496600	-0.86000400
H	-2.26798700	-0.54463800	-1.91987700
C	-3.07071100	0.14462900	-0.03483400
H	-2.63768400	1.15197500	-0.08585000
H	-3.02955400	-0.16849800	1.01977700
C	-4.53202800	0.19649100	-0.49721200
H	-4.56618300	0.53325800	-1.54498700
H	-4.93885200	-0.82211900	-0.48818000
C	-5.41345000	1.11746500	0.35591000
H	-4.99335300	2.13487700	0.35291800
H	-5.38376300	0.78139300	1.40353600
C	-6.87374900	1.17514900	-0.11171100
H	-6.90611200	1.51423500	-1.15732600
H	-7.29413900	0.15918800	-0.10940200
O	0.96181800	-3.00351700	0.79425100
S	0.00327100	0.92445700	-0.50679600
O	-2.76651300	-2.14761000	-0.78265700

H	-2.40329500	-2.58419800	0.02397300
H	-1.67663900	-4.45809400	0.96251000
C	-7.75174000	2.09097400	0.74627700
H	-8.78856200	2.10807900	0.38752800
H	-7.76832500	1.75975600	1.79264200
H	-7.37973200	3.12363900	0.73474500
O	-1.61728400	-3.59568600	1.40285300
H	-0.65042700	-3.36281900	1.29310600
O	1.47433700	-0.74605300	2.18061300
H	1.22501300	-1.60371200	1.72452100
H	0.82676300	-0.10667800	1.83619200

TS_{1t}

Charge/multiplicity: -1 1

N	-4.12214000	-1.11049200	0.13485900
H	-4.40399400	-0.93119700	1.09340900
C	-2.68433000	-1.09548400	-0.06595700
H	-2.39733400	-1.98250100	-0.64170300
C	-2.26326500	0.16933800	-0.86265300
C	-2.06168100	-1.15221900	1.34611600
H	-2.97576400	0.27847700	-1.68364400
H	-2.31410200	1.05795400	-0.23216000
O	-2.76256000	-1.00708800	2.35214900
N	-0.73263200	-1.38265400	1.38540800
H	-0.23502300	-1.33677300	0.50137700
C	0.03713800	-1.26918700	2.62023300
H	0.94129300	-1.87855700	2.52922200
H	0.31461200	-0.22628000	2.82306100
H	-0.56913000	-1.65030300	3.44460600
C	-5.00802700	-1.52520700	-0.80438600
C	-6.46521600	-1.53008100	-0.36347700
H	-6.60599700	-1.26697400	0.68952500
H	-7.02589200	-0.82002100	-0.98134900
H	-6.88741100	-2.52409400	-0.54406100
O	-4.67629800	-1.86349800	-1.94105600
C	0.51260100	1.29280000	-0.71850300
H	0.42357900	1.04738100	0.34330300
C	0.17242100	2.76307800	-0.89161600
H	0.35879200	3.15748300	-1.89304200
C	-0.99278500	3.33574000	-0.26664500
H	-1.29178000	4.32135200	-0.69781700
C	1.96183700	0.92494800	-1.22416600
H	1.87054000	0.54235800	-2.25286500
C	2.58461100	-0.18672100	-0.35492800
H	1.89055500	-1.03771100	-0.29621600
H	2.70226800	0.20423500	0.66573700
C	3.93960900	-0.67192100	-0.88193700
H	3.81055800	-1.07317800	-1.89933600
H	4.60368000	0.19575100	-0.97638000
C	4.59833300	-1.73955900	0.00082000
H	3.92767000	-2.60808100	0.09175500
H	4.72062200	-1.34368600	1.02028100
C	5.96159200	-2.21109100	-0.52235200
H	5.84189500	-2.60479300	-1.54221200
H	6.63355700	-1.34520900	-0.60845200
O	-1.60328500	2.93603400	0.73861300
S	-0.59523600	0.07605500	-1.65109100
O	2.83200900	2.03148900	-1.32872800
H	2.76369800	2.55372300	-0.47379700
H	2.32170400	4.31754200	0.84225100
C	6.61630700	-3.27790800	0.36031000
H	7.58857200	-3.59186300	-0.03980300
H	6.78193900	-2.90409000	1.37893900

H	5.98502700	-4.17263800	0.43759000
O	2.10452800	3.37262200	0.79861200
H	1.08834800	3.27175100	-0.08635800
O	0.51968200	2.12191800	2.66267700
H	-0.30808400	2.29113000	2.17529700
H	1.18530900	2.60297700	2.10513900

MIN_2

Charge/multiplicity: -1 1

N	-4.63072700	0.80071200	-0.11810500
H	-4.70172800	1.55993400	-0.78746600
C	-3.30407900	0.63855700	0.45245700
H	-3.39399600	0.57051200	1.54269900
C	-2.65656800	-0.67425700	-0.06341200
C	-2.52494500	1.91712700	0.07952700
H	-3.39551100	-1.46368600	0.09462400
H	-2.45313600	-0.62047900	-1.13443700
O	-2.98336000	2.73322000	-0.72754200
N	-1.34327900	2.08956100	0.70686900
H	-0.95865600	1.29784600	1.21743300
C	-0.47482000	3.21148100	0.39174300
H	-1.01800000	4.15327600	0.51572500
H	0.37609500	3.19426600	1.07570500
H	-0.10295500	3.16448000	-0.63924700
C	-5.73359400	0.16424400	0.35224300
C	-7.03940200	0.53693000	-0.33577100
H	-7.45037200	-0.35346800	-0.82406500
H	-7.76165100	0.85531200	0.42304300
H	-6.93184500	1.32978600	-1.08256700
O	-5.69605700	-0.66758300	1.25853600
C	0.22304000	-0.96668300	-0.45578100
H	-0.14436300	-0.22663400	-1.17631500
C	0.51540900	-2.29693400	-1.15197800
H	0.71559400	-3.07537600	-0.40633800
C	-0.48826700	-2.81109600	-2.14242300
H	-0.27036400	-3.84292000	-2.50503300
C	1.48287400	-0.43914000	0.31050700
H	1.13140300	0.50649700	0.79893800
C	2.58243300	0.02826700	-0.69226900
H	2.14679600	0.66647500	-1.47944800
H	3.00679100	-0.85320700	-1.19606400
C	3.71069700	0.78855000	0.01750800
H	3.29323700	1.70374800	0.46701900
H	4.07211900	0.17966300	0.85559000
C	4.87924200	1.17310000	-0.89918500
H	4.50849000	1.77563800	-1.74367800
H	5.30835300	0.26273200	-1.34679900
C	5.99226300	1.94667200	-0.17919900
H	5.56912500	2.86040700	0.26292400
H	6.35965700	1.34575400	0.66401100
O	-1.44478300	-2.20994300	-2.59383200
S	-1.12226800	-1.19329900	0.82536300
O	1.91030200	-1.35517500	1.22106700
H	3.02626300	-2.46089100	0.77313400
H	1.45781800	-2.22787800	-1.72346400
C	7.16445700	2.32046700	-1.09142100
H	7.93938100	2.87388700	-0.54616900
H	7.63622200	1.42667800	-1.52003600
H	6.83393100	2.95026000	-1.92789800
O	3.83123200	-3.05994700	0.60295100
H	4.45756600	-2.44205100	0.19597400
O	4.02180500	-1.23450500	2.91179400
H	3.15470300	-1.07559800	2.44946600

H	4.27781000	-2.04634500	2.43651300

TS_2

Charge/multiplicity: -1 1

N	4.67696200	0.69456400	0.15583700
H	4.74736800	1.38443600	0.89643200
C	3.36384500	0.61527500	-0.45906200
H	3.48178400	0.64009200	-1.54825400
C	2.67493800	-0.72592100	-0.08789900
C	2.59878300	1.87236900	0.00520900
H	3.39058400	-1.51705100	-0.32412100
H	2.47972200	-0.76795500	0.98790900
O	3.04002000	2.59258700	0.90681100
N	1.45053800	2.13678000	-0.65200900
H	1.07565300	1.40988000	-1.25714000
C	0.59668600	3.25051700	-0.27288200
H	0.19828400	3.13326600	0.74224400
H	1.15990300	4.18807300	-0.31124700
H	-0.23658200	3.30351800	-0.97633200
C	5.78023400	0.09465800	-0.36307700
C	7.08148500	0.38140400	0.37172000
H	6.96530800	1.06066800	1.22203300
H	7.50292100	-0.56397600	0.72955100
H	7.79963700	0.81235900	-0.33382800
O	5.74196900	-0.63901300	-1.34996000
C	-0.19639400	-0.85633500	0.26273400
H	0.15874000	-0.04662500	0.91556500
C	-0.41139300	-2.15907900	1.08259400
H	-0.01180400	-3.03573600	0.56998600
C	0.19682800	-2.06397000	2.45288700
H	-0.13059600	-1.17162100	3.04010500
C	-1.48930500	-0.39294700	-0.49108700
H	-1.16174600	0.51409900	-1.06438300
C	-2.53308500	0.15155500	0.53278600
H	-2.06187800	0.88269600	1.21118000
H	-2.89085400	-0.67674300	1.16252900
C	-3.73315200	0.80232200	-0.16666100
H	-3.37947500	1.67149600	-0.74403400
H	-4.13833300	0.09642300	-0.90201300
C	-4.84267600	1.25646400	0.79088400
H	-4.43151200	1.95507400	1.53709700
H	-5.20874700	0.38941700	1.36301100
C	-6.02896100	1.92022900	0.07866800
H	-5.66971900	2.79514500	-0.48249200
H	-6.43140700	1.22548000	-0.67135200
O	0.98425900	-2.85090200	2.94224500
S	1.12946800	-1.10368700	-1.02478200
O	-1.95331800	-1.37410700	-1.30401600
H	-2.92997100	-2.48860500	-0.62375100
H	-1.49165600	-2.32918300	1.20037600
C	-7.14920400	2.35137000	1.02985200
H	-7.98008900	2.82030900	0.48785300
H	-7.55619800	1.49289000	1.57977600
H	-6.78749100	3.07502700	1.77226200
O	-3.66685500	-3.09471700	-0.26806000
H	-4.28833500	-2.45265800	0.10806000
O	-4.25111600	-1.54987000	-2.73427200
H	-3.35187900	-1.29364700	-2.39531300
H	-4.39706300	-2.32627000	-2.16396800

MIN_3

Charge/multiplicity: -1 1

N	4.81371500	0.49482400	0.25355200
H	4.90258100	1.26635000	0.90687400
C	3.52638500	0.43851600	-0.41813800
H	3.69212900	0.34186500	-1.49713200
C	2.72678600	-0.80795000	0.04986000
C	2.83808200	1.78894900	-0.12549500
H	3.38443800	-1.66695700	-0.10472300
H	2.52127800	-0.73787200	1.12354500
O	3.29226500	2.56634800	0.72119300
N	1.74777600	2.06544600	-0.87060100
H	1.33798500	1.30098200	-1.40340000
C	0.96168000	3.26869500	-0.65179300
H	0.45620900	3.25903500	0.32191600
H	1.60887300	4.14965300	-0.69207600
H	0.20871200	3.33900000	-1.43934800
C	5.89050200	-0.24209000	-0.12417200
C	7.17346600	0.04447400	0.64280200
H	7.06728600	0.82686600	1.40074000
H	7.50976400	-0.87710100	1.12972900
H	7.95262400	0.34007300	-0.06774500
O	5.84501500	-1.09166400	-1.01304500
C	-0.10691900	-0.61950900	0.38344100
H	0.30434800	0.25915800	0.90117500
C	-0.35767600	-1.74747700	1.40150600
H	0.59830500	-2.23610300	1.65257300
C	-0.89251200	-1.26588400	2.72994900
H	-0.44881900	-0.30591800	3.08971600
C	-1.36315000	-0.22248100	-0.46094900
H	-1.04907500	0.71868700	-0.98631900
C	-2.53391900	0.21071300	0.46718900
H	-2.18562500	0.95617300	1.20333500
H	-2.88004600	-0.66151600	1.04031200
C	-3.71675700	0.78754200	-0.32033800
H	-3.37172400	1.66339300	-0.89310200
H	-4.03913400	0.04424600	-1.05889600
C	-4.90330000	1.20066800	0.55994100
H	-4.57358400	1.93910100	1.30832800
H	-5.25277600	0.32815900	1.13319400
C	-6.08146600	1.78161100	-0.23350200
H	-5.73654100	2.65496700	-0.80632700
H	-6.41259200	1.04394700	-0.97741400
O	-1.69391000	-1.85785200	3.42386600
S	1.16326800	-1.15070800	-0.87339300
O	-1.67530800	-1.20916100	-1.34151000
H	-2.38699800	-2.55671200	-0.80102400
H	-1.01413400	-2.51865600	0.98574800
C	-7.26721200	2.18820300	0.64664200
H	-8.09155600	2.59801200	0.04932000
H	-7.65941300	1.32929000	1.20644400
H	-6.97687000	2.95257600	1.37957900
O	-2.95954600	-3.35528700	-0.53035500
H	-3.58432800	-2.95581300	0.09485500
O	-3.90765700	-1.71523200	-2.81838300
H	-3.07046700	-1.31522900	-2.46689300
H	-3.92439000	-2.51132600	-2.25513000

TS_3

Charge/multiplicity: -1 1

N	4.81529500	0.48425800	0.25704900
H	4.90794100	1.26172500	0.90378000

C	3.52907600	0.43185800	-0.41692900
H	3.69525300	0.33398400	-1.49585700
C	2.72450900	-0.81141400	0.05082400
C	2.84467600	1.78536200	-0.12821300
H	3.38031200	-1.67238100	-0.10102200
H	2.51721700	-0.73938600	1.12403400
O	3.30378200	2.56626600	0.71264200
N	1.75206500	2.06083500	-0.87033200
H	1.33909700	1.29530200	-1.39925200
C	0.97054100	3.26768800	-0.65542300
H	0.47094200	3.26627000	0.32135400
H	1.61955300	4.14684100	-0.70582400
H	0.21298800	3.33433800	-1.43889000
C	5.89607700	-0.24811300	-0.12444100
C	7.17087800	0.06016700	0.65057200
H	7.44852300	1.11645300	0.55134100
H	7.03789300	-0.14905100	1.71873800
H	7.98038400	-0.56111000	0.26340900
O	5.84882600	-1.09959300	-1.01045500
C	-0.10926900	-0.62267500	0.38255000
H	0.30255600	0.25434300	0.90265800
C	-0.36160200	-1.75297600	1.39768000
H	0.59379400	-2.24315900	1.64791300
C	-0.89650800	-1.27404200	2.72703500
H	-0.45118900	-0.31590600	3.08968500
C	-1.36488400	-0.22208100	-0.46105600
H	-1.04963200	0.72014800	-0.98384000
C	-2.53512300	0.20987300	0.46836800
H	-2.18570600	0.95175200	1.20759300
H	-2.88302200	-0.66400600	1.03785500
C	-3.71663400	0.79203900	-0.31717600
H	-3.36999300	1.67003700	-0.88566100
H	-4.03970600	0.05256600	-1.05926000
C	-4.90314200	1.20272000	0.56429500
H	-4.57259300	1.93628000	1.31709300
H	-5.25492100	0.32773600	1.13233000
C	-6.07938000	1.79051500	-0.22694800
H	-5.73221800	2.66662300	-0.79419200
H	-6.41106700	1.05789800	-0.97559100
O	-1.69958800	-1.86625100	3.41879900
S	1.16152100	-1.15165000	-0.87462000
O	-1.67836400	-1.20592500	-1.34428400
H	-2.39109600	-2.55414000	-0.80744800
H	-1.01870600	-2.52242000	0.97971600
C	-7.26537500	2.19405000	0.65426300
H	-8.08840400	2.60860100	0.05840100
H	-7.65959800	1.33260600	1.20872600
H	-6.97458600	2.95375900	1.39185200
O	-2.96433200	-3.35293800	-0.53875500
H	-3.58835800	-2.95459500	0.08793100
O	-3.91172500	-1.70510900	-2.82202600
H	-3.07391200	-1.30717100	-2.46964300
H	-3.92944900	-2.50260300	-2.26079500

MIN_4

Charge/multiplicity: -1 1

N	4.78357700	-0.68255900	-0.28651500
H	4.86886700	-1.48607800	-0.90039100
C	3.47610300	-0.55069500	0.33333500
H	3.60831900	-0.39272500	1.40958300
C	2.72923200	0.68474600	-0.23948000
C	2.75625400	-1.89478200	0.09455800
H	3.41061600	1.53266800	-0.13526600

H	2.53672400	0.54374700	-1.30811500
O	3.20838500	-2.72908200	-0.69715700
N	1.63854100	-2.09892700	0.82247900
H	1.23924800	-1.29512200	1.30240200
C	0.81939800	-3.28648900	0.64251800
H	0.32599600	-3.30209300	-0.33737800
H	1.44056200	-4.18282500	0.72681200
H	0.05531800	-3.30306700	1.42241000
C	5.87334800	0.02795400	0.10533100
C	7.17297100	-0.33877300	-0.59685200
H	7.06777000	-1.15540400	-1.31791600
H	7.55823900	0.54498300	-1.11655300
H	7.91498400	-0.62236600	0.15699100
O	5.82658800	0.91468000	0.95671500
C	-0.10657600	0.59836000	-0.62965900
H	0.29846000	-0.30023700	-1.11463700
C	-0.31018200	1.68323200	-1.71343400
H	-0.96751500	1.26258600	-2.48864100
C	-0.92585300	2.98362600	-1.22616600
H	-2.02222200	2.98774200	-1.10273800
C	-1.39608900	0.25834200	0.16633000
H	-1.09666900	-0.59372700	0.82807700
C	-2.49372100	-0.32328400	-0.77002500
H	-2.05920400	-1.04820100	-1.47935200
H	-2.91187900	0.49736200	-1.36893900
C	-3.62380300	-0.99784400	0.01995200
H	-3.23580600	-1.92107500	0.47944200
H	-3.91279400	-0.34453700	0.85229200
C	-4.85400600	-1.33667000	-0.83090500
H	-4.55499800	-1.96401500	-1.68647400
H	-5.25781500	-0.40811200	-1.26091600
C	-5.96508000	-2.05011300	-0.04949600
H	-5.56789400	-2.98254100	0.37814900
H	-6.25940500	-1.42581300	0.80534700
O	-0.27764200	4.00024600	-1.05048100
S	1.16343900	1.13868900	0.62363600
O	-1.79652800	1.34869700	0.88852900
H	-3.16782700	2.13546900	0.48808200
H	0.65034500	1.92823700	-2.18161800
C	-7.19960100	-2.36659100	-0.89909900
H	-7.97512000	-2.87414100	-0.31145200
H	-7.64266100	-1.45073600	-1.31096600
H	-6.94610900	-3.01832700	-1.74586600
O	-4.01380700	2.68757900	0.38215300
H	-3.73488300	3.54743000	0.73571300
O	-3.68177400	1.15286400	2.87277700
H	-2.85303900	1.10261900	2.32759300
H	-4.21559800	1.69368500	2.26264900

TS_4

Charge/multiplicity: -1 1

N	-4.42948600	0.78898500	-0.30112900
H	-4.44490300	1.76702000	-0.57441600
C	-3.22212600	0.39798300	0.40674800
H	-3.50381900	-0.10974300	1.33675900
C	-2.39165100	-0.59780300	-0.44664900
C	-2.48439300	1.71190600	0.74588000
H	-3.08157800	-1.38151700	-0.76824900
H	-2.01478900	-0.09731500	-1.34458900
O	-2.86880900	2.79579500	0.29243400
N	-1.42917300	1.59611800	1.57708700
H	-1.08064600	0.65819400	1.76778200
C	-0.61363300	2.74484900	1.93456300
H	0.14229400	2.42255000	2.65343600

H	-0.11336700	3.17807800	1.06010100
H	-1.23411000	3.52263500	2.39100900
C	-5.56568900	0.04033200	-0.31737700
C	-6.75117500	0.71110000	-1.00010800
H	-7.60807500	0.03594200	-0.96699900
H	-7.01417300	1.65081700	-0.49941200
H	-6.51874300	0.94587800	-2.04563700
O	-5.63099400	-1.08876600	0.16441200
C	0.47459000	-0.71666100	-0.45980900
H	0.21571900	0.32223800	-0.70413500
C	0.72705800	-1.48026100	-1.78073500
H	1.53459500	-0.96363200	-2.32045300
C	1.11831200	-2.94031300	-1.62485400
H	2.17481500	-3.14102400	-1.37932000
C	1.66262200	-0.78069500	0.53643600
H	1.34847700	-0.12403100	1.38749300
C	2.95538000	-0.11499300	-0.01588600
H	3.31696100	-0.67594400	-0.88897400
H	3.70303400	-0.26873900	0.77301200
C	2.86206100	1.37879600	-0.35370400
H	2.18258000	1.53813600	-1.20518100
H	2.41185500	1.91457300	0.49658000
C	4.21934100	2.01848300	-0.68014100
H	4.67901200	1.48555200	-1.52624400
H	4.89914200	1.87356500	0.17237600
C	4.13543000	3.51404500	-1.01231200
H	3.45908400	3.65901300	-1.86751100
H	3.67460100	4.04710400	-0.16787900
O	0.34181800	-3.85633700	-1.83177900
S	-0.99665800	-1.42142500	0.44196600
O	1.85398300	-2.07703300	0.93682000
H	3.23007300	-2.81803100	0.44807100
H	-0.17240400	-1.44757100	-2.40674900
C	5.49502500	4.14464000	-1.32818100
H	5.40027200	5.21267100	-1.56139800
H	6.18376300	4.05018800	-0.47886000
H	5.96882000	3.65766000	-2.19031900
O	4.08113700	-3.33929700	0.26088300
H	3.82318300	-4.23983100	0.51464800
O	3.77310200	-1.98301700	2.88596500
H	4.33912900	-2.43814100	2.23722100
H	2.92752200	-1.98840900	2.36157100

MIN_5

Charge/multiplicity: -1 1

N	-4.07458300	1.36046100	0.22439800
H	-4.07451200	1.87632700	1.10036800
C	-3.16140800	0.22867300	0.23549600
H	-3.73647200	-0.69181400	0.06494000
C	-2.11417100	0.35979600	-0.89769000
C	-2.56801000	0.19018300	1.67100600
H	-2.63935900	0.69595600	-1.79476100
H	-1.36259800	1.10830500	-0.62791000
O	-2.96923900	0.98882400	2.52832900
N	-1.64426600	-0.75103700	1.92551100
H	-1.28266800	-1.31112600	1.15526900
C	-1.02310300	-0.88637600	3.23495900
H	-1.77335000	-1.13752800	3.99379300
H	-0.27839100	-1.68233700	3.16433900
H	-0.53485200	0.04727000	3.53741900
C	-5.10300400	1.47889300	-0.65527900
C	-6.05639800	2.63416500	-0.38300800
H	-6.16097800	3.23157000	-1.29424000
H	-7.04610900	2.22979900	-0.14251100
H	-5.73278200	3.28498300	0.43523500

O	-5.26204400	0.72207800	-1.61252900
C	0.39942600	-0.67107400	-1.78658300
H	0.21463000	0.08130700	-2.56344200
C	1.16361400	-1.86918100	-2.37298100
H	2.05671000	-1.48718900	-2.88283500
C	1.58267300	-2.84288800	-1.27086000
H	2.66603100	-3.03153500	-1.17855900
C	1.27732700	-0.12022400	-0.62297100
H	0.61454600	0.41937700	0.08654000
C	2.28615200	0.93220600	-1.15135200
H	1.74623400	1.74408800	-1.66516300
H	2.93890000	0.45830300	-1.89953000
C	3.14824900	1.51709100	-0.02683200
H	2.49611900	2.03890300	0.69111500
H	3.60661700	0.68714700	0.52471500
C	4.23541600	2.48254000	-0.51506100
H	3.77263500	3.30501200	-1.08319300
H	4.89382700	1.95802000	-1.22412800
C	5.08650400	3.07118400	0.61804300
H	4.43184500	3.60090300	1.32529900
H	5.54566000	2.25029600	1.18629800
O	0.76933800	-3.62996300	-0.76732700
S	-1.28690100	-1.25194200	-1.24126600
O	1.90791300	-1.18306300	-0.01291300
H	1.43938000	-2.07551000	1.35616000
H	0.55450900	-2.40590600	-3.11043800
C	6.18004600	4.02405600	0.12623200
H	6.76796200	4.42769900	0.96010600
H	6.87540400	3.51375700	-0.55261500
H	5.75193800	4.87490700	-0.42005500
O	1.30937800	-2.87999200	1.93320100
H	1.04348400	-3.50853600	1.23235000
O	4.10426300	-2.42797400	1.06755900
H	3.56777300	-1.79679100	0.54012800
H	3.38347900	-2.83411000	1.58694000

TS_5

Charge/multiplicity: -1 1

N	-4.07445700	1.36176100	0.21933200
H	-4.08303100	1.86562500	1.10289200
C	-3.16438500	0.22741500	0.22798700
H	-3.74017800	-0.69133200	0.04976500
C	-2.11186300	0.36267600	-0.89961900
C	-2.57860700	0.17742900	1.66646100
H	-2.63307000	0.70401800	-1.79714800
H	-1.36092100	1.10938900	-0.62314700
O	-2.98896700	0.96518000	2.52959300
N	-1.65137500	-0.76135600	1.91730700
H	-1.28415200	-1.31408600	1.14437700
C	-1.03905900	-0.90764500	3.22969200
H	-1.79314800	-1.17213200	3.98021400
H	-0.28864200	-1.69795300	3.15575100
H	-0.55928000	0.02572000	3.54626500
C	-5.10770500	1.48258200	-0.65723100
C	-6.04359800	2.65006700	-0.36879100
H	-6.86023500	2.63804500	-1.09294400
H	-6.45860100	2.58535200	0.64423800
H	-5.50907300	3.60430400	-0.44716600
O	-5.26377700	0.73208400	-1.61909900
C	0.40318400	-0.66645400	-1.78902100
H	0.22041000	0.08707800	-2.56524300
C	1.16810200	-1.86418200	-2.37537900
H	2.06196600	-1.48186000	-2.88364300
C	1.58566100	-2.83910300	-1.27364200

H	2.66899600	-3.02730300	-1.17995700
C	1.27890900	-0.11754700	-0.62289000
H	0.61513900	0.42151700	0.08608100
C	2.28934700	0.93501300	-1.14801100
H	1.75086100	1.74779000	-1.66191600
H	2.94327100	0.46164400	-1.89549900
C	3.14967600	1.51811200	-0.02123200
H	2.49659300	2.03982600	0.69592400
H	3.60626300	0.68726900	0.53042700
C	4.23861600	2.48306300	-0.50652200
H	3.77764600	3.30637400	-1.07491200
H	4.89794700	1.95853500	-1.21472900
C	5.08802000	3.07008700	0.62865800
H	4.43249000	3.59988000	1.33505500
H	5.54535000	2.24836300	1.19716700
O	0.77204700	-3.62754100	-0.77265400
S	-1.28439300	-1.24787200	-1.24832800
O	1.90771500	-1.18150700	-0.01294100
H	1.43930700	-2.07653000	1.35494800
H	0.56002600	-2.40013600	-3.11424100
C	6.18334300	4.02235600	0.13962100
H	6.77003700	4.42489100	0.97488900
H	6.87953600	3.51192900	-0.53827500
H	5.75702200	4.87397100	-0.40687300
O	1.31027100	-2.88255300	1.92995400
H	1.04568000	-3.50978800	1.22741100
O	4.10546400	-2.42377300	1.06767100
H	3.56780300	-1.79342900	0.54036400
H	3.38523800	-2.83217700	1.58603300

P(R)

Charge/multiplicity: -1 1

N	-3.54005500	0.59399500	0.18273300
H	-3.43818800	1.31408900	0.89012200
C	-2.39138200	-0.29594400	0.08226400
H	-2.74709300	-1.32227200	-0.04436700
C	-1.53148100	0.09053900	-1.15384800
C	-1.63702800	-0.13194600	1.41841100
H	-2.22732500	0.30090900	-1.96981800
H	-0.96502600	1.00422100	-0.94789500
O	-1.72384400	0.94437400	2.03439800
N	-0.91600300	-1.17289200	1.85268000
H	-0.78081300	-2.04937400	1.30639600
C	-0.14191800	-1.06523800	3.07803100
H	-0.79228400	-1.04612000	3.96196800
H	0.52084400	-1.93085200	3.13966500
H	0.45943800	-0.14973400	3.08639800
C	-4.66871400	0.46907500	-0.55811300
C	-5.75764200	1.49024600	-0.25459800
H	-6.65738300	0.96097000	0.07744500
H	-5.47477800	2.22049500	0.51016100
H	-6.01420600	2.02178200	-1.17701600
O	-4.82240500	-0.40020000	-1.41612100
C	1.28210400	-0.45605100	-1.63878700
H	1.22176500	0.46621100	-2.22456000
C	2.31469800	-1.43348900	-2.22101400
H	3.15908000	-0.85231300	-2.61703700
C	2.77496600	-2.29786300	-1.01961200
H	3.87338600	-2.47825300	-1.07644300
C	1.83882500	-0.18465200	-0.21391700
H	1.02059300	-0.15733800	0.51707900
C	2.61256700	1.14522700	-0.11918700
H	3.34081500	1.20015000	-0.94186800
H	3.20094300	1.10206300	0.80720600

C	1.73433200	2.40305700	-0.10360500
H	1.16730300	2.47887400	-1.04345200
H	0.98504700	2.31223500	0.69656700
C	2.53101300	3.69973700	0.09736600
H	3.28624000	3.79222300	-0.69797300
H	3.09204200	3.63654800	1.04177600
C	1.65768100	4.96099700	0.11332900
H	1.10281500	5.02972300	-0.83354600
H	0.89939800	4.86489400	0.90326200
O	2.06779500	-3.38093700	-0.77694700
S	-0.39655700	-1.24089000	-1.72692000
O	2.72243600	-1.25226400	0.10129800
H	2.60471800	-2.65621900	1.79543200
H	1.92203700	-2.06007500	-3.02665100
C	2.45676300	6.24967500	0.32845300
H	1.80428300	7.13157000	0.33398600
H	2.99419500	6.22912400	1.28525200
H	3.20235600	6.39373800	-0.46427300
O	2.49757400	-3.62461900	1.82808700
H	2.45421900	-3.77033000	0.83121300
O	-0.13444100	-3.62846000	0.82384500
H	0.59109800	-3.77424400	1.46963800
H	0.42618700	-3.42952900	0.02664300

TS_2’

Charge/multiplicity: -1 1

N	4.70441800	0.59218100	0.13010800
H	4.77932900	1.40263700	0.73649100
C	3.41254800	0.46455000	-0.52186000
H	3.57029600	0.31535200	-1.59640100
C	2.65296000	-0.77394000	0.02588900
C	2.68863900	1.80972700	-0.29195600
H	3.34739800	-1.61477100	-0.04117500
H	2.39616600	-0.62738000	1.07923000
O	3.15657400	2.66318000	0.46887800
N	1.55063500	1.99151900	-0.99360500
H	1.14898700	1.17742800	-1.45486700
C	0.72232600	3.17122700	-0.80551400
H	0.25215600	3.18843900	0.18563700
H	1.33003800	4.07439100	-0.91197800
H	-0.05988900	3.17147400	-1.56761900
C	5.79642200	-0.13565800	-0.21765200
C	7.07672400	0.22332500	0.52320400
H	6.96741400	1.07552300	1.20116500
H	7.40988100	-0.64601300	1.10050400
H	7.85891400	0.44713700	-0.20956600
O	5.76654800	-1.03429400	-1.05814900
C	-0.20012000	-0.82853400	0.32780200
H	0.17205900	0.03452200	0.89000300
C	-0.43686200	-2.00242300	1.29540400
H	0.11084200	-2.90607500	0.98791600
C	-0.04935100	-1.75695800	2.72566900
H	-0.33000400	-2.58528500	3.41723300
C	-1.48215900	-0.44243300	-0.47751200
H	-1.15961900	0.41523500	-1.12326900
C	-2.53816200	0.17217900	0.49202200
H	-2.07596700	0.96042100	1.10892300
H	-2.88422900	-0.60679700	1.18796200
C	-3.74833700	0.74776400	-0.25388500
H	-3.40884100	1.56752800	-0.90700400
H	-4.15260300	-0.02369200	-0.92054600
C	-4.85497600	1.27060900	0.67160000
H	-4.44440900	2.03490100	1.35057800
H	-5.20404500	0.45133200	1.31978800

C	-6.05707000	1.85806600	-0.07982500
H	-5.71576500	2.68767900	-0.71604700
H	-6.45912900	1.09843000	-0.76449600
O	0.53220900	-0.78185100	3.16362200
S	1.13043300	-1.23966100	-0.91352900
O	-1.93193500	-1.49309000	-1.21625900
H	-2.81644500	-2.57994600	-0.42678600
H	-1.48548000	-2.33432900	1.27626300
C	-7.17253400	2.35322100	0.84557900
H	-8.01505100	2.76645400	0.27671600
H	-7.56265400	1.53812400	1.46890000
H	-6.81186000	3.13950500	1.52184700
O	-3.49677700	-3.19512800	0.02711200
H	-4.15167400	-2.55730200	0.35079700
O	-4.23373300	-1.89650500	-2.57313200
H	-3.34581600	-1.56639000	-2.26542800
H	-4.33567300	-2.63267500	-1.94420800

MIN_3’

Charge/multiplicity: -1 1

N	-4.87998000	0.58203900	-0.32273600
H	-4.97120700	1.38044600	-0.94263500
C	-3.58165900	0.47962800	0.31989900
H	-3.72744900	0.34235300	1.39744500
C	-2.81389100	-0.75874200	-0.21652600
C	-2.87264300	1.82670100	0.06252200
H	-3.49304100	-1.60910700	-0.12123200
H	-2.58305800	-0.63090600	-1.27895300
O	-3.33240600	2.64502500	-0.74080600
N	-1.75527500	2.05160900	0.78378200
H	-1.35820000	1.26872300	1.29705300
C	-0.95286100	3.24880500	0.59035300
H	-1.57115900	4.14175300	0.72327300
H	-0.15159500	3.25289400	1.33194500
H	-0.50975700	3.28592800	-0.41208200
C	-5.95931700	-0.15334900	0.05270300
C	-7.25646100	0.18275000	-0.66800400
H	-7.62896400	-0.71756000	-1.16792000
H	-8.00718700	0.47783500	0.07285600
H	-7.15352300	0.98245100	-1.40800900
O	-5.90326900	-1.03745400	0.90647900
C	0.04935400	-0.70431900	-0.53402400
H	-0.36734800	0.13532100	-1.10354000
C	0.38219600	-1.87916300	-1.45994300
H	-0.53557300	-2.27261200	-1.92327700
C	1.07720500	-3.03846200	-0.76013000
H	0.57781100	-3.41565100	0.14756200
C	1.33446800	-0.30407100	0.24803100
H	1.00750700	0.40111200	1.04883800
C	2.31165600	0.49985200	-0.65343300
H	1.77983800	1.29285700	-1.20530400
H	2.73579900	-0.18579700	-1.39844200
C	3.45646100	1.11859000	0.16319600
H	3.06264300	1.95955000	0.75689400
H	3.81803600	0.37636000	0.88530500
C	4.62762400	1.60594600	-0.69835200
H	4.26142800	2.30251500	-1.47026900
H	5.04700800	0.74351800	-1.23574300
C	5.74276000	2.28741400	0.10494500
H	5.32966300	3.15611900	0.63907600
H	6.09975500	1.59528800	0.87987800
O	1.97506800	-3.68268100	-1.29744500
S	-1.27277400	-1.18618700	0.70082000
O	1.89299100	-1.44752200	0.76117800

H	3.42349600	-1.88108500	0.12326900
H	1.03665600	-1.54601900	-2.27409600
C	6.92441100	2.73828800	-0.75921100
H	7.70642400	3.21758400	-0.15651400
H	7.38157100	1.88654300	-1.27877200
H	6.60782300	3.45908400	-1.52497400
O	4.29088400	-2.28984100	-0.15912000
H	3.95951000	-3.09671200	-0.58789600
O	3.92108500	-1.58627800	2.64187100
H	3.05272100	-1.46389900	2.18721000
H	4.41088800	-2.00463600	1.90920400

TS_3'

Charge/multiplicity: -1 1

N	-4.88239900	0.57052900	-0.32455100
H	-4.97725500	1.37264000	-0.94010300
C	-3.58483400	0.47310200	0.32012800
H	-3.73060100	0.33543200	1.39771000
C	-2.81192600	-0.76237100	-0.21554100
C	-2.87989100	1.82291400	0.06521800
H	-3.48859700	-1.61491100	-0.12142900
H	-2.58069100	-0.63353400	-1.27777200
O	-3.34382800	2.64298500	-0.73394600
N	-1.76100500	2.04842300	0.78407800
H	-1.36087000	1.26513000	1.29443300
C	-0.96233400	3.24834500	0.59245800
H	-1.58254900	4.13929800	0.72985000
H	-0.15910000	3.25217600	1.33193700
H	-0.52194200	3.28989500	-0.41102300
C	-5.96506400	-0.16049100	0.05625400
C	-7.25313300	0.19155100	-0.67595200
H	-8.06160200	-0.43283600	-0.29170600
H	-7.51379100	1.24704800	-0.53245600
H	-7.14801300	0.01919000	-1.75372600
O	-5.90703600	-1.04348600	0.91007400
C	0.05128100	-0.70362100	-0.53283100
H	-0.36600100	0.13597300	-1.10200800
C	0.38420500	-1.87816900	-1.45907500
H	-0.53358000	-2.27188000	-1.92217100
C	1.07990800	-3.03732600	-0.75971800
H	0.58121300	-3.41457500	0.14832800
C	1.33662900	-0.30295600	0.24866600
H	1.00968900	0.40144400	1.05016600
C	2.31257500	0.50234800	-0.65290500
H	1.77983900	1.29582800	-1.20321100
H	2.73613600	-0.18225000	-1.39922600
C	3.45803100	1.12049800	0.16326800
H	3.06461100	1.96083200	0.75811100
H	3.82032700	0.37763900	0.88436500
C	4.62841700	1.60881900	-0.69878800
H	4.26153900	2.30610900	-1.46973300
H	5.04746700	0.74696200	-1.23735800
C	5.74413800	2.28959000	0.10429200
H	5.33141700	3.15779000	0.63953400
H	6.10171800	1.59675900	0.87832600
O	1.97741200	-3.68148900	-1.29773800
S	-1.27007200	-1.18609500	0.70253900
O	1.89641100	-1.44633200	0.76064200
H	3.42649700	-1.87894100	0.12124100
H	1.03824700	-1.54465900	-2.27342200
C	6.92514800	2.74127900	-0.76031200
H	7.70761300	3.21998800	-0.15773600
H	7.38191400	1.89002400	-1.28102100
H	6.60800900	3.46281100	-1.52515600

O	4.29373400	-2.28751200	-0.16189700
H	3.96211700	-3.09442900	-0.59041000
O	3.92582900	-1.58593500	2.63975700
H	3.05707400	-1.46335300	2.18590600
H	4.41507000	-2.00365200	1.90633900

MIN_4'

Charge/multiplicity: -1 1

N	4.84722000	0.32728800	0.32198300
H	4.99936400	0.56202500	1.29727000
C	3.50631600	0.60817500	-0.15758000
H	3.57774400	1.15248900	-1.10594600
C	2.74627200	-0.71887100	-0.42223200
C	2.84907900	1.50696500	0.91051000
H	3.40707000	-1.34241500	-1.02854900
H	2.55435000	-1.24635200	0.51680200
O	3.37434400	1.67354900	2.01467100
N	1.69538000	2.10695100	0.54514900
H	1.25735000	1.79805000	-0.31774300
C	0.93374000	2.92465100	1.47605800
H	0.17008500	3.47198200	0.91924400
H	0.44475300	2.32072500	2.25041900
H	1.59995600	3.63791000	1.96846000
C	5.88156500	0.02020900	-0.50515200
C	7.23246100	-0.13654000	0.17569700
H	7.19650700	0.01224800	1.25924000
H	7.62025000	-1.13928700	-0.03200400
H	7.93544900	0.58166700	-0.25968200
O	5.74375400	-0.13113700	-1.71822500
C	-0.10875500	-0.97350200	-0.07479700
H	0.09532100	-0.32911000	0.78654700
C	-0.18474600	-2.45284000	0.33685800
H	0.68626100	-3.03658400	0.01945600
C	-1.49360600	-3.04034800	-0.27160900
H	-1.35749400	-3.15254300	-1.37945100
C	-1.53345000	-0.65084800	-0.65322400
H	-1.47102700	-0.64205300	-1.76082800
C	-2.07758200	0.70377300	-0.19278500
H	-1.37668200	1.49000900	-0.51562500
H	-2.08414600	0.71471200	0.90716300
C	-3.48472200	1.02232300	-0.71496700
H	-3.47672700	0.99437200	-1.81544700
H	-4.17289400	0.23295500	-0.38939300
C	-4.00186800	2.38873900	-0.24772500
H	-3.30332600	3.17881000	-0.56736600
H	-4.00773900	2.41654300	0.85264500
C	-5.40793500	2.72260800	-0.76347200
H	-5.40533000	2.69988100	-1.86281400
H	-6.10366000	1.93432200	-0.44543700
O	-2.06913500	-4.02065500	0.32501400
S	1.16531700	-0.55592000	-1.35848000
O	-2.36214800	-1.69222500	-0.22125400
H	-3.29094800	-1.99428000	1.84232400
H	-0.27585900	-2.54328100	1.42596700
C	-5.92212200	4.08338500	-0.28473100
H	-6.92842500	4.29105500	-0.66919900
H	-5.97108800	4.12669000	0.81099700
H	-5.26566100	4.89842900	-0.61724500
O	-3.59440200	-2.85542300	2.17675300
H	-3.03457800	-3.44089400	1.57765300
O	-5.19666500	-2.13551100	-0.07386200
H	-4.31490300	-2.03256500	-0.47992700

H	-4.92112800	-2.51652800	0.78835100

TS_4’

Charge/multiplicity: -1 1

N	4.84755600	0.31634600	0.31978200
H	4.99986900	0.56116800	1.29322400
C	3.50868300	0.60064200	-0.16306500
H	3.58246500	1.14122500	-1.11347700
C	2.74399700	-0.72456900	-0.42337000
C	2.85307200	1.50734700	0.89967500
H	3.40336100	-1.35245900	-1.02685000
H	2.55032600	-1.24818100	0.51748000
O	3.38011100	1.68218200	2.00176500
N	1.69888100	2.10511700	0.53212000
H	1.25920400	1.79033900	-0.32786400
C	0.93943400	2.92993500	1.45848500
H	0.17471700	3.47330300	0.89923000
H	0.45188700	2.33194700	2.23836400
H	1.60677900	3.64670700	1.94425200
C	5.88838100	0.01565500	-0.50454600
C	7.22993400	-0.12854800	0.20027200
H	7.50380400	0.79750100	0.72003800
H	7.19341600	-0.93023700	0.94731700
H	7.99636000	-0.36421600	-0.54003500
O	5.75318600	-0.13956400	-1.71673100
C	-0.11085900	-0.97620100	-0.07637400
H	0.09501100	-0.33194800	0.78466400
C	-0.18894500	-2.45531400	0.33569600
H	0.68093100	-3.04049900	0.01786400
C	-1.49911000	-3.04079200	-0.27184200
H	-1.36381900	-3.15341000	-1.37974800
C	-1.53552500	-0.65131000	-0.65359500
H	-1.47407500	-0.64233600	-1.76124200
C	-2.07707100	0.70401600	-0.19221300
H	-1.37541200	1.48925400	-0.51582200
H	-2.08206100	0.71476300	0.90774600
C	-3.48447100	1.02487400	-0.71231500
H	-3.47802700	0.99774600	-1.81282400
H	-4.17333700	0.23624500	-0.38640400
C	-3.99900000	2.39165800	-0.24326800
H	-3.29990500	3.18100500	-0.56348400
H	-4.00300100	2.41866600	0.85712900
C	-5.40548300	2.72780200	-0.75641600
H	-5.40476900	2.70591900	-1.85577700
H	-6.10172700	1.94020500	-0.43780800
O	-2.07575100	-4.02019400	0.32527000
S	1.16347600	-0.56118500	-1.36065700
O	-2.36547700	-1.69150400	-0.22107100
H	-3.29411900	-1.99246700	1.84385100
H	-0.27954300	-2.54538000	1.42488500
C	-5.91701500	4.08889800	-0.27574400
H	-6.92369700	4.29821500	-0.65831700
H	-5.96402800	4.13141400	0.82010000
H	-5.26002300	4.90330900	-0.60875500
O	-3.59835900	-2.85345500	2.17794500
H	-3.03941800	-3.43929300	1.57830900
O	-5.20048500	-2.13145500	-0.07201100
H	-4.31880000	-2.02946400	-0.47848400
H	-4.92499000	-2.51293700	0.79001200

MIN_5’

Charge/multiplicity: -1 1

N	4.86018600	0.28851200	0.38504300
H	4.97429900	0.43653000	1.38256000
C	3.52932900	0.58879400	-0.11102100
H	3.61697100	1.23987900	-0.98838300
C	2.81554800	-0.71775700	-0.54993600
C	2.80938400	1.34264100	1.02787700
H	3.52221200	-1.26663500	-1.17612800
H	2.57952200	-1.33835700	0.31915900
O	3.30671000	1.41415800	2.15528600
N	1.63771700	1.92571700	0.69626000
H	1.23545800	1.68906500	-0.20637400
C	0.80359500	2.58715600	1.68822700
H	1.43175900	3.20295000	2.33612600
H	0.08194300	3.22524300	1.17308200
H	0.25902900	1.86864400	2.31286600
C	5.92557200	0.07172400	-0.42990800
C	7.25795600	-0.11749500	0.27946400
H	7.68819100	-1.07758200	-0.02364200
H	7.94931900	0.66717400	-0.04651300
H	7.18055000	-0.09161900	1.37073700
O	5.83034300	0.02308600	-1.65590700
C	-0.04584600	-1.07423800	-0.41463800
H	0.07983500	-0.55268100	0.53679500
C	-0.11505700	-2.57983100	-0.15696600
H	0.05126600	-3.14155200	-1.08429200
C	-1.58114200	-2.72431700	0.32992500
H	-2.00076800	-3.72908500	0.08556600
C	-1.45248200	-0.73661600	-1.01070500
H	-1.37383400	-0.58583200	-2.10179300
C	-2.05506100	0.52572300	-0.37494500
H	-1.34770200	1.36031600	-0.51679500
H	-2.13566200	0.33573700	0.70212400
C	-3.42649400	0.91986900	-0.93521200
H	-3.34848900	1.07708900	-2.02310400
H	-4.12219200	0.08602000	-0.78397300
C	-3.99758800	2.18478200	-0.28109400
H	-3.29967900	3.02612600	-0.42278900
H	-4.06667300	2.02649700	0.80544700
C	-5.37957100	2.58244000	-0.81598200
H	-5.31590700	2.74566800	-1.90190700
H	-6.07291500	1.74245100	-0.67418700
O	-1.79067100	-2.27285100	1.53738500
S	1.28619600	-0.48234300	-1.55526400
O	-2.24610300	-1.89149500	-0.79714400
H	-3.28417600	-2.45154400	2.00268900
H	0.59379000	-2.91714200	0.60632800
C	-5.95153400	3.83557500	-0.14629300
H	-6.93877900	4.09381800	-0.54977100
H	-6.06422600	3.69016200	0.93578700
H	-5.29538200	4.70362900	-0.29479400
O	-4.26444400	-2.63183400	2.26103600
H	-4.33438300	-3.59263500	2.15021000
O	-5.08816400	-2.15365500	-0.38704100
H	-4.16496600	-2.06563700	-0.69776900
H	-4.94390300	-2.21877700	0.58615400

TS_5’

Charge/multiplicity: -1 1

N	4.86063400	0.28054000	0.38165500
H	4.97588700	0.44152200	1.37770100
C	3.53147100	0.58347800	-0.11704100
H	3.62106700	1.23074000	-0.99717600

C	2.81341800	-0.72234800	-0.55087400
C	2.81301300	1.34633800	1.01710100
H	3.51876200	-1.27570100	-1.17469600
H	2.57588200	-1.33896500	0.32063900
O	3.31219300	1.42753700	2.14308600
N	1.64066500	1.92668400	0.68292100
H	1.23695700	1.68312400	-0.21728000
C	0.80866200	2.59673300	1.67079500
H	1.43852900	3.21602900	2.31367900
H	0.08761700	3.23242000	1.15181300
H	0.26337200	1.88374000	2.30112500
C	5.93120800	0.06753200	-0.43041100
C	7.25377700	-0.11167200	0.30247700
H	8.04690400	-0.27090000	-0.43012400
H	7.49297100	0.77221000	0.90598100
H	7.21100300	-0.97353700	0.97891300
O	5.83705800	0.01104400	-1.65546600
C	-0.04784900	-1.07711400	-0.41540900
H	0.07956700	-0.55543300	0.53575700
C	-0.11870600	-2.58257000	-0.15731800
H	0.04619600	-3.14468000	-1.08466600
C	-1.58452000	-2.72526400	0.33079700
H	-2.00554800	-3.72956500	0.08690100
C	-1.45463900	-0.73783500	-1.01013000
H	-1.37687000	-0.58712700	-2.10128500
C	-2.05512900	0.52516900	-0.37371500
H	-1.34695000	1.35893900	-0.51621000
H	-2.13488100	0.33522400	0.70342200
C	-3.42665200	0.92094500	-0.93259200
H	-3.34953300	1.07821900	-2.02054000
H	-4.12316200	0.08787300	-0.78078200
C	-3.99567700	2.18641900	-0.27772800
H	-3.29694300	3.02698700	-0.41996200
H	-4.06388600	2.02805100	0.80885400
C	-5.37772500	2.58574500	-0.81118800
H	-5.31492700	2.74918200	-1.89713100
H	-6.07186900	1.74649700	-0.66893000
O	-1.79253200	-2.27342200	1.53838300
S	1.28433400	-0.48743600	-1.55709100
O	-2.24943300	-1.89179300	-0.79584000
H	-3.28564400	-2.45136300	2.00519300
H	0.59042000	-2.92056000	0.60541600
C	-5.94762300	3.83935400	-0.14061200
H	-6.93496000	4.09884400	-0.54306700
H	-6.05944300	3.69377900	0.94153800
H	-5.29062100	4.70669800	-0.28950000
O	-4.26579200	-2.63117800	2.26437200
H	-4.33657800	-3.59180800	2.15260000
O	-5.09098500	-2.15108100	-0.38295700
H	-4.16795900	-2.06379500	-0.69441800
H	-4.94604300	-2.21655300	0.59010400

P(S)

Charge/multiplicity: -1 1

N	-4.65947300	-0.50443500	0.29898100
H	-4.79265000	-0.57164000	1.30342600
C	-3.28664500	-0.71603900	-0.12341200
H	-3.27097700	-1.47068500	-0.91837000
C	-2.69307200	0.59889200	-0.69524200
C	-2.53919200	-1.24969900	1.12185700
H	-3.44716600	1.02385600	-1.36090200
H	-2.50092400	1.31954800	0.10473800
O	-3.09341000	-1.26274900	2.22599200
N	-1.28926900	-1.70171300	0.90035000

H	-0.89228400	-1.53363100	-0.01913800
C	-0.39601300	-2.11825500	1.97768300
H	-1.00740600	-2.46291300	2.81361800
H	0.22738000	-2.94564900	1.62308300
H	0.24640900	-1.29130000	2.30767700
C	-5.70975300	-0.47683600	-0.56059000
C	-7.07871900	-0.35464600	0.09262100
H	-7.03935300	-0.30457000	1.18508200
H	-7.57455900	0.54538600	-0.28598900
H	-7.69152900	-1.21302600	-0.20287600
O	-5.57834200	-0.53519900	-1.78333100
C	0.13793500	1.18859900	-0.65385100
H	0.08438000	0.73414600	0.33771600
C	0.09280600	2.71112300	-0.52841200
H	-0.12362900	3.16834700	-1.50264200
C	1.54865000	3.01831200	-0.08158000
H	1.87464800	4.01741100	-0.44931000
C	1.54708900	0.93067300	-1.26431700
H	1.45889400	0.81742000	-2.36140200
C	2.23023300	-0.31939200	-0.69310400
H	1.61206900	-1.20093500	-0.93029600
H	2.25238800	-0.21996300	0.39858900
C	3.65052400	-0.53120900	-1.22812900
H	3.61954600	-0.65312000	-2.32289400
H	4.23039300	0.37816200	-1.03098100
C	4.36040200	-1.73755300	-0.60078900
H	3.76544200	-2.64872100	-0.77233000
H	4.40061100	-1.59919900	0.48930600
C	5.78256700	-1.95919100	-1.13197500
H	5.74657800	-2.10058400	-2.22237600
H	6.37459800	-1.04897600	-0.96232300
O	1.78460800	2.81595800	1.20552200
S	-1.16073800	0.39562000	-1.70468800
O	2.30219400	2.10559100	-1.01107200
H	2.44657400	0.59946400	2.68131900
H	-0.63425400	3.06730200	0.20809400
C	6.49143500	-3.15446100	-0.48792800
H	7.50529500	-3.28659200	-0.88664300
H	6.57639700	-3.02554900	0.59862900
H	5.94099500	-4.08772900	-0.66594100
O	1.46915600	0.60366800	2.70236600
H	1.32663800	1.41432600	2.13816400
O	4.03748200	1.79614400	2.16950600
H	3.28805900	2.23476500	1.65102000
H	4.00744100	2.28857000	3.00479900

TS_{1C1}

Charge/multiplicity: -1 1

N	-3.64441800	1.45694100	-0.31597800
H	-3.54896700	2.34829700	0.16331500
C	-2.67773600	0.46734100	0.13250400
H	-3.20543300	-0.45436700	0.39843300
C	-1.65521200	0.14549800	-0.99868400
C	-2.02189600	1.08819500	1.39538900
H	-2.14404100	0.33572800	-1.95650600
H	-0.78293100	0.80165400	-0.92808100
O	-2.19515300	2.30259700	1.61904400
N	-1.30297900	0.29696700	2.19628200
H	-1.03033500	-0.73257600	2.06516600
C	-0.68966700	0.87278300	3.38300400
H	0.04790200	1.64572400	3.12985200
H	-1.44118300	1.33376500	4.03566700

H	-0.19614600	0.05163200	3.90544600
C	-4.67170300	1.19080900	-1.15711500
C	-5.61191600	2.36161700	-1.41819900
H	-6.62692400	2.07313100	-1.12447200
H	-5.33427200	3.27527300	-0.88312400
H	-5.63170700	2.57191700	-2.49299400
O	-4.84753700	0.09423800	-1.68978300
C	0.70976200	-1.60390800	-1.14804200
H	0.90960800	-1.25664600	-2.16910500
C	1.06629200	-3.10616500	-1.07372500
H	0.42518600	-3.66084900	-1.77218700
C	2.45785900	-3.51604200	-1.34771500
H	2.55552500	-4.55516900	-1.73107700
C	1.45246700	-0.64341600	-0.15576000
H	0.70756800	-0.14631400	0.46959700
C	2.24481600	0.43159800	-0.92577400
H	1.56822300	0.93768600	-1.63070400
H	3.00951500	-0.06921700	-1.53799700
C	2.90551100	1.46773300	-0.00970300
H	2.12736300	1.97631800	0.57931900
H	3.54002900	0.94239000	0.71446100
C	3.73603000	2.51478700	-0.76275300
H	3.09616900	3.04246300	-1.48667000
H	4.51089300	2.00678700	-1.35704800
C	4.40366800	3.54201700	0.16090600
H	3.63046000	4.05227400	0.75292500
H	5.04132600	3.01493900	0.88497900
O	3.48863600	-2.87403100	-1.14774900
S	-1.14348600	-1.61960000	-0.94400000
O	2.29409200	-1.31202200	0.77684400
H	2.94992100	-1.80406000	0.24021500
H	-0.16119700	-3.14076700	1.92820400
C	5.23931800	4.58320200	-0.58941200
H	5.69849700	5.30283000	0.09976300
H	6.04815800	4.10882400	-1.16013500
H	4.62445400	5.15084700	-1.29977200
O	-0.13849900	-2.04818800	2.47731700
H	0.74872900	-1.77107600	2.19408700
O	0.01349200	-4.21488000	1.36357000
H	0.76373300	-3.54951200	-0.04659800
H	0.78162400	-4.55369100	1.85343800

MIN_{1C1}

Charge/multiplicity: -1 1

N	3.94037100	-1.51702400	-0.39381300
H	3.73889500	-2.51127400	-0.39709600
C	2.82921100	-0.69335400	0.06137400
H	3.21846500	0.10062500	0.70505500
C	2.10797500	-0.05005800	-1.15760500
C	1.91835300	-1.65547500	0.85006800
H	2.88044400	0.18773300	-1.89275800
H	1.42226500	-0.77240500	-1.61431200
O	1.90392400	-2.86087000	0.55289200
N	1.18114000	-1.13441900	1.83865600
H	1.13839200	-0.12497000	2.04625500
C	0.26996400	-1.97088700	2.60146000
H	-0.51851900	-2.39406600	1.96753000
H	0.80669900	-2.80252700	3.07182400
H	-0.18544600	-1.34804300	3.37273100
C	5.14993200	-1.02613600	-0.76100200
C	6.17189900	-2.07370500	-1.18305500
H	7.05707600	-1.98333600	-0.54446000
H	5.79729900	-3.10063700	-1.12699800

H	6.48952000	-1.86752200	-2.21080200
O	5.42012700	0.17468300	-0.75986600
C	-0.58664200	1.24439700	-1.40623900
H	-0.46215200	0.67743100	-2.33590800
C	-1.14464500	2.59794900	-1.74330800
H	-1.00334800	2.92257500	-2.77241500
C	-1.64236700	3.53100900	-0.87515200
H	-1.91267000	4.50113400	-1.33556800
C	-1.40391300	0.34414400	-0.44691600
H	-0.82228500	-0.57375700	-0.27578300
C	-2.74072600	-0.06370000	-1.10489900
H	-2.53903400	-0.50072000	-2.09492900
H	-3.33193000	0.84499900	-1.27737100
C	-3.53833500	-1.05782000	-0.25342800
H	-2.95205500	-1.98162600	-0.12688300
H	-3.66088200	-0.63175600	0.74958600
C	-4.91204000	-1.41067000	-0.83779100
H	-4.78869300	-1.82701100	-1.84971400
H	-5.50157100	-0.48945600	-0.95931900
C	-5.70366000	-2.40479500	0.02228600
H	-5.11845900	-3.32846100	0.13972300
H	-5.82239400	-1.99075000	1.03368800
O	-1.85747200	3.43869800	0.40650300
S	1.20185300	1.51955300	-0.81227600
O	-1.63471800	0.90977800	0.83152800
H	-1.80513100	1.90833000	0.71220100
H	0.43529700	2.18878100	2.64298500
C	-7.08161700	-2.74618800	-0.55235300
H	-7.61936200	-3.45829200	0.08607900
H	-7.70621900	-1.84854800	-0.64685800
H	-6.99733500	-3.19439700	-1.55093600
O	0.22231800	1.25208900	2.86663600
H	-0.48307000	1.05702300	2.20566900
O	0.48789600	3.82618700	1.78387900
H	1.07309800	3.49173700	1.08413100
H	-0.40404700	3.78364000	1.34396300

HNE_{c1}

Charge/multiplicity: 0 1

C	2.45226000	1.99229400	-0.04917400
O	1.92450700	1.87656600	-1.14504500
H	2.97982100	2.93579700	0.20928300
C	2.48297900	0.98158000	1.02357000
H	2.90780400	1.33050400	1.96360400
C	2.08080900	-0.30141800	0.92806500
H	2.19032200	-0.93910500	1.80682900
C	1.51650900	-1.02766300	-0.26482100
H	1.65816100	-0.43319000	-1.17298900
C	0.02355300	-1.34789200	-0.09501300
H	-0.10691000	-1.93216900	0.82661300
H	-0.24535500	-2.01306200	-0.92590500
C	-0.89748800	-0.12212000	-0.08295500
H	-0.63530900	0.52972900	0.76164800
H	-0.72599100	0.47257900	-0.98999200
C	-2.38212700	-0.49839700	0.01194800
H	-2.54973100	-1.10019500	0.91782900
H	-2.64908400	-1.14597200	-0.83643600
C	-3.31863400	0.71662600	0.03317100
H	-3.05403700	1.36277500	0.88243000
H	-3.15027900	1.31837900	-0.87108700
C	-4.79904900	0.33628300	0.12479800
H	-5.00678100	-0.23941600	1.03583100
H	-5.44110700	1.22512900	0.14089200

H	-5.10595000	-0.27879800	-0.73065800
O	2.18441600	-2.29576300	-0.37826600
H	3.11017000	-2.11517500	-0.60894900

TS_{1C2}

Charge/multiplicity: -1 1

N	-3.24770700	1.69473800	-0.08179600
H	-2.97597400	2.31756800	0.67091300
C	-2.52241500	0.43180000	-0.09483700
H	-3.21094500	-0.36321900	-0.39420600
C	-1.36214100	0.50076000	-1.12326700
C	-2.02583800	0.22981300	1.35000800
H	-1.78220500	0.89110800	-2.05430200
H	-0.59990900	1.20591500	-0.77747500
O	-1.70409500	1.22535000	2.01820900
N	-1.98236700	-1.02823800	1.81068900
H	-2.17019400	-1.83462000	1.19505300
C	-1.41866300	-1.32542200	3.11915100
H	-0.32348000	-1.28678000	3.09263300
H	-1.78589500	-0.60703000	3.85728500
H	-1.73186700	-2.33268800	3.40693700
C	-4.21264000	2.02906100	-0.97443900
C	-4.85019800	3.39470700	-0.75531900
H	-5.92795600	3.26409700	-0.61065800
H	-4.44065200	3.93779000	0.10222200
H	-4.71362900	4.00038600	-1.65750300
O	-4.56243100	1.29396000	-1.89793200
C	1.21966600	-1.01761900	-0.96775500
H	1.61171400	-0.21600500	-1.60796700
C	1.77693400	-2.38604700	-1.36634600
H	1.54724100	-2.63458300	-2.40760400
C	3.11532400	-2.78668800	-1.01552800
H	3.48575700	-2.40701900	-0.03631400
C	1.42861900	-0.56030300	0.50725000
H	0.57903200	0.08182900	0.78622800
C	2.69300200	0.31470500	0.66040600
H	3.54132300	-0.15497700	0.14644900
H	2.93778900	0.31668500	1.73034200
C	2.52454600	1.76283600	0.18286700
H	2.24567600	1.78191200	-0.88086100
H	1.68758900	2.22565000	0.72703100
C	3.78625300	2.61529800	0.37623700
H	4.62293900	2.15591000	-0.17114100
H	4.07470400	2.60185400	1.43810100
C	3.62066600	4.06966300	-0.08323700
H	3.33059600	4.08337900	-1.14372900
H	2.78666600	4.52996300	0.46587000
O	3.82601800	-3.58456800	-1.64629600
S	-0.59676700	-1.12815400	-1.50024500
O	1.53731300	-1.61610000	1.45089000
H	0.99657700	-2.39327600	1.15646700
H	0.97192400	-3.30153800	-0.50007400
C	4.88375000	4.91434500	0.10854500
H	4.73229600	5.94776100	-0.22728600
H	5.18257200	4.94899900	1.16421800
H	5.72806600	4.50159600	-0.45851400
O	0.32848400	-3.79660400	0.35499000
H	0.81463400	-4.60045700	0.60138700
O	-2.33259600	-3.47229400	0.33477700
H	-2.37749400	-3.08802500	-0.55608200
H	-1.36085800	-3.70663700	0.38474100

MIN_{1C2}

Charge/multiplicity: -1 1

N	-3.33224500	1.91745300	-0.07705400
H	-3.00288100	2.54963000	0.64371700
C	-2.66715300	0.62048400	-0.08121000
H	-3.40128500	-0.14028800	-0.36056100
C	-1.51944900	0.62065500	-1.12331200
C	-2.16475500	0.41266000	1.35972000
H	-1.93998700	0.98628300	-2.06447500
H	-0.74163100	1.32529000	-0.80749600
O	-1.76207500	1.39119300	2.00586900
N	-2.22062400	-0.83568600	1.85089500
H	-2.45279100	-1.63018300	1.24238100
C	-1.66966600	-1.14479500	3.16154800
H	-0.57408700	-1.13744800	3.13652300
H	-2.01587900	-0.41156500	3.89554500
H	-2.01690300	-2.13917300	3.45516100
C	-4.30871400	2.27449000	-0.94856800
C	-4.86264800	3.68038100	-0.75980800
H	-5.94764800	3.61872600	-0.62560300
H	-4.42832400	4.21336400	0.09186300
H	-4.67954700	4.26027500	-1.67102000
O	-4.72859200	1.52948400	-1.83397000
C	1.16219900	-0.86789200	-1.02022600
H	1.40173500	0.00566000	-1.63935700
C	1.79003500	-2.11382600	-1.53884100
H	1.71672800	-2.24238300	-2.62014600
C	2.75299000	-2.93177600	-0.90616300
H	2.87912300	-2.75776600	0.18751900
C	1.37968100	-0.44172200	0.44493500
H	0.66506300	0.37036200	0.65686800
C	2.78653000	0.13749600	0.70383500
H	3.54469800	-0.59772000	0.41408400
H	2.86606300	0.26272100	1.79276900
C	3.07114300	1.48080800	0.02132600
H	3.07965900	1.35314500	-1.06974500
H	2.25675100	2.18734200	0.24415800
C	4.40683000	2.10142200	0.45492600
H	5.22049400	1.39027500	0.24860000
H	4.40219200	2.24965900	1.54541400
C	4.71765800	3.43591400	-0.23429700
H	4.72715500	3.28707700	-1.32354500
H	3.90392900	4.14728800	-0.03160900
O	3.43402700	-3.83836400	-1.44327800
S	-0.75671300	-1.02825300	-1.43497800
O	1.17753500	-1.47741100	1.40507300
H	0.61480100	-2.17836200	1.02038500
H	0.52347400	-3.42961100	-0.56318500
C	6.05020000	4.04970600	0.20578500
H	6.24482500	5.00049700	-0.30596800
H	6.06062900	4.24628900	1.28571700
H	6.88928300	3.37709600	-0.01381900
O	0.02201600	-3.85435200	0.19470600
H	0.61480800	-4.56030400	0.49933200
O	-2.70583400	-3.27267200	0.30387700
H	-2.70114900	-2.83371100	-0.56346000
H	-1.77770000	-3.59985400	0.34659200

HNE_{c2}

Charge/multiplicity: 0 1

C	-2.72076000	-1.53561000	-0.38057700

O	-3.28235000	-2.61871000	-0.34539800
H	-2.31632900	-1.15043800	-1.33814500
C	-2.54956700	-0.68531100	0.80606200
H	-2.98570800	-1.09223600	1.71666700
C	-1.92111300	0.50540100	0.83954800
H	-1.87391500	1.03512600	1.79213600
C	-1.26168800	1.26451700	-0.28394800
H	-1.42385300	0.77009900	-1.25093200
C	0.24768900	1.42783400	-0.06049400
H	0.40545600	1.89264300	0.92234600
H	0.59995400	2.15019300	-0.80811900
C	1.04851300	0.12493700	-0.16862900
H	0.68360200	-0.59893600	0.57292500
H	0.87311600	-0.33134600	-1.15416200
C	2.55582400	0.33370300	0.02818600
H	2.73311700	0.79234700	1.01234300
H	2.92343800	1.05681000	-0.71480800
C	3.37068800	-0.96152200	-0.07981600
H	3.00240500	-1.68437500	0.66206500
H	3.19518100	-1.41930300	-1.06390700
C	4.87357700	-0.74808300	0.12039500
H	5.08822800	-0.32854100	1.11142600
H	5.42576500	-1.69133600	0.03325100
H	5.28084300	-0.05505400	-0.62665000
O	-1.80625600	2.59193900	-0.31880700
H	-2.76143200	2.51332400	-0.47715400

n-OCTANOL – IMPLICIT SOLVENT

Cysteinate($2H_2O$)$^-$

Charge/multiplicity: -1 1

N	1.69328500	-0.05817800	0.04895200
H	1.84453800	0.77527600	0.61324800
C	0.33170400	-0.39755500	-0.34190100
H	0.39510900	-0.97463000	-1.26888700
C	-0.35299300	-1.30236400	0.72596400
C	-0.45559000	0.89251700	-0.61604600
H	0.38787600	-2.06615100	0.98440200
H	-0.52473400	-0.70322000	1.63021200
S	-1.90965900	-2.14529000	0.18617800
O	-0.01236400	2.03036000	-0.35651600
N	-1.66337600	0.70435000	-1.17062700
H	-2.03129600	-0.25651100	-1.09239500
C	-2.60894100	1.79937800	-1.32833600
H	-2.12486600	2.64530900	-1.82336300
H	-3.43961900	1.45343200	-1.94807000
H	-3.00695900	2.13435300	-0.36297600
C	2.75719100	-0.82828600	-0.27213600
C	4.09959300	-0.34384300	0.24274000
H	4.03583300	0.58450000	0.81711800
H	4.53931500	-1.12378400	0.87437500
H	4.77328100	-0.19472900	-0.60840300
O	2.66703700	-1.86439300	-0.94829800
O	2.03139100	2.67532400	1.40568000
H	2.70275700	3.03934300	0.80508800
H	1.23822800	2.59941800	0.82727800
O	-3.95542400	0.07520200	1.36563900
H	-3.54937100	0.28034700	2.22298800
H	-3.36581000	-0.64255300	1.00850800

HNE_t

Charge/Multiplicity: 0 1

C	-4.36292400	-0.69308300	0.29759600
O	-5.29543900	-1.24486400	-0.27607700
H	-4.41692300	-0.48531800	1.38615600
C	-3.13046000	-0.26270200	-0.35955500
H	-3.05010900	-0.43729300	-1.43144300
C	-2.14448300	0.32161200	0.34236900
H	-2.27163100	0.48320300	1.41453800
C	-0.83627100	0.79529200	-0.22646400
H	-0.86677700	0.72803300	-1.32394800
C	0.33728100	-0.04388000	0.29581100
H	0.13250500	-1.09682500	0.06244500
H	0.36447300	0.04127200	1.39107800
C	1.69168300	0.36688200	-0.29734300
H	1.64327500	0.28938000	-1.39360800
H	1.88369500	1.42260100	-0.06844100
C	2.85344100	-0.48898100	0.22258600
H	2.65657200	-1.54807900	-0.00229400
H	2.89899400	-0.41279600	1.31933100
C	4.21276000	-0.09210700	-0.36713900
H	4.16887800	-0.17080500	-1.46305900
H	4.40872900	0.96666500	-0.14447500
C	5.37069600	-0.94511600	0.15778800
H	5.22215300	-2.00692400	-0.07790900
H	6.32649500	-0.63790700	-0.28430400
H	5.46660100	-0.85894000	1.24791800
O	-0.60668100	2.15425800	0.17650600
H	-1.30030100	2.70108600	-0.22930300

MIN_{1t}

Charge/multiplicity: -1 1

N	3.10965000	0.05204800	0.16034600
H	2.37103400	-0.22849100	0.81854900
C	2.84712000	1.08003000	-0.83264300
H	3.76175700	1.14070400	-1.43448500
C	1.71245900	0.72920700	-1.81537800
C	2.65754400	2.48470400	-0.23846800
H	1.77682800	1.41205600	-2.66615600
H	1.86146300	-0.29144900	-2.17890200
O	2.34079300	3.43626700	-0.96576900
N	2.88690200	2.62388600	1.08046300
H	3.16723400	1.80879200	1.60938500
C	2.78561600	3.91117000	1.74717400
H	1.78381100	4.33653700	1.62307100
H	2.98147800	3.76890100	2.81168800
H	3.51323300	4.62496700	1.34363700
C	4.26290300	-0.67442000	0.14579400
C	4.35418400	-1.77141500	1.18885300
H	3.59961900	-2.54289700	0.99777900
H	5.34962100	-2.21836800	1.14760800
H	4.17012600	-1.37887700	2.19437300
O	5.18088400	-0.46296300	-0.65864600
C	-0.56636600	-0.88425600	-0.72699000
H	-0.40203000	-0.95494300	0.34921700
C	0.20507500	-1.95809400	-1.40651100
H	0.16744300	-2.00989000	-2.49379800
C	0.89924300	-2.92683200	-0.74604800
H	1.40787700	-3.67490900	-1.38063900
C	-2.09989200	-0.95274600	-0.98088700
H	-2.28147900	-0.76102700	-2.04742300
C	-2.90118400	0.05792300	-0.14188900

H	-2.50613300	1.07059600	-0.29914600
H	-2.74102600	-0.17925000	0.92119300
C	-4.40328200	0.05336700	-0.45311300
H	-4.55140100	0.31077900	-1.51296300
H	-4.79239800	-0.96496500	-0.32616500
C	-5.20970100	1.02310900	0.41967400
H	-4.81130100	2.04210800	0.29973600
H	-5.06659000	0.76315200	1.47959700
C	-6.71046500	1.02887400	0.10151400
H	-6.85539100	1.29451400	-0.95574800
H	-7.10887900	0.01051000	0.21745800
O	1.03032900	-3.11480000	0.55161300
S	-0.01510100	0.88400300	-1.20380900
O	-2.57631500	-2.27921700	-0.74580800
H	-2.22887600	-2.57838900	0.13100300
H	-1.69103100	-4.18175800	1.58418300
C	-7.51237600	1.99190200	0.98126600
H	-8.57933100	1.97473500	0.72611400
H	-7.42126200	1.73054200	2.04363800
H	-7.15999300	3.02504000	0.86426100
O	-1.42768900	-3.24713700	1.61551000
H	-0.49448900	-3.24749500	1.24664100
O	1.37999900	-1.03688200	2.20305700
H	1.19403700	-1.81935000	1.60203400
H	0.50253300	-0.67475700	2.40579200

TS_{1t}

Charge/multiplicity: -1 1

N	-4.58189000	-0.39477400	0.21893500
H	-4.64859400	-0.15126200	1.20047000
C	-3.24563300	-0.70888700	-0.27234900
H	-3.34432400	-1.41818300	-1.09750400
C	-2.55806900	0.58025300	-0.78720300
C	-2.49085800	-1.33044000	0.90766000
H	-3.25727200	1.06826800	-1.47262800
H	-2.37663400	1.26267000	0.04963900
O	-2.59854100	-0.84754100	2.04361500
N	-1.73062600	-2.40599400	0.63875100
H	-1.66737000	-2.73478000	-0.31584700
C	-0.89662300	-3.02780700	1.65911300
H	-0.23042700	-2.28819900	2.11439600
H	-1.51342500	-3.47326900	2.44760800
H	-0.30066000	-3.81195900	1.18885000
C	-5.67618200	-0.33844200	-0.57655900
C	-6.97264200	0.03444800	0.11275200
H	-7.36468200	0.95136900	-0.34113200
H	-7.70780300	-0.75858400	-0.06195000
H	-6.86166000	0.18897200	1.18974600
O	-5.63103600	-0.58115100	-1.79038600
C	0.33043900	0.33594800	-0.45468300
H	0.12991200	-0.53574700	0.17606600
C	0.33514400	1.59187800	0.41649900
H	-0.36081400	2.37843000	0.10968900
C	0.34108300	1.40536800	1.83852700
H	0.09040800	2.32451300	2.41584700
C	1.65362700	0.01940500	-1.20422300
H	1.46726100	-0.84861800	-1.85275500
C	2.76919200	-0.37365400	-0.21519100
H	2.39940100	-1.18323400	0.42870600
H	2.98021300	0.47317600	0.45068700
C	4.06364200	-0.81737400	-0.90809300
H	3.84939000	-1.67950700	-1.55829400
H	4.41036200	-0.01378500	-1.57098400

C	5.18097200	-1.18951600	0.07453200
H	4.82913200	-1.98971300	0.74353600
H	5.39785000	-0.32657500	0.72240500
C	6.47653800	-1.64064400	-0.61167700
H	6.26340000	-2.50738700	-1.25415800
H	6.82755600	-0.84307500	-1.28248400
O	0.67742300	0.38227200	2.46773100
S	-1.01538600	0.36893600	-1.75449600
O	2.06047900	1.06049200	-2.08791900
H	2.25821700	1.85912300	-1.52834500
H	3.17713600	2.77904900	0.23533100
C	7.59040200	-2.00171100	0.37490100
H	8.50113100	-2.32066900	-0.14719200
H	7.85436400	-1.14496800	1.00862800
H	7.28455100	-2.82085200	1.03882700
O	2.40242700	3.07671100	-0.27290200
H	1.46127200	2.34200800	0.16913000
O	1.33212400	4.98070100	1.36758200
H	1.77723100	4.75859900	2.20023300
H	1.75947800	4.36176800	0.71578900

MIN_2

Charge/multiplicity: -1 1

N	-4.43569800	0.85881800	-0.20377800
H	-4.41037800	1.19844100	-1.15813800
C	-3.14539500	0.55171100	0.40736600
H	-3.26939500	0.61246500	1.49082800
C	-2.70815200	-0.87815600	0.01926000
C	-2.16537000	1.61624500	-0.09593000
H	-3.51001500	-1.55753300	0.32485900
H	-2.59107000	-0.95962900	-1.06315400
O	-2.07311200	1.85878800	-1.30913400
N	-1.45073200	2.26887200	0.83593600
H	-1.54641200	1.99851400	1.80603700
C	-0.47349300	3.29011700	0.48650000
H	-0.96437700	4.16769600	0.05050800
H	0.05314700	3.59085600	1.39367900
H	0.25111600	2.90503900	-0.23767400
C	-5.62560500	0.60007400	0.39086300
C	-6.85696600	0.93677800	-0.42504300
H	-7.42799200	0.01790300	-0.59907900
H	-7.49284700	1.61308200	0.15617200
H	-6.62717000	1.40033200	-1.38859700
O	-5.71272800	0.12396000	1.53052100
C	0.16626300	-1.11851400	-0.40977500
H	-0.24800900	-0.37746400	-1.10169400
C	0.54841900	-2.39382400	-1.16661300
H	0.83030900	-3.19522900	-0.47228100
C	-0.43603300	-2.94890000	-2.15129200
H	-0.15285300	-3.94182000	-2.56179200
C	1.38207100	-0.51588200	0.36326000
H	0.97120200	0.38771600	0.86614100
C	2.45286000	0.01365200	-0.63060300
H	1.97211200	0.61649500	-1.41751100
H	2.93189700	-0.83830300	-1.13553900
C	3.53758700	0.85456300	0.05567100
H	3.06791400	1.73085300	0.52928300
H	3.98135300	0.27030400	0.87123500
C	4.64150400	1.33069200	-0.89720500
H	4.19447800	1.91549100	-1.71620600
H	5.11392700	0.45699500	-1.37251700
C	5.72490500	2.17319300	-0.21136300
H	5.25793000	3.05033400	0.25995100
H	6.17189700	1.59041100	0.60676000

O	-1.45119900	-2.40316300	-2.55182200
S	-1.17835200	-1.48739400	0.84006800
O	1.87902100	-1.41613400	1.28610400
H	2.99224500	-2.47112400	0.81779200
H	1.45980500	-2.22368800	-1.76608300
C	6.82748700	2.63721800	-1.16715100
H	7.58381100	3.23799400	-0.64665300
H	7.34181200	1.78294300	-1.62656800
H	6.41786000	3.25139900	-1.97991900
O	3.77650600	-3.10680300	0.66086500
H	4.39705700	-2.56468300	0.14820800
O	3.92397400	-1.24645300	2.97206500
H	3.07782700	-1.11635400	2.44876900
H	4.27126600	-2.02031900	2.49054100

TS_2

Charge/multiplicity: -1 1

N	4.70553400	0.52804100	0.28712300
H	4.66495900	0.97370400	1.19701500
C	3.43381500	0.37509500	-0.40881900
H	3.63372400	0.37587800	-1.48291300
C	2.77376200	-0.97100400	-0.02235500
C	2.57242100	1.57931300	-0.01386800
H	3.48522700	-1.76366300	-0.27200900
H	2.60942800	-1.00296300	1.06033500
O	2.53125000	1.96258900	1.16586900
N	1.88972700	2.18056500	-1.00180500
H	1.91785800	1.77739500	-1.92924200
C	0.99189400	3.29956900	-0.75280900
H	0.57968700	3.63076200	-1.70736800
H	0.16888900	3.01229300	-0.08925500
H	1.53437700	4.13052700	-0.29021200
C	5.88151300	0.03690900	-0.17771500
C	7.07742100	0.28119500	0.72316600
H	7.24294800	1.35563600	0.86488500
H	6.91642500	-0.16410200	1.71189300
H	7.96592600	-0.16239300	0.26986600
O	5.97165600	-0.55653100	-1.25956400
C	-0.05481400	-0.72968700	0.30743400
H	0.36245600	0.18398700	0.74720600
C	-0.29956800	-1.76398500	1.42443400
H	0.66089800	-2.22012700	1.71391900
C	-0.82206600	-1.17043400	2.70653400
H	-0.31760900	-0.23486400	3.03290600
C	-1.32197200	-0.37989200	-0.53213700
H	-0.99502300	0.46504100	-1.18174700
C	-2.43571500	0.20029800	0.37978900
H	-2.01221700	0.96531600	1.05124200
H	-2.82818000	-0.60131700	1.02127700
C	-3.59738100	0.81677900	-0.41023500
H	-3.21095400	1.63165500	-1.04236300
H	-4.00147400	0.06095600	-1.09483600
C	-4.72590100	1.35865600	0.47624000
H	-4.32089500	2.11037200	1.17162500
H	-5.11613500	0.54376600	1.10513300
C	-5.88410700	1.97847400	-0.31628300
H	-5.49978000	2.80105800	-0.93709700
H	-6.28371800	1.23059900	-1.01623000
O	-1.69105400	-1.66687000	3.40332200
S	1.20930000	-1.37251600	-0.90147900
O	-1.72414100	-1.45903000	-1.29069600
H	-2.53543800	-2.62960900	-0.55688100
H	-0.95924400	-2.56945600	1.08846400

C	-7.01766600	2.49961200	0.57130700
H	-7.82851900	2.93351700	-0.02719400
H	-7.44936900	1.69385500	1.17927200
H	-6.66115500	3.27727900	1.25956600
O	-3.13936000	-3.37223800	-0.19898200
H	-3.71723800	-2.90039900	0.42213800
O	-3.92180500	-1.92730700	-2.71620700
H	-3.06999200	-1.57312400	-2.32519300
H	-4.09368300	-2.64185200	-2.07580500

MIN_3

Charge/multiplicity: -1 1

N	4.70316000	0.53243300	0.29377700
H	4.65936800	0.98771600	1.19811800
C	3.43398600	0.37925500	-0.40719400
H	3.63783600	0.37871900	-1.48056800
C	2.77363300	-0.96692200	-0.02097900
C	2.57190200	1.58408400	-0.01549400
H	3.48567400	-1.75949200	-0.26900500
H	2.60757400	-0.99813900	1.06142600
O	2.53254100	1.97193300	1.16279600
N	1.88668400	2.18013500	-1.00461900
H	1.91418000	1.77340600	-1.93054200
C	0.98745900	3.29868000	-0.75848700
H	0.16728000	3.01313800	-0.09073400
H	1.52979700	4.13311800	-0.30200400
H	0.57146000	3.62403500	-1.71339400
C	5.87761700	0.03854300	-0.16661800
C	7.08475500	0.27381000	0.71832100
H	6.85219300	0.81992300	1.63704100
H	7.52555700	-0.69433000	0.98003100
H	7.83609900	0.83325600	0.15032200
O	5.97060400	-0.56217200	-1.24536700
C	-0.05475500	-0.72839200	0.30673000
H	0.36175900	0.18491300	0.74803700
C	-0.29947700	-1.76454100	1.42203200
H	0.66099000	-2.22101900	1.71096500
C	-0.82232500	-1.17326400	2.70506200
H	-0.31826800	-0.23803700	3.03302600
C	-1.32173800	-0.37811500	-0.53289900
H	-0.99523700	0.46827100	-1.18083000
C	-2.43612000	0.19931700	0.37999100
H	-2.01325600	0.96300200	1.05335800
H	-2.82810800	-0.60409000	1.01952500
C	-3.59818400	0.81695000	-0.40854000
H	-3.21265200	1.63469100	-1.03749100
H	-4.00085100	0.06298500	-1.09603700
C	-4.72781900	1.35379900	0.47959200
H	-4.32404200	2.10307400	1.17832100
H	-5.11728300	0.53578300	1.10488700
C	-5.88652100	1.97551900	-0.31069900
H	-5.50309900	2.80144400	-0.92762400
H	-6.28478300	1.23023600	-1.01417200
O	-1.69114200	-1.67122300	3.40095700
S	1.21059500	-1.36869700	-0.90226100
O	-1.72269600	-1.45622800	-1.29357700
H	-2.53422000	-2.62797500	-0.56198400
H	-0.95893700	-2.56960600	1.08466100
C	-7.02117700	2.49098500	0.57880900
H	-7.83242100	2.92647200	-0.01800700
H	-7.45194300	1.68182200	1.18289400
H	-6.66603400	3.26599000	1.27076800
O	-3.13829700	-3.37111100	-0.20538500
H	-3.71652700	-2.90012600	0.41605200

O	-3.92061800	-1.92236800	-2.71987900
H	-3.06878800	-1.56881500	-2.32837900
H	-4.09230900	-2.63808800	-2.08072800

TS_3

Charge/multiplicity: -1 1

N	-4.31447200	0.67234200	-0.35841400
H	-4.18042300	1.29648300	-1.14609700
C	-3.11218400	0.28897800	0.37474600
H	-3.41647700	-0.00122000	1.38271600
C	-2.43080000	-0.91209700	-0.31867000
C	-2.20878800	1.52587000	0.40712900
H	-3.17067100	-1.71539000	-0.38312800
H	-2.15351200	-0.63564900	-1.34088100
O	-1.94847200	2.13775200	-0.64076700
N	-1.74864500	1.90700900	1.60990400
H	-1.96898600	1.34179300	2.41945200
C	-0.87761600	3.06198800	1.77588800
H	-0.66758800	3.18703200	2.83939200
H	0.06726900	2.92594700	1.23887900
H	-1.36313800	3.96789400	1.39790800
C	-5.53846100	0.13288000	-0.12659400
C	-6.63994200	0.62791100	-1.04460500
H	-7.57248400	0.11866500	-0.79406700
H	-6.77908700	1.70972100	-0.93382200
H	-6.39099000	0.42975500	-2.09360300
O	-5.74112900	-0.68943400	0.77486600
C	0.43816700	-0.79642700	-0.36824600
H	0.13559900	0.24125100	-0.54360300
C	0.67658600	-1.46438500	-1.74525200
H	1.39835600	-0.85018100	-2.30085300
C	1.20650800	-2.87902400	-1.68271500
H	2.30148300	-2.99347800	-1.62180300
C	1.67613800	-0.86463800	0.55857600
H	1.37444000	-0.33028100	1.48633200
C	2.88993300	-0.07247600	0.00506700
H	3.23151000	-0.52734500	-0.93523800
H	3.69686800	-0.23586500	0.73297300
C	2.68270800	1.43512700	-0.18914500
H	1.93341700	1.61860600	-0.97299700
H	2.26804600	1.86483500	0.73587900
C	3.97225100	2.18481600	-0.55223800
H	4.39804400	1.75284900	-1.47072200
H	4.72120200	2.01905800	0.23673300
C	3.77271800	3.69267100	-0.75128100
H	3.02705800	3.85853100	-1.54251700
H	3.34602900	4.12569800	0.16527300
O	0.49185800	-3.86811400	-1.78470100
S	-0.96665600	-1.60884800	0.54726200
O	1.98565800	-2.19294600	0.82366600
H	3.43152800	-2.73162900	0.24310200
H	-0.25915800	-1.47994400	-2.31528500
C	5.06461800	4.43303300	-1.10824600
H	4.88729300	5.50713300	-1.24516700
H	5.81952300	4.31915300	-0.31940600
H	5.49993600	4.04744300	-2.03941200
O	4.34030700	-3.09668900	-0.01559500
H	4.23581500	-4.05249400	0.12253900
O	3.76961700	-2.14347000	2.80448100
H	4.46164700	-2.46259400	2.19953600
H	2.98203800	-2.17181100	2.17917600

MIN_4

Charge/multiplicity: -1 1

N	-3.83034600	1.04826700	0.53250700
H	-3.70855400	1.46087200	1.45208500
C	-2.95278400	-0.07481900	0.24800300
H	-3.57162700	-0.93509100	-0.03773500
C	-1.99977100	0.26058900	-0.92926400
C	-2.22715400	-0.40768000	1.57260400
H	-2.56558000	0.82609600	-1.67216400
H	-1.16865800	0.87965400	-0.58339500
O	-2.47001700	0.24729300	2.59912900
N	-1.35894900	-1.43185500	1.56566100
H	-1.10246900	-1.87823300	0.68714000
C	-0.62246900	-1.79897000	2.76780100
H	-1.30659400	-2.13611900	3.55429000
H	0.06222700	-2.60831800	2.51566600
H	-0.04860700	-0.94945400	3.15557100
C	-4.92511400	1.33357800	-0.21087700
C	-5.80432600	2.45174400	0.31052400
H	-5.92530900	3.20565400	-0.47462000
H	-6.79803900	2.04611100	0.53176800
H	-5.40742100	2.93116100	1.20972000
O	-5.19527600	0.72798600	-1.25732100
C	0.42082000	-0.98496700	-2.08971200
H	0.45899500	-0.37244200	-2.99440000
C	1.09250000	-2.36177500	-2.31457600
H	1.74172100	-2.30615200	-3.19623200
C	1.94418500	-2.58778400	-1.03937700
H	2.90220000	-3.09607600	-1.28285900
C	1.27238000	-0.32639300	-0.95712400
H	0.70760800	-0.33057300	-0.01411900
C	1.73583000	1.09612600	-1.26915500
H	0.86069100	1.70272500	-1.54249900
H	2.38090800	1.05722900	-2.15862300
C	2.47879200	1.76931600	-0.10655400
H	1.79388100	1.85774200	0.75047100
H	3.30237300	1.12515900	0.22869500
C	3.02460900	3.15745700	-0.46353800
H	2.19917300	3.79620500	-0.81396300
H	3.71999200	3.06584500	-1.31152500
C	3.74035000	3.85312300	0.70100900
H	3.04471000	3.95207900	1.54697200
H	4.56158300	3.21335200	1.05432900
O	1.28866000	-3.09541300	-0.00148200
S	-1.36868900	-1.28690200	-1.70993500
O	2.41649100	-1.17039000	-0.82999300
H	2.38543300	-2.28032000	2.59991500
H	0.38076100	-3.17914200	-2.46860000
C	4.29223600	5.23322200	0.33341600
H	4.79619400	5.70359300	1.18688000
H	5.02045300	5.16566700	-0.48529100
H	3.49093400	5.90945600	0.00768300
O	2.72556000	-3.08115700	2.16889600
H	2.18257600	-3.11273700	1.29353000
O	4.60480200	-1.36822600	0.93476700
H	3.94171400	-1.15338100	0.24667500
H	4.11054900	-2.04236700	1.45538200

TS_4

Charge/multiplicity: -1 1

N	-3.86416000	0.61831200	0.19231800
H	-3.52493600	1.57173500	0.24900800
C	-2.86562100	-0.42385400	0.38339200
H	-3.35852600	-1.28054100	0.85069800
C	-2.29254700	-0.85946200	-0.98866300
C	-1.79060100	0.15410400	1.31449700
H	-3.13894000	-1.16236200	-1.61109800
H	-1.80382100	-0.01228100	-1.47536600
O	-1.44760800	1.34123300	1.20392000
N	-1.29371700	-0.69204800	2.23411200
H	-1.56250300	-1.66637100	2.17014900
C	-0.18389200	-0.36279700	3.11639600
H	-0.12872400	0.72070600	3.22825500
H	-0.35370200	-0.81758400	4.09655500
H	0.76626300	-0.73388100	2.71350900
C	-5.16399300	0.36379600	-0.09028800
C	-6.05001100	1.57889400	-0.27213500
H	-6.47161500	1.56138600	-1.28329000
H	-6.88589800	1.51609300	0.43289700
H	-5.52452200	2.52603400	-0.12139000
O	-5.60912800	-0.78737400	-0.19327600
C	0.46872200	-1.63266400	-1.61067500
H	0.23115500	-1.22077000	-2.59601900
C	1.46257100	-2.81971900	-1.73913600
H	1.81551300	-2.88845000	-2.77468600
C	2.63377800	-2.47211600	-0.78074400
H	3.61626600	-2.71084900	-1.24429200
C	1.24691000	-0.57624700	-0.76544700
H	0.94588900	-0.66955500	0.28705700
C	1.10476800	0.87268100	-1.22774800
H	0.04014800	1.12922000	-1.29458700
H	1.51512700	0.94645400	-2.24553600
C	1.79675900	1.88511000	-0.30262300
H	1.29558100	1.86296600	0.67530300
H	2.83581900	1.58040700	-0.12393700
C	1.76727200	3.31597800	-0.85399600
H	0.72457400	3.61038500	-1.04950000
H	2.27938600	3.34023400	-1.82802100
C	2.41358700	4.34726100	0.07937900
H	1.89477400	4.33316800	1.04879900
H	3.45192500	4.04950700	0.28403300
O	2.47271100	-2.90801300	0.46332200
S	-1.11817700	-2.27857900	-0.90412200
O	2.61271500	-0.97040600	-0.90837700
H	3.81342800	-1.48732500	2.66087500
H	1.02631300	-3.78603800	-1.46751500
C	2.39452300	5.76997600	-0.48655800
H	2.86067000	6.48326700	0.20462600
H	2.93884800	5.82698700	-1.43826400
H	1.36767400	6.11143800	-0.67249000
O	4.32909300	-2.05203700	2.06232400
H	3.61086500	-2.41332500	1.41316700
O	5.01101400	-0.03233700	0.25407100
H	4.21310100	-0.21316200	-0.28430900
H	4.90210500	-0.70825500	0.96654500

P(R)

Charge/multiplicity: -1 1

N	2.72814500	-2.44016900	0.29223700
H	2.25292700	-2.95349300	1.02594400
C	2.20454600	-1.10693100	0.02204800

H	3.03953500	-0.45414800	-0.24453800
C	1.20481000	-1.16109300	-1.16500400
C	1.54029900	-0.64509700	1.32777000
H	1.65711900	-1.78345100	-1.94181000
H	0.27008800	-1.63879500	-0.85510900
O	0.93446900	-1.47797600	2.03040000
N	1.65011400	0.64603500	1.65495100
H	2.05022400	1.34588300	1.00707300
C	0.98772800	1.16723600	2.84135000
H	1.37776700	0.69068300	3.74758600
H	1.17966600	2.24016900	2.89183000
H	-0.09499900	1.00222000	2.80572200
C	3.76306800	-2.99377000	-0.38001400
C	4.16648600	-4.38573800	0.06398800
H	5.21089300	-4.36243100	0.39428900
H	3.54566700	-4.78002100	0.87364400
H	4.10931400	-5.06374100	-0.79449100
O	4.35516700	-2.40709900	-1.29655900
C	-0.94426700	0.79320400	-1.60842700
H	-1.50737600	0.03905700	-2.16384800
C	-1.25731900	2.22251800	-2.08078800
H	-2.30916100	2.26734500	-2.38882400
C	-1.01163300	3.13715000	-0.84763200
H	-1.87928100	3.81876800	-0.71389700
C	-1.37382500	0.84636300	-0.12822700
H	-0.76923700	0.17993200	0.49644500
C	-2.85208300	0.45796400	0.07645800
H	-3.48369300	0.99876300	-0.64258800
H	-3.13819900	0.81884900	1.07387700
C	-3.12488300	-1.04946800	-0.01099000
H	-2.84694100	-1.42616000	-1.00609200
H	-2.47734800	-1.57413200	0.70757500
C	-4.58876300	-1.41597000	0.26756500
H	-5.23787500	-0.89104400	-0.44951600
H	-4.87249600	-1.04543200	1.26403800
C	-4.86799000	-2.92236400	0.19126000
H	-4.58221000	-3.29397400	-0.80359900
H	-4.22240500	-3.44720500	0.91023900
O	0.15225000	3.79890300	-0.83493500
S	0.85691100	0.47684200	-1.92719500
O	-1.13637300	2.18582700	0.30468300
H	0.15793100	4.17686000	2.11308400
H	-0.64948800	2.55370100	-2.92785100
C	-6.33082900	-3.28116600	0.46600800
H	-6.49634400	-4.36386800	0.40279200
H	-6.63945600	-2.95674500	1.46831100
H	-7.00155900	-2.80020600	-0.25784500
O	0.68402500	4.77796800	1.56124800
H	0.40739800	4.49821100	0.62467600
O	2.46191300	2.93844000	0.21043700
H	2.25201300	3.57905200	0.91996100
H	1.63547400	3.04928200	-0.34666300

TS_2’

Charge/multiplicity: -1 1

N	4.66030200	0.63669700	0.07385600
H	4.71504500	1.35058500	0.79222500
C	3.35251400	0.46642900	-0.53665700
H	3.48523900	0.33932400	-1.61580900
C	2.66703800	-0.80820500	0.02563000
C	2.56492800	1.75782400	-0.25909000
H	3.38674800	-1.62422400	-0.07755700

H	2.44918200	-0.68093300	1.08956500
O	2.91559200	2.54271500	0.63436300
N	1.49951800	1.98117500	-1.04873600
H	1.19421600	1.23073000	-1.65972400
C	0.60730400	3.11072000	-0.82790200
H	0.13009600	3.06222600	0.15778900
H	1.16170100	4.05208100	-0.89610800
H	-0.16430900	3.09726400	-1.59970400
C	5.76578800	-0.02715900	-0.33449700
C	7.04970300	0.31281800	0.39476200
H	6.91748300	1.05941100	1.18309500
H	7.46026600	-0.60250200	0.83487500
H	7.78146800	0.68430000	-0.33107700
O	5.73951000	-0.86399000	-1.24801100
C	-0.19789900	-0.85747300	0.35894100
H	0.14164300	0.07291600	0.82459900
C	-0.37921500	-1.93352300	1.44484700
H	0.10639300	-2.88326700	1.17798800
C	0.12482600	-1.58139500	2.81380200
H	-0.06349700	-2.36137600	3.58143600
C	-1.49954700	-0.58221300	-0.45351400
H	-1.20565300	0.18967400	-1.20205800
C	-2.54501600	0.11752400	0.45841500
H	-2.06338700	0.94242200	1.00655000
H	-2.90591100	-0.59276000	1.21680200
C	-3.74260900	0.67258000	-0.32297100
H	-3.37577500	1.38762200	-1.07629900
H	-4.21934200	-0.14037200	-0.88474700
C	-4.78328200	1.37136700	0.56133800
H	-4.29631000	2.17792300	1.13119600
H	-5.16448000	0.65991700	1.31036500
C	-5.96535500	1.95470100	-0.22360600
H	-5.58627800	2.66222200	-0.97546500
H	-6.45961100	1.14953400	-0.78603200
O	0.69996400	-0.55215500	3.12930400
S	1.13491700	-1.33281300	-0.85506400
O	-1.95811200	-1.72793700	-1.07224800
H	-2.90370800	-2.67089800	-0.18037700
H	-1.43601300	-2.21618900	1.56059000
C	-6.99381000	2.66158400	0.66358200
H	-7.82360400	3.06698200	0.07118400
H	-7.42114000	1.97359900	1.40489100
H	-6.53921800	3.49681600	1.21236500
O	-3.59019800	-3.26026500	0.29440000
H	-4.25514800	-2.61847200	0.59055000
O	-4.15611300	-2.18494600	-2.49013700
H	-3.28958600	-1.85929800	-2.10040700
H	-4.39127700	-2.84619500	-1.81536300

MIN_3’

Charge/multiplicity: -1 1

N	-4.74308800	0.58242700	-0.38840100
H	-4.71029800	0.98831300	-1.31636800
C	-3.46314600	0.42934800	0.29257500
H	-3.64844100	0.46472600	1.36859400
C	-2.83335600	-0.93724800	-0.06560300
C	-2.58754400	1.60537400	-0.15414700
H	-3.56006500	-1.71242000	0.19342700
H	-2.65248500	-0.99415200	-1.14373200
O	-2.52800600	1.92090100	-1.35247400
N	-1.92007000	2.26019900	0.80977500
H	-1.97342300	1.91829800	1.76033100
C	-1.03166300	3.37596900	0.51560300

H	-1.57143200	4.16437700	-0.01869800
H	-0.65583700	3.77640300	1.45858800
H	-0.18321000	3.05827100	-0.10066300
C	-5.91938300	0.14830900	0.12641600
C	-7.14203400	0.37358000	-0.73907200
H	-7.59223700	-0.59690600	-0.97571000
H	-7.87938800	0.94597200	-0.16607000
H	-6.92462500	0.90226700	-1.67152900
O	-6.00015100	-0.39454900	1.23614300
C	0.02299800	-0.81533400	-0.39134100
H	-0.39313100	0.04504800	-0.92373400
C	0.34302800	-1.94286400	-1.37921400
H	-0.58008500	-2.30458100	-1.85654700
C	1.01654700	-3.13631000	-0.73724600
H	0.53087200	-3.52744400	0.17167300
C	1.32686100	-0.43715100	0.37128600
H	1.01943000	0.14693400	1.26331500
C	2.20898400	0.50618400	-0.48495300
H	1.59905900	1.32558800	-0.89581100
H	2.60113300	-0.06090900	-1.33983700
C	3.38115400	1.10077800	0.30914600
H	2.98358800	1.79127400	1.06969900
H	3.88924900	0.30124100	0.86266900
C	4.39842400	1.84125300	-0.56753100
H	3.88312100	2.61723600	-1.15521400
H	4.82035100	1.13445700	-1.29755800
C	5.54214900	2.48688000	0.22502400
H	5.12408800	3.19404100	0.95649100
H	6.05746100	1.71200200	0.81038500
O	1.88101100	-3.80541600	-1.31144200
S	-1.28405400	-1.34245400	0.83621200
O	1.97974300	-1.61001100	0.73265800
H	3.38415100	-1.91774600	-0.12359200
H	0.99549500	-1.57487400	-2.18038000
C	6.55778500	3.21418400	-0.66064500
H	7.36323200	3.66141400	-0.06466000
H	7.02064200	2.52712500	-1.38100300
H	6.08175000	4.02102800	-1.23342100
O	4.24412400	-2.22402300	-0.54682600
H	3.95053200	-3.03765900	-0.99133000
O	4.10874200	-1.92302700	2.37668700
H	3.21947100	-1.74036200	1.96970400
H	4.57945200	-2.23677600	1.58221100

TS_3’

Charge/multiplicity: -1 1

N	-4.79246200	0.53180500	-0.35734700
H	-4.79001200	0.94054000	-1.28519000
C	-3.49580600	0.41990300	0.29914600
H	-3.65993300	0.44487300	1.37891800
C	-2.82605400	-0.92274500	-0.07775700
C	-2.66814200	1.62650200	-0.15671300
H	-3.52256900	-1.72229300	0.19039700
H	-2.66663300	-0.96749100	-1.16017900
O	-2.64830700	1.95666900	-1.35248500
N	-1.99484600	2.29037800	0.79731400
H	-2.01073300	1.93452100	1.74412400
C	-1.14261000	3.43102800	0.49235300
H	-0.76806200	3.84353900	1.43065100
H	-0.29179900	3.13881500	-0.13338700
H	-1.71183800	4.20222300	-0.03622200
C	-5.94204800	0.03121000	0.16190000
C	-7.17186200	0.22101400	-0.70539300

H	-7.37294800	1.28703400	-0.86372700
H	-7.02930400	-0.24074800	-1.68932200
H	-8.03229500	-0.23745800	-0.21427500
O	-5.98365800	-0.52701100	1.26509500
C	0.01364500	-0.68012300	-0.44347500
H	-0.41787900	0.20834200	-0.91543600
C	0.31029400	-1.74356400	-1.50989200
H	-0.62898200	-2.10334200	-1.95606700
C	1.04620700	-2.95599000	-0.98405700
H	0.57739300	-3.47037300	-0.12993900
C	1.31952000	-0.34300300	0.32317900
H	1.02670800	0.30963000	1.17242900
C	2.28909200	0.48601400	-0.55680300
H	1.74755500	1.28899700	-1.08072600
H	2.70469700	-0.17568500	-1.32829800
C	3.43944100	1.09672500	0.25857600
H	3.04759500	1.92580700	0.86816900
H	3.81549200	0.34925800	0.96867000
C	4.59979300	1.60172800	-0.60759200
H	4.21630000	2.29458500	-1.37320900
H	5.02785000	0.74736000	-1.15246600
C	5.70944700	2.29823900	0.18993900
H	5.28527200	3.15824600	0.72891200
H	6.08598400	1.61066200	0.96085900
O	1.97650600	-3.48530300	-1.59495300
S	-1.24864800	-1.28957100	0.79063200
O	1.88245200	-1.53429000	0.76459400
H	3.37981700	-1.92803500	0.14154800
H	0.90597300	-1.31125100	-2.32247500
C	6.87593200	2.77140700	-0.68202200
H	7.65247400	3.26285200	-0.08241800
H	7.34559400	1.92987400	-1.20759800
H	6.54042400	3.48929300	-1.44217000
O	4.28322800	-2.26802300	-0.14239100
H	4.03950700	-3.06619400	-0.64052900
O	3.69557800	-1.71710800	2.74072900
H	2.89875300	-1.58616800	2.15334900
H	4.30761400	-2.10907800	2.09267500

MIN_4’

Charge/multiplicity: -1 1

N	4.72779500	0.24520400	0.42884400
H	4.73049300	0.04883700	1.42301400
C	3.42328800	0.46127500	-0.18746100
H	3.57975700	1.04958400	-1.09419800
C	2.78917400	-0.89622600	-0.56484600
C	2.57836900	1.23022000	0.83446800
H	3.49424300	-1.42289300	-1.21429300
H	2.64143000	-1.50366200	0.33330600
O	2.48457600	0.82150800	2.00139100
N	1.97527700	2.34962500	0.40037800
H	2.09643900	2.63038700	-0.56374600
C	1.15387900	3.17556000	1.27481200
H	0.70871000	3.97434700	0.67936800
H	0.35628300	2.58397400	1.73436200
H	1.75775000	3.61998200	2.07416800
C	5.88527600	0.19184400	-0.27603400
C	7.13513300	-0.09100500	0.53148300
H	7.86470600	0.70414900	0.34488900
H	6.95025700	-0.16326500	1.60694500
H	7.57678700	-1.03081100	0.18171000
O	5.92703300	0.36649000	-1.50072400
C	-0.05735600	-0.97536600	-0.14629300

H	0.23038500	-0.29594000	0.65910000
C	-0.25491600	-2.40732900	0.36978100
H	0.61508200	-3.05408600	0.21580800
C	-1.50909500	-2.94477300	-0.35870400
H	-1.24301300	-3.13722000	-1.42798300
C	-1.46071500	-0.58018300	-0.72520700
H	-1.38898100	-0.46918300	-1.82243400
C	-1.99946400	0.72479400	-0.13858600
H	-1.27170500	1.51841500	-0.36335500
H	-2.03270900	0.62368800	0.95601300
C	-3.38304100	1.13056300	-0.66279800
H	-3.35512100	1.17547600	-1.76225700
H	-4.11042800	0.35179900	-0.40162900
C	-3.85995600	2.48090900	-0.11308800
H	-3.13007000	3.26197800	-0.37667200
H	-3.87842900	2.43956800	0.98660500
C	-5.24656700	2.89374800	-0.62331700
H	-5.23123400	2.93399700	-1.72219100
H	-5.97568700	2.11555300	-0.35677300
O	-2.18330600	-3.92875300	0.20079200
S	1.20518100	-0.79173200	-1.49164800
O	-2.32843100	-1.66075500	-0.41780200
H	-3.45813400	-2.20073500	2.25916900
H	-0.48199600	-2.39165200	1.44385000
C	-5.71669500	4.24262300	-0.07218700
H	-6.71068800	4.50706400	-0.45382900
H	-5.77618600	4.22587100	1.02388200
H	-5.02799800	5.05027300	-0.35318700
O	-3.78866700	-3.09819500	2.08976100
H	-3.15959500	-3.42365500	1.34955500
O	-5.14712200	-2.07738000	-0.16060200
H	-4.26216300	-1.94436200	-0.55458200
H	-4.88912800	-2.47679800	0.70253700

TS_4’

Charge/multiplicity: -1 1

N	4.71590700	0.25533800	0.42855300
H	4.71623600	0.03476500	1.41814900
C	3.41216900	0.47339200	-0.18816700
H	3.56716700	1.07757000	-1.08462000
C	2.78629300	-0.88112800	-0.58953300
C	2.55968100	1.22154700	0.84278900
H	3.49645300	-1.39321600	-1.24511700
H	2.63955600	-1.50370500	0.29838300
O	2.46238000	0.79331900	2.00245100
N	1.95380000	2.34575600	0.42495700
H	2.07811500	2.64353600	-0.53360300
C	1.12633200	3.15405000	1.30997800
H	0.67674900	3.95847400	0.72553000
H	0.33201200	2.55089700	1.75999700
H	1.72628400	3.59084100	2.11651800
C	5.87850000	0.21628800	-0.27228300
C	7.11585400	-0.06814800	0.55720500
H	7.01600500	-1.01915900	1.09296000
H	7.98620200	-0.11459700	-0.10011700
H	7.26963000	0.72012800	1.30354300
O	5.92333800	0.41263900	-1.49259400
C	-0.06100200	-0.97505500	-0.18115900
H	0.22225800	-0.30334600	0.63214900
C	-0.25479300	-2.41262100	0.32162500
H	0.61509700	-3.05685300	0.15679600
C	-1.51235400	-2.94562600	-0.40432500

H	-1.25185700	-3.13701100	-1.47461900
C	-1.46454500	-0.57818400	-0.75851200
H	-1.39240500	-0.46134500	-1.85525100
C	-2.00594500	0.72286900	-0.16548900
H	-1.28548700	1.52160900	-0.39561500
H	-2.02925400	0.62062900	0.92927300
C	-3.39738300	1.11915000	-0.67614100
H	-3.38291100	1.15848200	-1.77603500
H	-4.11715400	0.33784800	-0.40143800
C	-3.87494500	2.46959800	-0.12722700
H	-3.15252300	3.25324500	-0.40338300
H	-3.87986200	2.43341300	0.97279100
C	-5.26980600	2.87274700	-0.62244800
H	-5.26779600	2.90883900	-1.72157200
H	-5.99138800	2.09162800	-0.34415900
O	-2.18900900	-3.92879000	0.15375000
S	1.20472100	-0.77261500	-1.52028000
O	-2.33066700	-1.66070100	-0.45688300
H	-3.30194900	-2.15774000	2.26767500
H	-0.47484900	-2.40692900	1.39722700
C	-5.74077100	4.22112600	-0.07080200
H	-6.74051600	4.47887600	-0.44184500
H	-5.78748700	4.20803200	1.02593300
H	-5.05971100	5.03139700	-0.36265600
O	-3.61472400	-3.07154700	2.16549600
H	-3.00427400	-3.42935400	1.42286300
O	-5.11541800	-2.12493500	-0.02561000
H	-4.25948200	-1.98626300	-0.47693300
H	-4.79725900	-2.51641400	0.82115500

MIN_5’

Charge/multiplicity: -1 1

N	4.69266400	0.20927800	0.46928700
H	4.67379100	-0.14398100	1.41895400
C	3.39901000	0.51559800	-0.12984800
H	3.55523500	1.28337100	-0.89083200
C	2.81924700	-0.75240500	-0.79732600
C	2.50500100	1.03342000	1.00232400
H	3.56403900	-1.12391000	-1.50658600
H	2.65279300	-1.52852600	-0.04486800
O	2.44883000	0.42527100	2.08096800
N	1.81943600	2.16347100	0.76185400
H	1.89389600	2.59712200	-0.14876900
C	0.92305300	2.74797200	1.75016600
H	1.48014300	3.07347200	2.63580300
H	0.43051100	3.61278300	1.30264800
H	0.16386300	2.02594800	2.06646000
C	5.86400400	0.27708300	-0.20936300
C	7.10072600	-0.11910000	0.57017400
H	7.60303200	-0.93850800	0.04464000
H	7.79273000	0.72994500	0.59206600
H	6.88576000	-0.43140800	1.59593400
O	5.92910800	0.64812800	-1.38890900
C	-0.01992600	-1.10600200	-0.56762500
H	0.18816800	-0.66181800	0.40877900
C	-0.13245000	-2.62777400	-0.42528700
H	-0.02319400	-3.11492000	-1.40178000
C	-1.57433800	-2.78578000	0.10225600
H	-2.02969300	-3.74933200	-0.21463800
C	-1.43816000	-0.67606300	-1.04839100
H	-1.42693800	-0.47624800	-2.13222000
C	-1.96681700	0.56482300	-0.31906600
H	-1.22831800	1.37251000	-0.43544300
H	-2.02444800	0.32511400	0.75054000

C	-3.33374900	1.04403900	-0.82276900
H	-3.28158000	1.20774300	-1.91056900
H	-4.07360600	0.25005300	-0.66125600
C	-3.81691900	2.33199500	-0.14349200
H	-3.07408600	3.13009200	-0.29810200
H	-3.87108900	2.17161900	0.94375600
C	-5.18331000	2.81051300	-0.65018700
H	-5.13160800	2.96695700	-1.73767600
H	-5.92528200	2.01524900	-0.49125300
O	-1.71956300	-2.48223400	1.38509000
S	1.26483600	-0.49789800	-1.74877900
O	-2.27527000	-1.82097200	-0.84776900
H	-3.16015300	-2.74735800	1.88128900
H	0.60041400	-3.04882800	0.26995000
C	-5.66416100	4.09786100	0.02517100
H	-6.64237400	4.41193000	-0.35999300
H	-5.76256900	3.96518800	1.11044400
H	-4.96074900	4.92390000	-0.14402000
O	-4.13254500	-2.93181500	2.18541400
H	-4.22687600	-3.89002200	2.05998400
O	-5.04489300	-2.16606700	-0.32939800
H	-4.14035100	-1.98679100	-0.66169600
H	-4.85614700	-2.37977600	0.61733500

TS_5’

Charge/multiplicity: -1 1

N	4.75097900	0.24402900	0.45028200
H	4.76472600	-0.00853200	1.43225800
C	3.43825300	0.49512000	-0.12966800
H	3.55992000	1.21353600	-0.94372300
C	2.85177100	-0.81837800	-0.69976400
C	2.56906700	1.07590600	0.99173800
H	3.59567800	-1.24404200	-1.37877700
H	2.68180400	-1.53615900	0.10808800
O	2.61182900	0.59017600	2.13149100
N	1.78776500	2.12106400	0.67156800
H	1.77631000	2.45065400	-0.28448900
C	0.89420900	2.74026500	1.64140200
H	1.46465300	3.18209900	2.46587900
H	0.32896800	3.52687600	1.13894800
H	0.19649200	2.00746400	2.05895000
C	5.90019600	0.24844500	-0.27062300
C	7.15502400	-0.06583400	0.52108300
H	8.01542000	-0.05744500	-0.15083000
H	7.30878100	0.67593200	1.31353300
H	7.07794500	-1.05027500	0.99701600
O	5.92087000	0.50107700	-1.48186700
C	-0.00729900	-1.11115500	-0.47043600
H	0.19563200	-0.58992600	0.46827700
C	-0.15485800	-2.61497500	-0.20658900
H	0.01549200	-3.18572100	-1.12720600
C	-1.63349200	-2.72536700	0.22762300
H	-2.07272400	-3.70722800	-0.05439200
C	-1.40608000	-0.68759400	-1.01797400
H	-1.35538600	-0.50520900	-2.10297600
C	-1.95175900	0.56850700	-0.32599500
H	-1.21052900	1.37362700	-0.44258000
H	-2.03132000	0.35044400	0.74642300
C	-3.30837900	1.04029100	-0.86289300
H	-3.22869600	1.22136000	-1.94626800
H	-4.04452100	0.23715400	-0.73360800
C	-3.82134700	2.31143500	-0.17361200
H	-3.08665500	3.12185100	-0.30109100

H	-3.89235700	2.13170300	0.90962400
C	-5.18556200	2.78091900	-0.69423200
H	-5.11773100	2.96421400	-1.77659600
H	-5.91765200	1.97097700	-0.56685100
O	-1.87318400	-2.33287800	1.47189400
S	1.30550100	-0.62519500	-1.67738200
O	-2.25163500	-1.82793900	-0.83502500
H	-3.34163900	-2.59940500	1.87420000
H	0.52259700	-2.98046500	0.57142000
C	-5.69798700	4.04378100	0.00390200
H	-6.67417800	4.35263100	-0.39047000
H	-5.81313800	3.88213000	1.08360200
H	-5.00465000	4.88436700	-0.13190900
O	-4.33040700	-2.79292000	2.11432500
H	-4.39276600	-3.75899800	2.03984300
O	-5.04930000	-2.16670100	-0.49994000
H	-4.12274200	-1.99326600	-0.76885700
H	-4.93286300	-2.33759700	0.46693500

P(S)

Charge/multiplicity: -1 1

N	-4.60002400	-0.49850600	0.37077700
H	-4.68101800	-0.28815800	1.35969000
C	-3.24765800	-0.72128600	-0.11430700
H	-3.26830300	-1.53736100	-0.84253600
C	-2.71995700	0.55745700	-0.81588200
C	-2.40604000	-1.11908800	1.10784000
H	-3.48536600	0.87413000	-1.52871100
H	-2.58246600	1.36234100	-0.08822900
O	-2.73119500	-0.75214500	2.24625100
N	-1.32798500	-1.88359200	0.86514300
H	-1.07503600	-2.06899400	-0.09772000
C	-0.39638200	-2.25922100	1.92216900
H	-0.92671800	-2.78515400	2.72248100
H	0.35545600	-2.92680000	1.49749600
H	0.10149000	-1.38257600	2.34872500
C	-5.69798100	-0.58636400	-0.41474800
C	-7.02399200	-0.33796700	0.27413100
H	-6.92283600	-0.11250200	1.33942500
H	-7.53040400	0.49748600	-0.22154200
H	-7.65751900	-1.22357600	0.15373200
O	-5.63177500	-0.85505100	-1.62259800
C	0.09600300	1.15749900	-0.71138200
H	0.00176000	0.73522400	0.29202600
C	0.03852500	2.68641900	-0.65147300
H	-0.19197700	3.09604200	-1.64273200
C	1.48455900	3.05356700	-0.24505000
H	1.78511400	4.02601700	-0.68961000
C	1.52010000	0.87658600	-1.26654100
H	1.46807000	0.70432400	-2.35557200
C	2.20779800	-0.32415900	-0.60896500
H	1.58221500	-1.21450000	-0.77484400
H	2.23914000	-0.14825700	0.47324100
C	3.62364200	-0.58843400	-1.13500400
H	3.58659200	-0.75213800	-2.22335900
H	4.23480800	0.30908200	-0.97433100
C	4.29990200	-1.78926300	-0.46195200
H	3.67596100	-2.68623800	-0.59874700
H	4.34788300	-1.61205700	0.62271300
C	5.71226000	-2.07496900	-0.98789200
H	5.66705600	-2.25425000	-2.07216900
H	6.33579300	-1.17975100	-0.85196900
O	1.74292200	2.98278800	1.06912000

S	-1.16743400	0.34122800	-1.78258900
O	2.26378100	2.08350200	-1.06655900
H	2.46398300	0.87746200	2.70856300
H	-0.69179100	3.06636800	0.06921900
C	6.38183000	-3.26969700	-0.30318400
H	7.38851200	-3.44862500	-0.70127200
H	6.47697100	-3.10584700	0.77806800
H	5.79991300	-4.18955800	-0.44762900
O	1.49022100	0.93519600	2.76551100
H	1.34788700	1.67389800	2.10565600
O	4.05956600	1.91638900	1.84751500
H	3.26093600	2.39101000	1.45377500
H	4.28509700	2.46608500	2.61566600

TS_{1C1}

Charge/multiplicity: -1 1

N	3.66080800	-1.67469500	-0.22466600
H	3.33416600	-2.58169000	0.09087400
C	2.79724200	-0.55451700	0.11719700
H	3.42409500	0.28506200	0.43233300
C	1.96784300	-0.12047500	-1.12234200
C	1.92097200	-1.03450300	1.29041400
H	2.64079200	-0.12173800	-1.98345400
H	1.16972300	-0.84338200	-1.31836500
O	1.72235300	-2.25281400	1.44932900
N	1.41597900	-0.10910700	2.11924400
H	1.42933700	0.89149500	1.89839900
C	0.54406400	-0.50254400	3.21878600
H	-0.39874200	-0.93138800	2.85845900
H	1.04112600	-1.24415700	3.85178400
H	0.32615600	0.38809300	3.80888600
C	4.84469900	-1.54282800	-0.86391500
C	5.61090400	-2.82861600	-1.10224800
H	5.09251000	-3.71758600	-0.73168800
H	5.79075800	-2.94091100	-2.17703300
H	6.58810600	-2.75472700	-0.61238100
O	5.28555800	-0.44581200	-1.23531500
C	-0.55526300	1.36299900	-1.26377100
H	-0.61519000	0.89533200	-2.25271400
C	-1.07725400	2.81499300	-1.38089900
H	-0.69726800	3.25777600	-2.30772900
C	-2.48736300	3.16454700	-1.24277900
H	-2.78430900	4.05862800	-1.82717000
C	-1.25997400	0.40290000	-0.26775200
H	-0.53024300	-0.34195800	0.06267500
C	-2.41221200	-0.37279000	-0.93937700
H	-1.99498400	-0.91017100	-1.80291000
H	-3.15639100	0.32869500	-1.33571800
C	-3.09500200	-1.37389800	0.00104700
H	-2.33771600	-2.05742000	0.41473400
H	-3.51944100	-0.83408200	0.85712100
C	-4.19595100	-2.19279200	-0.68410200
H	-3.76800500	-2.73943100	-1.53827600
H	-4.94868800	-1.50959600	-1.10596500
C	-4.88943000	-3.18898300	0.25408300
H	-4.13763300	-3.86995600	0.67893500
H	-5.32185000	-2.64332000	1.10507100
O	-3.33258600	2.67546800	-0.47641300
S	1.27712700	1.57158400	-0.93389200
O	-1.68499700	1.04917000	0.93414200
H	-2.39864700	1.67087000	0.65234000

H	0.35397000	3.33804300	1.64796000
C	-5.98431300	-4.00806000	-0.43479500
H	-6.45742800	-4.71109700	0.26204100
H	-6.77293500	-3.35951700	-0.83814500
H	-5.57786900	-4.59248900	-1.27059600
O	0.31745500	2.59216300	2.35580500
H	-0.39454000	2.03667300	1.98030500
O	0.13149600	4.42932500	0.51361500
H	-0.57063000	3.52304500	-0.51410900
H	-0.66779800	4.83957500	0.88797800

MIN_{1C1}

Charge/multiplicity: -1 1

N	3.81932400	-1.63840200	-0.36254800
H	3.53530000	-2.60439100	-0.47987700
C	2.76208600	-0.71286300	0.02926700
H	3.20193200	0.06079700	0.66288600
C	2.13961400	-0.05514000	-1.23023700
C	1.74488600	-1.55388600	0.81299600
H	2.96215300	0.17949000	-1.91121100
H	1.47877000	-0.76580900	-1.73799800
O	1.47598600	-2.70584400	0.42775400
N	1.20792800	-1.00341500	1.90922900
H	1.32294400	-0.00565700	2.10764000
C	0.19188200	-1.70495000	2.68184200
H	-0.72651800	-1.85703600	2.10297500
H	0.56475400	-2.68310500	3.00147000
H	-0.04050500	-1.10496400	3.56304500
C	5.09272300	-1.25844800	-0.61721800
C	6.04151600	-2.36640900	-1.02868200
H	6.88345500	-2.39036000	-0.32825500
H	5.57149700	-3.35368000	-1.05601900
H	6.44659900	-2.13601600	-2.02026800
O	5.47089400	-0.08284200	-0.51869800
C	-0.55663800	1.19561000	-1.46906900
H	-0.45313600	0.59745700	-2.38072100
C	-1.14221000	2.53227700	-1.84101700
H	-1.03814800	2.81617800	-2.88667500
C	-1.65392100	3.48172700	-1.00701600
H	-1.95934000	4.42573800	-1.49340200
C	-1.33891800	0.32176600	-0.45994900
H	-0.76125700	-0.59889300	-0.30144300
C	-2.71101700	-0.07801500	-1.03888300
H	-2.56696500	-0.48001300	-2.05254100
H	-3.32380500	0.82721200	-1.14418700
C	-3.45013300	-1.11226700	-0.18089200
H	-2.84180800	-2.02721100	-0.11158300
H	-3.54426700	-0.72563200	0.84241000
C	-4.84020900	-1.47195700	-0.72051400
H	-4.74690600	-1.85387000	-1.74879100
H	-5.45071600	-0.55885300	-0.78902800
C	-5.57870300	-2.50800700	0.13649200
H	-4.97026900	-3.42160000	0.20512800
H	-5.67249200	-2.12639600	1.16346500
O	-1.84937300	3.43099300	0.29168500
S	1.23108000	1.52205900	-0.93384200
O	-1.49234100	0.91984500	0.82490400
H	-1.70709300	1.90170100	0.67749100
H	0.56449800	2.50404800	2.46270400
C	-6.96725700	-2.86206100	-0.40286300
H	-7.46719500	-3.60386700	0.23238500
H	-7.61380700	-1.97606500	-0.44987700
H	-6.90638200	-3.28026700	-1.41616200

O	0.39629300	1.58903800	2.79269800
H	-0.27854200	1.27468800	2.14796500
O	0.44516500	4.11583900	1.58772500
H	1.09823300	3.95415300	0.88699300
H	-0.42421600	3.93151300	1.13211000

HNE_{c1}

Charge/multiplicity: 0 1

C	2.40807600	2.01006700	-0.04922600
O	1.84342300	1.89697300	-1.13310100
H	2.94090500	2.95218600	0.19079100
C	2.46981600	0.99983200	1.01561700
H	2.90071300	1.35380100	1.95043500
C	2.09680800	-0.29268500	0.91899600
H	2.23209800	-0.92791600	1.79575800
C	1.53457100	-1.02826100	-0.26758400
H	1.67970700	-0.44701900	-1.18340400
C	0.04112100	-1.34719700	-0.09517100
H	-0.08894900	-1.91789100	0.83511000
H	-0.22884800	-2.02162300	-0.91889400
C	-0.88389400	-0.12456600	-0.09840900
H	-0.61651100	0.54472900	0.73082400
H	-0.72692300	0.45060700	-1.02099900
C	-2.36483800	-0.50804000	0.01953700
H	-2.51797700	-1.09213600	0.93950400
H	-2.63605900	-1.17359300	-0.81363500
C	-3.30910400	0.70068200	0.02707700
H	-3.04121700	1.36437100	0.86186300
H	-3.15491500	1.28610500	-0.89068300
C	-4.78534700	0.31087900	0.14069200
H	-4.97926800	-0.24915800	1.06479700
H	-5.43425500	1.19536000	0.14671600
H	-5.09580500	-0.32248000	-0.70045400
O	2.20529400	-2.29730600	-0.37441800
H	3.13430400	-2.11693900	-0.59674600

TS_{1C2}

Charge/multiplicity: -1 1

N	-3.15579700	1.90457900	-0.07398900
H	-2.82741200	2.54870300	0.63642300
C	-2.49122700	0.60797200	-0.10506400
H	-3.22107200	-0.14091900	-0.42231600
C	-1.32310300	0.63537700	-1.12525000
C	-2.01728000	0.33131700	1.32985300
H	-1.71103200	1.06188200	-2.05446800
H	-0.52271800	1.28961800	-0.76674200
O	-1.57444500	1.26891400	2.01974100
N	-2.11937400	-0.92616300	1.77474400
H	-2.38978600	-1.69475300	1.14568900
C	-1.62861200	-1.29941900	3.09427300
H	-0.54564300	-1.15664100	3.17287800
H	-2.11954500	-0.70557200	3.87249800
H	-1.85813900	-2.35497100	3.25445800
C	-4.12630100	2.27065400	-0.94272100

C	-4.68734200	3.66599400	-0.75670200
H	-5.77150800	3.59579300	-0.61713000
H	-4.25108900	4.20037700	0.09205900
H	-4.51113800	4.24345700	-1.67109700
O	-4.53953000	1.51913900	-1.83710000
C	1.15156800	-1.03790500	-0.98259100
H	1.61829800	-0.28595600	-1.62948600
C	1.60916600	-2.45466600	-1.35823500
H	1.35953700	-2.70610600	-2.39484400
C	2.91035600	-2.94560400	-1.00259300
H	3.32249100	-2.58605400	-0.03820200
C	1.39092200	-0.58810700	0.48689400
H	0.60082100	0.12701600	0.75633100
C	2.72650600	0.16530500	0.65860800
H	3.54220700	-0.39481500	0.18375500
H	2.93923000	0.17298500	1.73614600
C	2.72157300	1.61144600	0.14576000
H	2.50637100	1.63395200	-0.93237000
H	1.90664000	2.16546600	0.63515000
C	4.04952600	2.33667800	0.40215300
H	4.86610600	1.78230300	-0.08444200
H	4.26891900	2.31888500	1.48030200
C	4.06332200	3.78916400	-0.09091400
H	3.84851500	3.80871600	-1.16927200
H	3.24698300	4.34441700	0.39347600
O	3.54996300	-3.81733900	-1.62645500
S	-0.65962400	-1.03384500	-1.51625700
O	1.38658400	-1.65472800	1.43471400
H	0.77708400	-2.38183200	1.13288700
H	0.77582200	-3.26459000	-0.52822200
C	5.39110900	4.50354800	0.17543900
H	5.36922100	5.53882800	-0.18702200
H	5.61886400	4.53243500	1.24894700
H	6.22466100	3.99415500	-0.32535000
O	0.03479600	-3.71923900	0.34540300
H	0.46539100	-4.54014800	0.64029900
O	-2.61719100	-3.38664000	0.34493000
H	-2.77566500	-3.09340500	-0.56721700
H	-1.63475700	-3.59199900	0.33836200

MIN_{1C2}

Charge/multiplicity: -1 1

N	3.31884900	-2.02725200	-0.10242600
H	2.94752700	-2.72381700	0.53308500
C	2.63682600	-0.73671200	-0.10012100
H	3.36706000	0.03071500	-0.36711200
C	1.49336200	-0.74226600	-1.14234600
C	2.12114600	-0.52623500	1.32916300
H	1.91073900	-1.10004300	-2.08804400
H	0.71603400	-1.44825500	-0.83058600
O	1.56458300	-1.46558000	1.92606500
N	2.32814700	0.67748300	1.87622700
H	2.70491100	1.44612300	1.30859500
C	1.81799000	0.99745500	3.20173500
H	0.72495100	0.93493200	3.22870400
H	2.22743800	0.31158000	3.95102800
H	2.12365800	2.01635000	3.44931300
C	4.32411800	-2.34262000	-0.95184100
C	4.87710800	-3.74801200	-0.82798700
H	5.95471200	-3.68933900	-0.64062600
H	4.40684600	-4.33222000	-0.03183400
H	4.73801100	-4.26864100	-1.78206600
O	4.77535700	-1.53869700	-1.77961000

C	-1.17444100	0.73464500	-1.06317500
H	-1.42228000	-0.16213500	-1.64091500
C	-1.83119300	1.93201000	-1.65366000
H	-1.86100300	1.94952400	-2.74548500
C	-2.44770500	2.99948000	-1.00967500
H	-2.42119700	2.97586900	0.09936800
C	-1.40923100	0.37332500	0.41492100
H	-0.78267100	-0.50471500	0.63604200
C	-2.86391700	-0.02452600	0.72027300
H	-3.52594500	0.81614200	0.48388000
H	-2.92017300	-0.17756400	1.80748200
C	-3.35746300	-1.29089000	0.00939900
H	-3.40995400	-1.11470000	-1.07381100
H	-2.63180400	-2.10509100	0.15783600
C	-4.73608400	-1.74698500	0.50594400
H	-5.45749800	-0.92624400	0.37655600
H	-4.68536700	-1.94119500	1.58796700
C	-5.26456400	-2.99796100	-0.20702000
H	-5.32124000	-2.80262200	-1.28766600
H	-4.54354000	-3.81901900	-0.08213700
O	-3.04935800	3.98044700	-1.56584100
S	0.72698000	0.91031100	-1.44235900
O	-1.06748600	1.41030700	1.34385400
H	-0.38181400	1.99106400	0.95743500
H	-0.02947900	3.51982100	-0.50564800
C	-6.63779100	-3.44652200	0.30046400
H	-6.98840100	-4.34117800	-0.22901500
H	-6.60781700	-3.68515000	1.37161600
H	-7.39066500	-2.66035500	0.15834300
O	0.42880400	3.69210700	0.34104900
H	-0.00139800	4.48980100	0.69444000
O	3.15561100	3.09074200	0.48977800
H	3.42883400	2.85823700	-0.41271800
H	2.22181800	3.38580000	0.37831200

HNE_{c2}

Charge/multiplicity: 0 1

C	-2.64478700	-1.56682500	-0.38064800
O	-3.15815200	-2.68117200	-0.34489600
H	-2.25011500	-1.17536600	-1.33595600
C	-2.53049600	-0.70845900	0.79946800
H	-2.96412200	-1.12194600	1.70861100
C	-1.94738600	0.50639100	0.82969000
H	-1.93548300	1.04417700	1.77871200
C	-1.28827300	1.27252900	-0.28791900
H	-1.45019600	0.78915000	-1.25880700
C	0.22032600	1.43523100	-0.05617100
H	0.37415700	1.90014000	0.92752400
H	0.57706200	2.15455000	-0.80538600
C	1.02271300	0.13344800	-0.15989800
H	0.66407100	-0.58566500	0.58938400
H	0.84325300	-0.32869900	-1.14177900
C	2.52972000	0.35084000	0.02809900
H	2.70917600	0.82046900	1.00686300
H	2.89042500	1.06705300	-0.72517600
C	3.35014100	-0.94118500	-0.06971700
H	2.99160700	-1.65645800	0.68452100
H	3.17048100	-1.41202500	-1.04713500
C	4.85307200	-0.71677400	0.11671900
H	5.07227200	-0.28263000	1.10082600
H	5.41036600	-1.65833000	0.03819700

H	5.25090000	-0.03142000	-0.64291000
O	-1.83698600	2.60115500	-0.31385700
H	-2.78293600	2.52596300	-0.52519600

WATER – IMPLICIT SOLVENT

Cysteinate$(H_2O)^-$

Charge/multiplicity: -1 1

N	1.17858000	1.05478800	0.23402100
H	0.98654100	2.03241400	0.42640400
C	0.00745100	0.21919600	-0.00369100
H	0.15647200	-0.32934500	-0.93905700
C	-0.20942500	-0.82072100	1.13103500
C	-1.18953700	1.16700300	-0.17138600
H	0.77785700	-1.21628200	1.38665000
H	-0.58662700	-0.29945700	2.01973500
S	-1.32464900	-2.22562800	0.66929300
O	-1.05906100	2.40373600	-0.07809000
N	-2.36314400	0.57043500	-0.42817100
H	-2.38894800	-0.44986600	-0.27589600
C	-3.60121300	1.33357100	-0.49226100
H	-3.81040800	1.85249900	0.45077400
H	-3.55306700	2.08069300	-1.29014300
H	-4.42088600	0.64548500	-0.70552900
C	2.44404000	0.65150600	0.02735500
C	3.52341400	1.68313400	0.26380300
H	4.21546300	1.30604800	1.02409100
H	4.09282600	1.81862000	-0.66184300
H	3.12754900	2.64921700	0.58658600
O	2.74364900	-0.50644900	-0.33486500
O	1.18428400	-2.71947600	-1.35303300
H	1.71622300	-1.98135100	-0.99014100
H	0.37398500	-2.69982400	-0.78250300

HNE$(H_2O)_t$

Charge/multiplicity: 0 1

C	-3.77524900	-0.42776100	-0.98808200
O	-4.80687200	0.24771300	-0.92086900
H	-3.70581300	-1.23922000	-1.73491600
C	-2.60961700	-0.23917900	-0.13985400
H	-2.65937800	0.54454500	0.61284500
C	-1.52217100	-1.01549700	-0.29725600
H	-1.52464000	-1.79508400	-1.06062200
C	-0.25797900	-0.90068100	0.50568800
H	-0.41656800	-0.20828300	1.34393900
C	0.90160800	-0.38783300	-0.35798200
H	0.59113600	0.56246200	-0.81022100
H	1.06355300	-1.09613400	-1.18200300
C	2.20322500	-0.18511700	0.42885400
H	2.01447200	0.50365400	1.26497100
H	2.51498200	-1.13793400	0.87459300
C	3.34041100	0.36730000	-0.43866700
H	3.02805200	1.32400700	-0.88283500
H	3.52168100	-0.31703300	-1.28066200
C	4.64839700	0.57268500	0.33500100
H	4.46639900	1.25373800	1.17844600
H	4.96143400	-0.38430200	0.77595900
C	5.77989200	1.12834800	-0.53360900

H	5.51002800	2.10246500	-0.96080200
H	6.70078400	1.26313000	0.04620600
H	6.00776000	0.45291500	-1.36793300
O	0.10734400	-2.19841900	1.00580100
H	-0.57574200	-2.46176400	1.64526600
O	-4.65045300	2.27247200	1.09394800
H	-4.19395800	2.99207000	0.62922200
H	-4.75543300	1.59305000	0.39295100

MIN_{1t}

Charge/multiplicity: -1 1

N	3.10976000	0.05557700	0.13435800
H	2.38177200	-0.24358600	0.79543800
C	2.82453200	1.09206800	-0.84357100
H	3.73540800	1.18248200	-1.44625700
C	1.69627500	0.73065800	-1.82990900
C	2.60803700	2.48375300	-0.23249900
H	1.75531200	1.41772100	-2.67704100
H	1.85722800	-0.28500700	-2.20070800
O	2.27597000	3.43882900	-0.95660100
N	2.82946900	2.61776900	1.08485200
H	3.12351100	1.80532300	1.61057900
C	2.71217500	3.90294300	1.75764800
H	1.70324300	4.31164500	1.64337900
H	2.91865600	3.75935500	2.81875900
H	3.42547900	4.62747100	1.35073800
C	4.29247000	-0.61645300	0.14276800
C	4.41174100	-1.71660700	1.17740100
H	3.63074000	-2.47007800	1.03012400
H	5.39317900	-2.18537200	1.08755400
H	4.29440300	-1.31294500	2.18859300
O	5.22067600	-0.35512100	-0.64080600
C	-0.56077700	-0.89882800	-0.72618200
H	-0.38981700	-0.96197800	0.34919500
C	0.21209900	-1.96969300	-1.41079000
H	0.17136900	-2.01610000	-2.49794000
C	0.91055300	-2.94027500	-0.75936000
H	1.41448700	-3.68610300	-1.39806700
C	-2.09475200	-0.98238000	-0.96825900
H	-2.28715600	-0.80157800	-2.03418600
C	-2.89814000	0.02449200	-0.12974700
H	-2.51050100	1.03804900	-0.29743700
H	-2.72797500	-0.20339600	0.93327800
C	-4.40206700	0.01378200	-0.43073600
H	-4.55660800	0.23584500	-1.49724900
H	-4.79959600	-0.99580700	-0.26505100
C	-5.19467500	1.01860600	0.41384100
H	-4.79127400	2.02940300	0.25200100
H	-5.04311400	0.79675400	1.48082400
C	-6.69756700	1.02180100	0.10861600
H	-6.84939600	1.24425200	-0.95720800
H	-7.10176100	0.01253000	0.27108200
O	1.05460300	-3.12930100	0.54089100
S	-0.03382700	0.86682900	-1.22308200
O	-2.55443300	-2.31654800	-0.71939000
H	-2.20449000	-2.59713100	0.16315600
H	-1.66018100	-4.19547700	1.56634800
C	-7.48194600	2.02778400	0.95513800
H	-8.55126300	2.00901000	0.71278100
H	-7.37966700	1.81029800	2.02591300
H	-7.12122000	3.05097600	0.78987700
O	-1.40140000	-3.26240400	1.64640300
H	-0.47751200	-3.23914100	1.25972600

O	1.38799400	-1.05280200	2.21476200
H	1.19548400	-1.81613100	1.59446900
H	0.52286200	-0.63510100	2.35396600

TS_{1t}

Charge/multiplicity: -1 1

N	-4.56267900	-0.42540300	0.26313200
H	-4.63178500	-0.15411900	1.23695300
C	-3.22390900	-0.70393500	-0.24865200
H	-3.31727200	-1.42730100	-1.06083700
C	-2.58199300	0.59464900	-0.79313000
C	-2.42403800	-1.28783300	0.91721300
H	-3.30103200	1.05389600	-1.47708800
H	-2.40275500	1.29592200	0.02810400
O	-2.42429800	-0.71949800	2.02323000
N	-1.75080900	-2.42443400	0.68205000
H	-1.76129300	-2.81365000	-0.25200200
C	-0.86896500	-3.01090900	1.68454500
H	-0.14639300	-2.27010200	2.04065500
H	-1.44284300	-3.37748100	2.54183300
H	-0.33646200	-3.84704900	1.23058500
C	-5.65953300	-0.37518500	-0.52746400
C	-6.95764800	-0.02069100	0.16191200
H	-7.37303300	0.87819000	-0.30577300
H	-7.67418200	-0.83419700	0.00702800
H	-6.83988000	0.15444700	1.23432600
O	-5.61241300	-0.61669800	-1.74585100
C	0.30105300	0.37296100	-0.48415700
H	0.08690000	-0.47565700	0.17292700
C	0.33107500	1.65714600	0.34546500
H	-0.34614600	2.44693300	0.00644500
C	0.32322500	1.52777300	1.77103700
H	0.10181000	2.47262800	2.31240800
C	1.61572800	0.00714100	-1.22275400
H	1.41249500	-0.87361900	-1.84638400
C	2.72578000	-0.37430900	-0.22567400
H	2.33922900	-1.15475300	0.44346200
H	2.95831900	0.48986700	0.41015600
C	4.00786100	-0.87183900	-0.90412600
H	3.77302000	-1.75238300	-1.52071700
H	4.37525700	-0.10207900	-1.59524300
C	5.11690800	-1.23055600	0.09203100
H	4.74994700	-2.00128000	0.78633700
H	5.34891800	-0.34980000	0.70945200
C	6.40354200	-1.72723500	-0.57804000
H	6.17507700	-2.61234200	-1.18866200
H	6.76678400	-0.95955000	-1.27613200
O	0.61640400	0.51408500	2.44468600
S	-1.04822000	0.39762800	-1.77681700
O	2.03957500	1.02109800	-2.13750500
H	2.26581100	1.82144200	-1.59194000

H	3.19836200	2.71731800	0.12858100
C	7.51050700	-2.07041800	0.42228600
H	8.41609100	-2.42204300	-0.08640400
H	7.78596300	-1.19536000	1.02467400
H	7.18959600	-2.85977300	1.11385800
O	2.44174000	3.07220100	-0.37002100
H	1.47415000	2.36952800	0.08058100
O	1.52123500	4.92751600	1.41765800
H	1.84588200	4.54877700	2.24979400
H	1.89989600	4.31020100	0.73530900

MIN_2

Charge/multiplicity: -1 1

N	-4.36913100	0.94709200	-0.24636900
H	-4.34039000	1.24737400	-1.21377400
C	-3.09563100	0.58197900	0.37304800
H	-3.21871700	0.67655800	1.45346700
C	-2.73398800	-0.87532900	0.02382400
C	-2.05072500	1.57341000	-0.14485100
H	-3.56861300	-1.50781700	0.33966600
H	-2.61100200	-0.98952100	-1.05451600
O	-1.81407900	1.65845100	-1.36363100
N	-1.45023800	2.34977400	0.76956800
H	-1.66157700	2.20569200	1.74836700
C	-0.41433100	3.30857900	0.40752700
H	-0.79773700	4.03533900	-0.31497500
H	-0.10066500	3.83492300	1.30945200
H	0.45250700	2.80396500	-0.03232100
C	-5.56727600	0.71154400	0.34016700
C	-6.78867800	1.06670400	-0.47744000
H	-7.37317000	0.15672200	-0.65111800
H	-7.41384200	1.75466400	0.10088300
H	-6.54566800	1.52380800	-1.43999700
O	-5.66538900	0.23970800	1.48532500
C	0.13294000	-1.25721200	-0.37117900
H	-0.26205200	-0.55783000	-1.11406800
C	0.51160300	-2.57952400	-1.04303400
H	0.74967100	-3.35070100	-0.29997900
C	-0.45998700	-3.16317500	-2.02285200
H	-0.19188600	-4.17835300	-2.37925700
C	1.34061200	-0.60987400	0.36933500
H	0.92690300	0.31113400	0.83094300
C	2.41000600	-0.12716300	-0.64609400
H	1.92159800	0.37432000	-1.49530600
H	2.93995300	-0.99938900	-1.05307100
C	3.43073300	0.83384700	-0.02159700
H	2.90949800	1.74947400	0.29806500
H	3.84198200	0.38373500	0.89070900
C	4.57856000	1.21121600	-0.96580000
H	4.16675400	1.64153700	-1.89132900
H	5.11540800	0.29863300	-1.26693500
C	5.57653400	2.20053600	-0.35151900
H	5.04276700	3.11448800	-0.05424200
H	5.98719000	1.77200500	0.57387100
O	-1.45672500	-2.61343700	-2.46863300
S	-1.23954200	-1.53279200	0.87231500
O	1.84919700	-1.46859500	1.34360100
H	3.20391700	-2.26376400	0.92858500
H	1.44323100	-2.46113200	-1.62252100
C	6.72462100	2.56611400	-1.29614800
H	7.41961500	3.27375600	-0.82832900
H	7.29957400	1.67691500	-1.58451400

H	6.34831800	3.02925700	-2.21716100
O	4.10300200	-2.72007600	0.78819300
H	4.65169200	-1.99756100	0.44334700
O	3.67166200	-0.87904400	3.16942500
H	2.89345100	-0.96189400	2.53264100
H	4.26823800	-1.53566400	2.76943300

TS_2

Charge/multiplicity: -1 1

N	4.67222600	0.58620000	0.36613200
H	4.63748600	0.87460000	1.33748000
C	3.39432800	0.45883400	-0.33027100
H	3.58312300	0.59194700	-1.39724000
C	2.79248000	-0.94364400	-0.09426500
C	2.48547900	1.56933700	0.20170000
H	3.53772400	-1.68070900	-0.40452900
H	2.59793000	-1.09211500	0.97263400
O	2.27677800	1.67729800	1.42419200
N	1.96029800	2.40764700	-0.70336400
H	2.14594800	2.24746300	-1.68493500
C	1.05793800	3.48725100	-0.32378100
H	0.80606700	4.05748800	-1.21820300
H	0.13760800	3.09340800	0.11996800
H	1.53678900	4.15166000	0.40143900
C	5.84386900	0.14197300	-0.15286900
C	7.04637700	0.27914800	0.75652900
H	7.20433600	1.32736100	1.03302800
H	6.89527900	-0.28941400	1.68094400
H	7.93262200	-0.09684000	0.24279400
O	5.92272400	-0.33024900	-1.29835400
C	-0.06837500	-0.92289800	0.19905300
H	0.28542000	-0.07065700	0.78820100
C	-0.25029500	-2.15085400	1.11808200
H	0.73626100	-2.44290300	1.50797800
C	-1.08629100	-1.90048300	2.33955200
H	-0.73972700	-1.08518500	3.00388900
C	-1.34296200	-0.50727300	-0.59946700
H	-0.99886000	0.34517600	-1.22521800
C	-2.42035000	0.08717300	0.34793100
H	-1.94090800	0.69369500	1.13176000
H	-2.94610100	-0.73312200	0.85151300
C	-3.44960200	0.96002700	-0.38425100
H	-2.92781200	1.79401400	-0.87804200
H	-3.91676200	0.37014100	-1.18241500
C	-4.53596700	1.52315100	0.53960800
H	-4.06429300	2.10469400	1.34636100
H	-5.06166500	0.69116900	1.03195100
C	-5.56027100	2.40714400	-0.18309500
H	-5.03682400	3.23909200	-0.67560700
H	-6.03602600	1.82704200	-0.98657400
O	-2.07342500	-2.55562900	2.65311100
S	1.26376200	-1.30080900	-1.05085900
O	-1.80623400	-1.55146300	-1.39515700
H	-2.66571300	-2.67989200	-0.53393900
H	-0.66320800	-2.99186900	0.55762100
C	-6.63870800	2.96521200	0.74926800
H	-7.35581100	3.59146500	0.20502100
H	-7.20218600	2.15663400	1.23205100
H	-6.19637200	3.57964300	1.54384200
O	-3.21921900	-3.36993900	-0.04286400
H	-2.95888700	-3.23057100	0.88568700
O	-4.07366700	-1.58343000	-2.75027600
H	-3.19107600	-1.47082100	-2.26750400

H	-4.60375900	-2.03388600	-2.07315500

MIN_3

Charge/multiplicity: -1 1

N	4.66154800	0.58869700	0.38250600
H	4.61275000	0.89383600	1.34748500
C	3.39388800	0.45922700	-0.33230900
H	3.59760200	0.58873400	-1.39702400
C	2.79113500	-0.94349900	-0.09897900
C	2.47781800	1.57101000	0.18475100
H	3.53790700	-1.68041300	-0.40579000
H	2.59222900	-1.09147300	0.96711800
O	2.25954100	1.68652400	1.40487000
N	1.95784700	2.40172800	-0.72999300
H	2.15082600	2.23488600	-1.70904900
C	1.04687200	3.47928600	-0.36534500
H	0.12327900	3.08361300	0.06994700
H	1.51508900	4.14890600	0.36197000
H	0.80269700	4.04434400	-1.26517500
C	5.84042800	0.15100100	-0.11994900
C	7.04269700	0.28971500	0.78691200
H	6.81175900	0.76872700	1.74205700
H	7.45701400	-0.70625100	0.97709600
H	7.81091100	0.87249500	0.26833100
O	5.93808200	-0.32928200	-1.26185200
C	-0.06762600	-0.92914300	0.19188600
H	0.28701300	-0.08011600	0.78511200
C	-0.24918700	-2.16203400	1.10431000
H	0.73767600	-2.45722100	1.49104300
C	-1.08281900	-1.91762000	2.32864700
H	-0.73388700	-1.10668900	2.99707400
C	-1.34305300	-0.50850600	-0.60259700
H	-0.99938600	0.34691300	-1.22451500
C	-2.41784300	0.08183600	0.35042800
H	-1.93592900	0.68097900	1.13841300
H	-2.94527200	-0.74086200	0.84825600
C	-3.44544200	0.96365700	-0.37325900
H	-2.92175800	1.79987200	-0.86121400
H	-3.91598000	0.38172200	-1.17531800
C	-4.52829700	1.52285100	0.55709400
H	-4.05309700	2.09564800	1.36804400
H	-5.05626800	0.68862100	1.04314000
C	-5.55047400	2.41694300	-0.15608600
H	-5.02472900	3.25102200	-0.64250100
H	-6.03010800	1.84562200	-0.96356300
O	-2.07027800	-2.57320400	2.64020000
S	1.26505800	-1.30030200	-1.05984000
O	-1.80899000	-1.54794100	-1.40286100
H	-2.66894300	-2.67923600	-0.54545500
H	-0.66388200	-2.99946000	0.53976500
C	-6.62495500	2.97122200	0.78307600
H	-7.34104700	3.60425400	0.24537800
H	-7.19019000	2.16074000	1.26057000
H	-6.17886600	3.57778600	1.58158700
O	-3.22307800	-3.37047100	-0.05682000
H	-2.96010100	-3.23691600	0.87185100
O	-4.08115600	-1.56733700	-2.75011100
H	-3.19648500	-1.45920400	-2.27005500
H	-4.60934500	-2.02100100	-2.07363500

TS_3

Charge/multiplicity: -1 1

N	-4.28302000	0.66810000	-0.34642100
H	-4.14963700	1.27844400	-1.14505100
C	-3.08099100	0.26006900	0.37704200
H	-3.38542900	-0.03017200	1.38438200
C	-2.42163000	-0.94632300	-0.32403900
C	-2.15553000	1.47877100	0.42001600
H	-3.17076400	-1.73984300	-0.39146900
H	-2.13374900	-0.67186800	-1.34331100
O	-1.79946100	2.03394100	-0.63590700
N	-1.78546600	1.91470600	1.63271100
H	-2.09629000	1.40630200	2.45010500
C	-0.91582700	3.07099200	1.80777500
H	-0.78725000	3.24759500	2.87590600
H	0.06493900	2.89763000	1.35326000
H	-1.35911200	3.96010400	1.34906200
C	-5.49935600	0.10373600	-0.14163900
C	-6.59887900	0.58968400	-1.06221800
H	-7.53036600	0.07868000	-0.81323600
H	-6.73961300	1.67120200	-0.95838600
H	-6.34275100	0.38654100	-2.10801000
O	-5.69756600	-0.73844900	0.74845700
C	0.44392000	-0.86192400	-0.37639300
H	0.12914100	0.16557600	-0.57946000
C	0.69776000	-1.55707500	-1.73816600
H	1.40288900	-0.93958800	-2.30906800
C	1.26385500	-2.95258300	-1.63660400
H	2.36241900	-3.04015700	-1.63849300
C	1.68316300	-0.87629900	0.54839900
H	1.36203400	-0.36045300	1.47767700
C	2.85210000	-0.02833800	-0.01416500
H	3.19986400	-0.46054900	-0.96265600
H	3.67707800	-0.15349300	0.70072400
C	2.57152100	1.46866500	-0.19752800
H	1.80496700	1.61987800	-0.97061600
H	2.15036600	1.87609100	0.73438300
C	3.82210400	2.27369000	-0.57554400
H	4.25342100	1.86212300	-1.50038700
H	4.58761800	2.14064300	0.20342600
C	3.55414300	3.77119100	-0.76906900
H	2.79237100	3.90457400	-1.55041100
H	3.12130700	4.18334500	0.15366200
O	0.57136900	-3.96648000	-1.64100600
S	-0.96601000	-1.65772400	0.54476200
O	2.06456000	-2.19414600	0.81856500
H	3.55180400	-2.63055900	0.21059000
H	-0.24012600	-1.60790200	-2.30187300
C	4.80930700	4.56487500	-1.14139600
H	4.58596800	5.63019300	-1.27471000
H	5.57714400	4.48079400	-0.36188900
H	5.24731400	4.19698000	-2.07794000
O	4.47770900	-2.92922600	-0.06511800
H	4.49213500	-3.86284500	0.20208700
O	3.84600000	-2.05259300	2.78522400
H	4.57538800	-2.31201000	2.19651900
H	3.07762500	-2.11247700	2.13440800

MIN_4

Charge/multiplicity: -1 1

N	-3.55351200	0.89691600	0.56448100

H	-3.10240900	1.66890600	1.04204600
C	-2.71270100	-0.25438300	0.26570600
H	-3.33399600	-1.15172400	0.31556300
C	-2.12511400	-0.12600700	-1.16335200
C	-1.62134700	-0.30020700	1.34143800
H	-2.95668600	0.07082000	-1.84402500
H	-1.44265600	0.72562800	-1.20716800
O	-1.11593400	0.75319400	1.77045800
N	-1.26673000	-1.51506900	1.78574700
H	-1.63424700	-2.32382200	1.30056500
C	-0.14347700	-1.70906000	2.69670100
H	-0.33666300	-1.20394500	3.64773500
H	-0.03484300	-2.77843000	2.88128500
H	0.79042400	-1.32104700	2.27943600
C	-4.83730600	1.00576000	0.15431900
C	-5.54244200	2.29418100	0.51407900
H	-5.84669600	2.79944700	-0.40891500
H	-6.45220200	2.05587800	1.07471600
H	-4.92225300	2.97304800	1.10497800
O	-5.41218100	0.10221900	-0.47735400
C	0.46761200	-1.08094000	-2.13310900
H	0.39740400	-0.47578300	-3.03996100
C	1.36105700	-2.32074200	-2.36230500
H	2.01063200	-2.13656900	-3.22550200
C	2.21174700	-2.44387300	-1.07521900
H	3.24393500	-2.77687400	-1.30897800
C	1.20024500	-0.28351500	-1.01130400
H	0.60652500	-0.29611500	-0.08981600
C	1.50633800	1.16735300	-1.38513500
H	0.56645600	1.65559500	-1.67690900
H	2.15050400	1.16937000	-2.27597900
C	2.16127600	1.97134100	-0.25428800
H	1.51632800	1.92259700	0.63554400
H	3.11334300	1.50291900	0.02765300
C	2.41003100	3.43841300	-0.62384400
H	1.45563800	3.91195900	-0.89856900
H	3.04425200	3.48528600	-1.52171600
C	3.06878200	4.24678400	0.50062200
H	2.43655300	4.19850300	1.39862900
H	4.02343300	3.77485800	0.77303500
O	1.62790600	-3.10698800	-0.07372000
S	-1.25827600	-1.64746300	-1.73974100
O	2.43701200	-0.97949700	-0.78893000
H	2.41542300	-3.54637200	2.70285400
H	0.79912200	-3.23989300	-2.55455700
C	3.31261200	5.71126200	0.12723600
H	3.78402300	6.26179800	0.95016000
H	3.97018800	5.79319900	-0.74753600
H	2.37165900	6.22016600	-0.11762700
O	3.10072700	-3.53798700	2.01399500
H	2.55156800	-3.39643900	1.15272500
O	3.35866500	-0.76459600	1.86657300
H	3.04452900	-0.74929400	0.93416000
H	3.37139100	-1.73615400	2.04298300

TS_4

Charge/multiplicity: -1 1

N	-3.55067700	0.88191400	0.56108600
H	-3.10285800	1.65540100	1.03930200
C	-2.70553300	-0.26623800	0.26240600
H	-3.32422000	-1.16550100	0.30982000
C	-2.11479300	-0.13398900	-1.16484300
C	-1.61582100	-0.30996000	1.33971600

H	-2.94478500	0.06213000	-1.84764800
H	-1.43398300	0.71910200	-1.20498000
O	-1.11188000	0.74439000	1.76809600
N	-1.26078000	-1.52390700	1.78602600
H	-1.62755100	-2.33377500	1.30219500
C	-0.13829100	-1.71520700	2.69846000
H	-0.33635000	-1.21629500	3.65182200
H	-0.02287900	-2.78481800	2.87753100
H	0.79341400	-1.31880700	2.28437600
C	-4.83418100	0.98666800	0.14889800
C	-5.54448200	2.27221100	0.50874600
H	-5.85102900	2.77616500	-0.41419100
H	-6.45314900	2.03016600	1.06957800
H	-4.92700800	2.95362100	1.09957100
O	-5.40488500	0.08163900	-0.48441700
C	0.48037300	-1.08148300	-2.13698700
H	0.40711200	-0.47668000	-3.04387100
C	1.37598600	-2.31975200	-2.36819400
H	2.01883200	-2.13724400	-3.23674600
C	2.23616400	-2.43587500	-1.08666600
H	3.26814700	-2.76562200	-1.32654100
C	1.21342900	-0.28166900	-1.01691500
H	0.62782800	-0.30674500	-0.09046100
C	1.50108400	1.17446300	-1.38457600
H	0.55479600	1.65306800	-1.67146700
H	2.14234500	1.18813800	-2.27741000
C	2.14967200	1.98093400	-0.25185700
H	1.50638500	1.92255900	0.63856100
H	3.10664500	1.52100600	0.02734100
C	2.38235000	3.45178100	-0.61677800
H	1.42285600	3.91526200	-0.89096300
H	3.01672900	3.50854200	-1.51396500
C	3.03067700	4.26447700	0.51060500
H	2.39845100	4.20586300	1.40799500
H	3.99078000	3.80331000	0.78229700
O	1.66138700	-3.09309100	-0.07743200
S	-1.24260600	-1.65298300	-1.73970500
O	2.45941500	-0.96614900	-0.81040300
H	2.36327200	-3.52374600	2.73010100
H	0.81513300	-3.24114800	-2.55284800
C	3.25699300	5.73295400	0.14186000
H	3.72124000	6.28664100	0.96674000
H	3.91400100	5.82551400	-0.73227600
H	2.31007100	6.23116700	-0.10198100
O	3.07458400	-3.52139300	2.06825700
H	2.56174400	-3.37757000	1.18936800
O	3.34685100	-0.75195600	1.83924000
H	3.03485600	-0.82726800	0.90762300
H	3.36553500	-1.70416700	2.09666800

P(R)

Charge/multiplicity: -1 1

N	2.62798700	-2.51073200	0.30907600
H	2.12884800	-3.03593800	1.01763100
C	2.13722800	-1.16382600	0.04077000
H	2.99157800	-0.53615900	-0.22213600
C	1.13926300	-1.18185300	-1.14728900
C	1.48415000	-0.67732500	1.34011700
H	1.56058300	-1.82855000	-1.92077700
H	0.18015700	-1.60738200	-0.83753500
O	0.79737100	-1.47158800	2.01536900
N	1.69759300	0.59308900	1.70173700
H	2.12261400	1.26862300	1.04928900

C	1.02651000	1.15330000	2.86801500
H	1.28191000	0.58692100	3.76840600
H	1.36145800	2.18415200	2.99143700
H	-0.06283500	1.14427900	2.75213800
C	3.62731300	-3.08994600	-0.39211500
C	3.98154100	-4.50597200	0.00354700
H	5.03825100	-4.53994900	0.28876600
H	3.37429700	-4.88596200	0.82904100
H	3.85391700	-5.15908800	-0.86625200
O	4.23071100	-2.49762400	-1.30403500
C	-0.92059800	0.84481500	-1.60989900
H	-1.49859100	0.09952300	-2.16023500
C	-1.19859700	2.27528100	-2.09799200
H	-2.25090800	2.34154700	-2.39763600
C	-0.92920200	3.19230200	-0.87674200
H	-1.75720100	3.92173600	-0.76798000
C	-1.35710900	0.91957200	-0.13344200
H	-0.75842600	0.26357300	0.50614900
C	-2.83480000	0.53955100	0.06938400
H	-3.46076600	1.06770400	-0.66324000
H	-3.12934400	0.91101400	1.06017300
C	-3.09758200	-0.97036200	-0.00120800
H	-2.80730300	-1.35582200	-0.98890900
H	-2.45257000	-1.48123700	0.72933200
C	-4.56151300	-1.34085400	0.26711600
H	-5.20579900	-0.82362800	-0.45926700
H	-4.85587000	-0.96630000	1.25871200
C	-4.83178200	-2.84868800	0.19597700
H	-4.53395300	-3.22264000	-0.79400700
H	-4.19078700	-3.36589500	0.92404000
O	0.27503000	3.80035800	-0.85069800
S	0.87293700	0.47156600	-1.90779600
O	-1.11689400	2.27086000	0.28284100
H	0.34211100	4.03855700	2.11538200
H	-0.58904000	2.57945600	-2.95368800
C	-6.29574700	-3.21160500	0.45760400
H	-6.45689600	-4.29463900	0.39784700
H	-6.61455400	-2.88261100	1.45480300
H	-6.95922400	-2.73554400	-0.27548600
O	0.78069000	4.72321600	1.58440200
H	0.52240100	4.45419900	0.64130200
O	2.56693400	2.87973400	0.20519300
H	2.36556100	3.49745300	0.93623400
H	1.72913800	2.99508000	-0.33211700

TS_2’

Charge/multiplicity: -1 1

N	4.69345400	0.43952200	0.12630900
H	4.71749300	0.91027500	1.02391100
C	3.37781600	0.23119400	-0.47344600
H	3.52240600	0.09801600	-1.54698100
C	2.71931200	-1.03722500	0.11278800
C	2.55611500	1.48993800	-0.18769100
H	3.41704300	-1.86648500	-0.03423300
H	2.57062700	-0.91379600	1.19045400
O	2.40703300	1.89102000	0.98084900
N	2.03885100	2.12735700	-1.24825600
H	2.17453500	1.73347200	-2.17009900
C	1.21543700	3.32114400	-1.10434500
H	0.29761900	3.10251800	-0.54862500
H	1.76387800	4.10535000	-0.57420500
H	0.95177700	3.68069800	-2.09930000

C	5.82479200	-0.13553800	-0.35154700
C	7.07437800	0.12412400	0.46300000
H	6.94918800	-0.24079200	1.48846900
H	7.92024100	-0.38561300	-0.00115300
H	7.28351700	1.19833800	0.51564000
O	5.83561800	-0.81171500	-1.39263500
C	-0.11446500	-0.67462100	0.38715000
H	0.26922300	0.33314600	0.56345800
C	-0.29176300	-1.38074600	1.73927600
H	0.59936800	-1.96295900	2.02290800
C	-0.52902400	-0.48007200	2.91818800
H	-0.76037000	-1.01460500	3.86170400
C	-1.42053600	-0.58512400	-0.45897200
H	-1.14301300	0.04168100	-1.33467600
C	-2.50817100	0.21352600	0.30333500
H	-2.07537700	1.14491200	0.69582600
H	-2.84004200	-0.37103100	1.17413700
C	-3.72459100	0.55593600	-0.56608400
H	-3.39156000	1.15472200	-1.42799400
H	-4.14701600	-0.36796900	-0.97927900
C	-4.81741800	1.32487700	0.18676400
H	-4.39271200	2.24913300	0.60706900
H	-5.15579900	0.72738400	1.04680700
C	-6.02855800	1.67939600	-0.68492400
H	-5.69376100	2.28152500	-1.54160300
H	-6.45265800	0.75713400	-1.10689600
O	-0.44781100	0.73963300	2.91794900
S	1.13984700	-1.55237200	-0.67179100
O	-1.83776100	-1.84750900	-0.87177000
H	-2.70973600	-2.65690600	0.20306700
H	-1.10337500	-2.11975700	1.70568600
C	-7.11853500	2.43888400	0.07627200
H	-7.97034000	2.67682000	-0.57214900
H	-7.49742400	1.84797300	0.91984400
H	-6.73450700	3.38393800	0.48110400
O	-3.33936200	-3.20186400	0.79749400
H	-3.96846800	-2.52940600	1.10550500
O	-4.06172000	-2.67838700	-2.08044600
H	-3.21247200	-2.23264300	-1.78361800
H	-4.28868400	-3.13884800	-1.25259600

MIN_3’

Charge/multiplicity: -1 1

N	-4.73873900	0.59193600	-0.38362700
H	-4.73608200	0.95181300	-1.33085800
C	-3.44047300	0.44470900	0.26922600
H	-3.60336900	0.49401600	1.34743200
C	-2.81811300	-0.92320700	-0.08756000
C	-2.56993000	1.61088400	-0.20537400
H	-3.54078900	-1.69746400	0.18287400
H	-2.64434100	-0.98703100	-1.16608700
O	-2.40624300	1.81464300	-1.42246400
N	-2.02487300	2.38630600	0.74263600
H	-2.17856800	2.15311100	1.71507600
C	-1.15147800	3.50630900	0.41552100
H	-1.66653200	4.21862500	-0.23571800
H	-0.87149300	4.00791800	1.34212000
H	-0.24477600	3.16239800	-0.09340700
C	-5.89058400	0.11804400	0.14796800
C	-7.13178300	0.28614400	-0.69922200
H	-7.52467000	-0.70542400	-0.94929000
H	-7.89480200	0.80403100	-0.10935800
H	-6.95197500	0.84169100	-1.62325200

O	-5.93423100	-0.41832300	1.26798700
C	0.03274300	-0.76704300	-0.42065100
H	-0.38147300	0.11098400	-0.92343000
C	0.32843300	-1.85605000	-1.46256900
H	-0.61049700	-2.18082600	-1.93524600
C	0.98151700	-3.09153800	-0.89863600
H	0.48271800	-3.54576300	-0.02757600
C	1.32838000	-0.40373400	0.34941100
H	1.02240400	0.25816000	1.18467400
C	2.28130300	0.42929500	-0.54264100
H	1.71777800	1.21534400	-1.06697300
H	2.70370800	-0.22935900	-1.31239400
C	3.42354700	1.07487500	0.25525000
H	3.01589500	1.89320200	0.86774900
H	3.83158600	0.34202200	0.96265800
C	4.55603900	1.61264500	-0.62710800
H	4.14232800	2.29942900	-1.38118800
H	4.99758400	0.77350900	-1.18510900
C	5.65951900	2.33249800	0.15769000
H	5.22036400	3.17665400	0.70831900
H	6.06619000	1.65020500	0.91785400
O	1.89446200	-3.69455700	-1.46906000
S	-1.26204200	-1.32500600	0.80371700
O	1.91420500	-1.57976700	0.82558400
H	3.37892300	-1.97171100	0.13350500
H	0.96869400	-1.45908200	-2.25858400
C	6.79789100	2.84152300	-0.73052300
H	7.57026100	3.35044100	-0.14136300
H	7.28019700	2.01570400	-1.26877800
H	6.42854300	3.55325300	-1.47983300
O	4.23102000	-2.29661000	-0.29277900
H	3.88206400	-2.93170000	-0.94089200
O	3.56974600	-1.46566900	2.90615500
H	2.88536700	-1.47080300	2.16784500
H	4.31898100	-1.91078400	2.47861600

TS_3’

Charge/multiplicity: -1 1

N	-4.74506300	0.58959800	-0.37453500
H	-4.74570000	0.92970400	-1.32959900
C	-3.44375500	0.44740200	0.27305600
H	-3.60222400	0.49984800	1.35171900
C	-2.81823400	-0.91950700	-0.08189900
C	-2.57770700	1.61437300	-0.20747300
H	-3.53863800	-1.69505700	0.19097600
H	-2.64590200	-0.98495400	-1.16060600
O	-2.41423100	1.81270800	-1.42552900
N	-2.03566300	2.39684200	0.73664600
H	-2.18885500	2.16821000	1.71024700
C	-1.16738200	3.51913600	0.40402900
H	-0.88767300	4.02513300	1.32833200
H	-0.26022500	3.17702900	-0.10529900
H	-1.68625500	4.22724100	-0.24880600
C	-5.89331600	0.10189400	0.15761200
C	-7.12559700	0.26516700	-0.70645500
H	-7.31550800	1.32464700	-0.91074300
H	-6.99010900	-0.24012100	-1.66915900
H	-7.98705600	-0.16347300	-0.19178000
O	-5.93013400	-0.42606700	1.28061100
C	0.03318200	-0.75889500	-0.41772600
H	-0.37979400	0.12125800	-0.91779500
C	0.32501600	-1.84600400	-1.46266000
H	-0.61531600	-2.16781400	-1.93460200

C	0.97650800	-3.08414800	-0.90275000
H	0.47819800	-3.53938200	-0.03196100
C	1.33079200	-0.40035000	0.35134400
H	1.02748400	0.25981900	1.18893300
C	2.28427900	0.43308400	-0.53965600
H	1.72191200	1.22216100	-1.06066700
H	2.70378600	-0.22425300	-1.31211400
C	3.42941700	1.07311500	0.25860400
H	3.02514700	1.89164300	0.87306700
H	3.83538100	0.33738800	0.96422500
C	4.56334000	1.60848700	-0.62336300
H	4.15178400	2.29821800	-1.37594100
H	5.00150300	0.76876100	-1.18313400
C	5.66982200	2.32273600	0.16231300
H	5.23409800	3.16759800	0.71458400
H	6.07410200	1.63754800	0.92116100
O	1.88714200	-3.68779500	-1.47625300
S	-1.26005300	-1.31696000	0.80797900
O	1.91490100	-1.57890100	0.82344000
H	3.37742600	-1.97207600	0.12716900
H	0.96470300	-1.44839700	-2.25883100
C	6.80993900	2.82893500	-0.72526900
H	7.58449800	3.33360000	-0.13532200
H	7.28879500	2.00224100	-1.26525100
H	6.44325800	3.54361100	-1.47308100
O	4.22804400	-2.29742400	-0.30170800
H	3.87647300	-2.92936000	-0.95148800
O	3.57566000	-1.47703200	2.90079500
H	2.88962300	-1.47711500	2.16405000
H	4.32214700	-1.92382700	2.47019100

MIN_4’

Charge/multiplicity: -1 1

N	4.69173300	0.32355700	0.48652000
H	4.65153000	0.18460000	1.48959600
C	3.41767600	0.50211100	-0.20525500
H	3.62012200	1.03082900	-1.13819400
C	2.79256600	-0.87267500	-0.52432900
C	2.52548100	1.33848700	0.71503800
H	3.51319800	-1.43779300	-1.12119600
H	2.61175600	-1.42772600	0.40066700
O	2.28758700	0.95351300	1.87430400
N	2.04780600	2.48804700	0.21684700
H	2.27168200	2.74029100	-0.73706400
C	1.18110400	3.36423900	0.99509300
H	0.92441700	4.22866600	0.38234800
H	0.26202900	2.84663100	1.28715900
H	1.68980800	3.70675400	1.90152900
C	5.86777900	0.15418700	-0.16427000
C	7.07807500	-0.09991200	0.70591900
H	7.81813400	0.68557600	0.52003600
H	6.84519900	-0.12743500	1.77334300
H	7.52878700	-1.05368200	0.41211300
O	5.95766900	0.21696100	-1.40175100
C	-0.05450700	-0.92118900	-0.16816400
H	0.22415800	-0.20727400	0.60887500
C	-0.25746300	-2.32944800	0.40055700
H	0.63976600	-2.95424400	0.35137800
C	-1.42839700	-2.92775500	-0.40305600
H	-1.07626600	-3.16560800	-1.43335100
C	-1.44721700	-0.55260800	-0.78077200
H	-1.34672600	-0.36756700	-1.86353700
C	-2.05995400	0.68711500	-0.12853400

H	-1.36113900	1.52204000	-0.28267900
H	-2.11625600	0.51542000	0.95621700
C	-3.44477000	1.06872300	-0.66550500
H	-3.39507200	1.17008500	-1.75996800
H	-4.14956900	0.25390800	-0.45756400
C	-3.98152700	2.37104200	-0.05961700
H	-3.27602300	3.18882700	-0.26964200
H	-4.01933200	2.27378700	1.03569700
C	-5.37170700	2.75879000	-0.57845300
H	-5.33558200	2.85424500	-1.67305100
H	-6.07743700	1.94341000	-0.36548700
O	-2.12489200	-3.92001800	0.14645700
S	1.23390900	-0.80947000	-1.49798000
O	-2.28469300	-1.69070300	-0.57845300
H	-3.17165600	-2.09376900	2.25249000
H	-0.57225500	-2.26555600	1.45045200
C	-5.89934900	4.06108200	0.02905700
H	-6.89400000	4.31054200	-0.35939800
H	-5.97772700	3.98600000	1.12106100
H	-5.23290000	4.90301800	-0.19742800
O	-3.45926500	-3.02072300	2.20454900
H	-2.88412000	-3.38825000	1.43776500
O	-5.03416700	-2.23892700	-0.00533000
H	-4.19166600	-2.05122900	-0.46565700
H	-4.68684000	-2.54816400	0.86314900

TS_4’

Charge/multiplicity: -1 1

N	4.76341700	0.15931500	0.37935600
H	4.79440800	-0.04233200	1.37201300
C	3.44671100	0.39664100	-0.20704700
H	3.59495000	0.96808200	-1.12472700
C	2.76891700	-0.94687500	-0.54795100
C	2.63961700	1.20410800	0.81244500
H	3.43378400	-1.49674500	-1.21923400
H	2.63610500	-1.54312300	0.35928900
O	2.45692000	0.76143300	1.96093600
N	2.17408900	2.39468200	0.40731100
H	2.34387000	2.68943500	-0.54556600
C	1.36852100	3.24416700	1.27553900
H	1.10059300	4.14565000	0.72398400
H	0.45406300	2.72962400	1.58719600
H	1.93051200	3.52691900	2.17105500
C	5.88830700	0.02197700	-0.36331800
C	7.15274600	-0.29539800	0.40243100
H	7.89058100	0.48980600	0.20708100
H	6.99371500	-0.37797600	1.48055200
H	7.56612500	-1.23738200	0.02696900
O	5.89141200	0.16123500	-1.59773200
C	-0.05025200	-0.97927300	-0.01120600
H	0.28087200	-0.30949200	0.78498500
C	-0.24193900	-2.41285700	0.51196200
H	0.56813700	-3.09326100	0.23207600
C	-1.60887700	-2.88147100	-0.03650600
H	-1.50174800	-3.11019600	-1.12511600
C	-1.46937200	-0.56034200	-0.51497500
H	-1.48605700	-0.57467300	-1.61863100
C	-1.91587200	0.81585000	-0.02915700
H	-1.15018200	1.54617700	-0.32519800
H	-1.93466700	0.80206100	1.06974800
C	-3.28055300	1.25815500	-0.57317200
H	-3.23654500	1.28498500	-1.67216500

H	-4.04032600	0.50878500	-0.31579000
C	-3.71765600	2.63159700	-0.05021200
H	-2.95499600	3.38045900	-0.31136900
H	-3.75715200	2.60612800	1.04896300
C	-5.07814700	3.08622000	-0.59233100
H	-5.03964600	3.11272100	-1.69060900
H	-5.83941900	2.33766900	-0.33082500
O	-2.24074600	-3.82268400	0.65751600
S	1.15053300	-0.80412800	-1.41047600
O	-2.35613600	-1.56448500	-0.02376600
H	-4.64891400	-2.55032800	1.94094100
H	-0.32230000	-2.40758600	1.60602400
C	-5.50881600	4.45711600	-0.06422800
H	-6.48430700	4.75403900	-0.46760600
H	-5.58856500	4.45306900	1.03025500
H	-4.78430800	5.23387500	-0.34001600
O	-4.70118500	-3.40303400	1.47866900
H	-3.74495200	-3.54203400	1.16032100
O	-4.96278700	-2.03061800	-0.94565400
H	-4.02086700	-1.77549600	-0.83508600
H	-5.08367000	-2.57327100	-0.13196900

MIN_5’

Charge/multiplicity: -1 1

N	4.66934600	0.18367300	0.47423500
H	4.65684700	-0.27949400	1.37558800
C	3.37475500	0.49676700	-0.12563800
H	3.52901200	1.30949600	-0.83752100
C	2.82648100	-0.73821300	-0.86986700
C	2.44787200	0.93620000	1.01016100
H	3.57269200	-1.04417900	-1.60778900
H	2.68201300	-1.56603500	-0.17048800
O	2.22326100	0.17419200	1.96768000
N	1.92587900	2.16789300	0.91971600
H	2.14534800	2.73482700	0.11121600
C	1.01252200	2.69505600	1.92554900
H	1.48940900	2.71255700	2.91029400
H	0.73887000	3.71213800	1.64410200
H	0.10584700	2.08505100	1.98903600
C	5.84179600	0.31353100	-0.19228400
C	7.07993600	-0.13738700	0.54908800
H	7.56947600	-0.92724300	-0.03047500
H	7.77790200	0.70366300	0.61577600
H	6.86836000	-0.50985000	1.55453800
O	5.90497500	0.78586700	-1.33945600
C	-0.01270200	-1.06031400	-0.60294500
H	0.19838600	-0.60603500	0.36742600
C	-0.12000400	-2.58072900	-0.44360600
H	-0.01186500	-3.07824100	-1.41428500
C	-1.55855000	-2.73950800	0.08528700
H	-2.00942600	-3.70712000	-0.21301400
C	-1.43201600	-0.63632200	-1.07737400
H	-1.43579900	-0.45637200	-2.16327400
C	-1.95268900	0.61506400	-0.36241600
H	-1.22364900	1.42372300	-0.51642500
H	-1.97880100	0.40426900	0.71500900
C	-3.33536300	1.07585700	-0.83771900
H	-3.31087300	1.23037400	-1.92701400
H	-4.06475500	0.27730900	-0.65196200
C	-3.81237500	2.36393400	-0.15542500
H	-3.08465900	3.16801600	-0.34146300
H	-3.82976000	2.21345900	0.93435200
C	-5.19968500	2.82048800	-0.62248800

H	-5.18281000	2.97131100	-1.71131500
H	-5.92581800	2.01657300	-0.43629700
O	-1.70549700	-2.42930600	1.37963900
S	1.26128400	-0.45895100	-1.79650800
O	-2.27003200	-1.78304700	-0.84769600
H	-3.12681500	-2.81953100	1.85511500
H	0.61707000	-2.99130900	0.25257500
C	-5.67467400	4.10487800	0.06207400
H	-6.66783700	4.40525900	-0.29286400
H	-5.73556000	3.97521000	1.15010600
H	-4.98597900	4.93663700	-0.13358200
O	-4.08506200	-3.07249400	2.15325000
H	-4.14379900	-4.01655500	1.93315600
O	-5.01364400	-2.19072600	-0.31282200
H	-4.11645500	-1.97723000	-0.64659800
H	-4.80753900	-2.47010900	0.61342800

P(S)

Charge/multiplicity: -1 1

N	-4.44873000	-0.47225200	0.38200700
H	-4.52332500	0.06065400	1.24062100
C	-3.10381900	-0.68118400	-0.15016200
H	-3.12436200	-1.58619600	-0.76042800
C	-2.69340200	0.51845800	-1.03006300
C	-2.17637100	-0.85027500	1.05684500
H	-3.46516200	0.65432600	-1.79210600
H	-2.64834000	1.42956700	-0.42747000
O	-2.11814600	0.03824700	1.92560400
N	-1.46986600	-1.98788300	1.12625200
H	-1.58749100	-2.68323000	0.40091700
C	-0.57230100	-2.27416500	2.23906200
H	-1.13424400	-2.47323200	3.15833400
H	0.02089900	-3.15403500	1.98809000
H	0.09404200	-1.42657700	2.41570500
C	-5.57312800	-0.78873700	-0.30377200
C	-6.87995200	-0.43257800	0.36851800
H	-6.74575200	0.07536900	1.32700700
H	-7.45814000	0.21134000	-0.30228100
H	-7.45824400	-1.34928200	0.52582100
O	-5.54114200	-1.35098200	-1.41117000
C	0.09539000	1.17746500	-0.83533700
H	-0.05463700	0.80659700	0.18086700
C	0.04251800	2.70692800	-0.84739100
H	-0.10002000	3.07055800	-1.87205100
C	1.44676900	3.09154000	-0.33610800
H	1.79610700	4.03133900	-0.80750400
C	1.54374200	0.87472000	-1.29077600
H	1.56598200	0.73703800	-2.38504400
C	2.16167600	-0.35549900	-0.62413800
H	1.52654200	-1.22394800	-0.84966800
H	2.13064400	-0.20790300	0.46286500
C	3.60033400	-0.64359400	-1.06917000
H	3.62809800	-0.75697800	-2.16329900
H	4.23027400	0.22323900	-0.82936100
C	4.19246500	-1.89631000	-0.41301300
H	3.55498200	-2.76354300	-0.64170200
H	4.16774600	-1.77819600	0.68050800
C	5.62988100	-2.19735900	-0.85433300
H	5.65562600	-2.31516800	-1.94705400
H	6.26721400	-1.33160800	-0.62476500
O	1.58593800	3.11419900	1.00877300
S	-1.10684800	0.31776200	-1.93907300
O	2.29887900	2.06113500	-0.99217300

H	2.17817600	0.97803100	2.70426100
H	-0.74541100	3.12035000	-0.21169000
C	6.21310900	-3.44892800	-0.19322100
H	7.24006900	-3.63792800	-0.52812000
H	6.23276500	-3.34760200	0.89931500
H	5.61621800	-4.33834700	-0.43205700
O	1.20795900	1.08009100	2.68987500
H	1.14130900	1.81442500	2.00835600
O	3.87425000	2.00041400	1.85218000
H	3.07905300	2.48853000	1.47149100
H	4.03573400	2.46144000	2.69144000

TS_{1C1}

Charge/multiplicity: -1 1

N	3.69992000	-1.68070400	-0.19582500
H	3.38216200	-2.59330600	0.11126100
C	2.83810900	-0.56063900	0.14959600
H	3.46970500	0.27720800	0.45860100
C	1.99610300	-0.12350200	-1.07917000
C	1.96870400	-1.02246200	1.33003500
H	2.66107600	-0.10589400	-1.94550500
H	1.20359800	-0.85147100	-1.27557000
O	1.75185600	-2.23429600	1.51127000
N	1.48860600	-0.07276100	2.15117900
H	1.50627300	0.90021400	1.85299900
C	0.55913700	-0.41698500	3.22214200
H	-0.37593600	-0.83258900	2.83096700
H	1.01242800	-1.15215400	3.89226800
H	0.33850700	0.48979400	3.78530200
C	4.86628200	-1.54376300	-0.86233700
C	5.63489500	-2.81949600	-1.12516200
H	5.14659700	-3.70793500	-0.71646300
H	5.75675700	-2.94287400	-2.20661000
H	6.63525900	-2.72610100	-0.68970300
O	5.29111700	-0.43751600	-1.24069900
C	-0.54370900	1.30469000	-1.24665200
H	-0.55245600	0.79623400	-2.21619300
C	-1.10817000	2.72834700	-1.44553200
H	-0.76383300	3.12756800	-2.40441300
C	-2.49886400	3.08475600	-1.25726300
H	-2.81662300	3.95441500	-1.86398500
C	-1.25195800	0.35990300	-0.24386100
H	-0.52833800	-0.38874600	0.09231200
C	-2.40855300	-0.41003700	-0.91182900
H	-1.99185400	-0.94871600	-1.77376500
H	-3.14940800	0.29374600	-1.30936200
C	-3.09643900	-1.41054700	0.02507800
H	-2.34165900	-2.09239000	0.44512800
H	-3.53365200	-0.87305200	0.87644900
C	-4.18680400	-2.23067100	-0.67435600
H	-3.74646100	-2.77052700	-1.52589800
H	-4.93740600	-1.54843200	-1.10073400
C	-4.88598700	-3.23472900	0.25025300
H	-4.13594600	-3.91475300	0.67876200
H	-5.33101200	-2.69618500	1.09890400
O	-3.31854200	2.63945300	-0.42703700
S	1.27622300	1.55455500	-0.86632300
O	-1.67229400	1.02632000	0.95323500
H	-2.38058200	1.65205700	0.65686700
H	0.16963100	3.50434400	1.54360100
C	-5.96809600	-4.05296600	-0.45911600
H	-6.44734500	-4.76322800	0.22521500
H	-6.75253400	-3.40342300	-0.86787300
H	-5.54660100	-4.62757600	-1.29368000

O	0.11661200	2.84079900	2.31109100
H	-0.46011600	2.15431900	1.91767600
O	0.03744300	4.51404500	0.25842000
H	-0.58209400	3.54879200	-0.62062500
H	-0.78482200	4.94019000	0.55656500

MIN_{1C1}

Charge/multiplicity: -1 1

N	3.74465900	-1.69016300	-0.35668600
H	3.46450700	-2.64070000	-0.56832700
C	2.67584400	-0.76074700	0.00094800
H	3.09203200	-0.01507100	0.68107500
C	2.13766100	-0.05547300	-1.26959400
C	1.60388800	-1.60255500	0.70038800
H	2.99806500	0.17142800	-1.90385800
H	1.47883900	-0.72735200	-1.82884400
O	1.23908100	-2.67995400	0.19196100
N	1.13293500	-1.14950400	1.87071500
H	1.30450300	-0.18056400	2.14648800
C	0.04363000	-1.83802700	2.55336900
H	-0.87411700	-1.83845800	1.95450700
H	0.32188800	-2.87464800	2.76179400
H	-0.14751200	-1.32526200	3.49668600
C	5.02427000	-1.30154400	-0.55869200
C	5.98886300	-2.38547900	-0.98520100
H	6.77818800	-2.47417900	-0.23101800
H	5.51119800	-3.35939600	-1.11921200
H	6.46360500	-2.08543200	-1.92517200
O	5.39605900	-0.12710400	-0.39132100
C	-0.53765400	1.26875600	-1.46053000
H	-0.48272400	0.69968100	-2.39373000
C	-1.10290200	2.63189700	-1.76741200
H	-1.04227000	2.94107500	-2.80871000
C	-1.56132900	3.56647400	-0.88922000
H	-1.86825900	4.52839400	-1.33318000
C	-1.30713100	0.37866800	-0.45802900
H	-0.74695600	-0.55838500	-0.34598800
C	-2.70060400	0.02503400	-1.01259400
H	-2.58585800	-0.35316300	-2.03825000
H	-3.29772400	0.94418300	-1.08085500
C	-3.44190700	-1.01826400	-0.16811300
H	-2.83524500	-1.93470800	-0.11087000
H	-3.54034000	-0.64793100	0.86082300
C	-4.83067400	-1.36702300	-0.71706800
H	-4.73329900	-1.73445200	-1.74963700
H	-5.43942800	-0.45228200	-0.77453400
C	-5.57258900	-2.41416300	0.12232500
H	-4.96437200	-3.32816800	0.17975300
H	-5.67079300	-2.04687000	1.15378400
O	-1.70343500	3.48203000	0.42155500
S	1.27369200	1.54909000	-0.99364100
O	-1.41356000	0.94002400	0.85197300
H	-1.58556500	1.93428800	0.74199200
H	0.65411900	2.37123900	2.56338600
C	-6.95812100	-2.75865400	-0.43023300
H	-7.46193600	-3.50984700	0.18975500
H	-7.60244400	-1.87103200	-0.46694900
H	-6.88989600	-3.15982900	-1.44943600
O	0.43132700	1.47586900	2.91417900
H	-0.24375300	1.18255000	2.26159700

O	0.74204600	3.90604600	1.56096100
H	1.29599600	3.44413200	0.90708000
H	-0.17230200	3.80431100	1.17338200

HNE_{c1}

Charge/multiplicity: 0 1

C	-2.37798900	-2.02280100	-0.04711000
O	-1.79237900	-1.91473100	-1.12415000
H	-2.91378800	-2.96293600	0.18551000
C	-2.45747100	-1.01032900	1.01157600
H	-2.89087500	-1.36659100	1.94360300
C	-2.10321600	0.28766300	0.91373300
H	-2.25317600	0.92117400	1.78864200
C	-1.54350400	1.02864500	-0.26976900
H	-1.68531200	0.45055900	-1.18780300
C	-0.05177700	1.35225100	-0.09260000
H	0.07643100	1.90935200	0.84561000
H	0.21883200	2.03635100	-0.90773300
C	0.87587700	0.13240500	-0.11035100
H	0.60257000	-0.55252600	0.70370900
H	0.72980900	-0.42494500	-1.04543700
C	2.35403500	0.51718000	0.02820300
H	2.49762000	1.08009200	0.96232400
H	2.63025800	1.20131300	-0.78769700
C	3.29963400	-0.68992000	0.01628400
H	3.02473600	-1.37241600	0.83292200
H	3.15445000	-1.25332300	-0.91626400
C	4.77355000	-0.29922400	0.15249300
H	4.95566300	0.23911900	1.09128300
H	5.42497000	-1.18126400	0.14315000
H	5.08789900	0.35534100	-0.67028400
O	-2.22257100	2.29492700	-0.37846600
H	-3.15531800	2.10391600	-0.57536400

TS_{1C2}

Charge/multiplicity: -1 1

N	-3.13498500	1.93310900	-0.02687800
H	-2.81342900	2.56729000	0.69502800
C	-2.47646400	0.63303600	-0.08846800
H	-3.20463100	-0.09560600	-0.45222700
C	-1.27967700	0.68416200	-1.07315600
C	-2.03861200	0.29085200	1.34053000
H	-1.63044800	1.15450300	-1.99509400
H	-0.47561400	1.30355000	-0.66573400
O	-1.53090400	1.17685900	2.05713100
N	-2.24357400	-0.96347000	1.76211400
H	-2.50664800	-1.69957600	1.09537900
C	-1.73534300	-1.40935000	3.05438000
H	-0.64225400	-1.35720200	3.09287300
H	-2.14472800	-0.79570400	3.86172400
H	-2.04645400	-2.44445000	3.20390300
C	-4.04213900	2.34737800	-0.93972000
C	-4.58646900	3.74571300	-0.75093800
H	-5.67808800	3.69408400	-0.68356900
H	-4.19420300	4.24474600	0.13892800
H	-4.33878900	4.34296100	-1.63511100

O	-4.41788300	1.62440300	-1.87911500
C	1.16235800	-1.04130900	-0.96177900
H	1.65420200	-0.29935500	-1.59954100
C	1.58266000	-2.46814100	-1.34565300
H	1.29875300	-2.72148800	-2.37260500
C	2.88267500	-2.97527100	-1.02191800
H	3.34313000	-2.59845600	-0.08871500
C	1.41116800	-0.61277000	0.51390500
H	0.61747300	0.08690400	0.80681400
C	2.74093100	0.14797800	0.68232200
H	3.55760900	-0.40547100	0.20135200
H	2.96046200	0.15861400	1.75831100
C	2.71923800	1.59366800	0.16959500
H	2.50084100	1.61335000	-0.90744200
H	1.89956300	2.13866100	0.66051100
C	4.04029500	2.33099800	0.42324400
H	4.86133900	1.78214400	-0.06143300
H	4.25963500	2.32033700	1.50120200
C	4.03964600	3.78057600	-0.07702700
H	3.82526000	3.79155000	-1.15515100
H	3.21777600	4.32944300	0.40437700
O	3.48193000	-3.88096100	-1.64738500
S	-0.64236000	-0.98461500	-1.50730500
O	1.42636300	-1.69979400	1.44579000
H	0.79756000	-2.41154800	1.14639200
H	0.75186500	-3.25722400	-0.51328400
C	5.36082700	4.50744500	0.18714200
H	5.33059100	5.54037600	-0.17972500
H	5.58631100	4.54173700	1.26056500
H	6.19793700	4.00179500	-0.31065200
O	-0.00902900	-3.71084900	0.35750600
H	0.41736000	-4.53713200	0.64347200
O	-2.67097800	-3.36920300	0.15364800
H	-2.70135900	-2.89480200	-0.69397100
H	-1.69589300	-3.58110600	0.23827600

MIN_{1C2}

Charge/multiplicity: -1 1

N	3.21729700	-1.71094600	-1.00650900
H	2.77135100	-2.58907100	-1.24548400
C	2.35252800	-0.62963400	-0.53237800
H	2.98026300	0.25726400	-0.46400200
C	1.21478600	-0.38019800	-1.53477300
C	1.81509200	-1.01454300	0.85776100
H	1.63039400	-0.38463100	-2.54549900
H	0.46814100	-1.17747100	-1.47019200
O	0.95608200	-1.90925800	0.97539200
N	2.35463600	-0.37160900	1.90130400
H	3.11652100	0.30051200	1.74407900
C	1.91759300	-0.64874100	3.26230400
H	0.85020900	-0.43062000	3.37261700
H	2.08702700	-1.69696500	3.53089800
H	2.48337900	-0.01202500	3.94409700
C	4.56811300	-1.65197600	-1.00588000
C	5.28777100	-2.88889100	-1.48934000
H	5.92466800	-3.26319200	-0.68086100
H	4.60903700	-3.68341000	-1.80852700
H	5.94059900	-2.61413400	-2.32417200
O	5.20743100	-0.64483300	-0.64485200

C	-1.53750600	0.93087200	-0.92366000
H	-1.79130700	0.20680100	-1.70197600
C	-2.24677400	2.20652500	-1.16142900
H	-2.56570700	2.39090400	-2.18902200
C	-2.42835100	3.23328700	-0.25116900
H	-2.03730500	3.04545700	0.76911400
C	-1.66540100	0.20337600	0.43088000
H	-1.16448500	-0.76829800	0.32212900
C	-3.11449100	-0.06156900	0.85198500
H	-3.62804700	0.89680100	0.99222100
H	-3.07801500	-0.55418400	1.83354000
C	-3.90482100	-0.93931100	-0.12563800
H	-4.02304200	-0.41122000	-1.08156800
H	-3.33285800	-1.85328900	-0.34328900
C	-5.28966300	-1.32556800	0.40842300
H	-5.86105600	-0.41244400	0.63207600
H	-5.17499400	-1.85676800	1.36490800
C	-6.09497600	-2.19983600	-0.56029000
H	-6.21272000	-1.66829600	-1.51524700
H	-5.52258400	-3.11094600	-0.78575800
O	-3.00985300	4.36047900	-0.46320000
S	0.36846400	1.25015500	-1.29392200
O	-1.03840700	0.91325700	1.51357000
H	-0.18329200	1.22698000	1.16205900
H	2.02472500	2.63901800	-0.08030100
C	-7.47375800	-2.58592600	-0.01844700
H	-8.02360900	-3.21221800	-0.73112700
H	-7.38766700	-3.14734200	0.92054400
H	-8.08417600	-1.69650400	0.18286000
O	2.78622200	3.20083800	0.16998100
H	3.17608700	3.44316600	-0.68697200
O	4.58543800	1.38335800	1.28202000
H	4.81719400	0.75132900	0.56750300
H	3.99615600	2.04226500	0.84115200

HNE_{c2}

Charge/multiplicity: 0 1

C	2.55010800	1.60445300	-0.37969600
O	3.01003200	2.74634800	-0.34864800
H	2.16209700	1.19723800	-1.32909400
C	2.49622200	0.74143000	0.79812200
H	2.92357500	1.16792400	1.70364800
C	1.96769700	-0.49845200	0.82683000
H	1.98998300	-1.04284400	1.77130500
C	1.32095600	-1.27551600	-0.28913200
H	1.47863400	-0.79202800	-1.25974900
C	-0.18598300	-1.45203400	-0.05696400
H	-0.33731700	-1.91558000	0.92743500
H	-0.53889900	-2.17238100	-0.80669800
C	-0.99472400	-0.15475500	-0.16194500
H	-0.64108100	0.56477600	0.58879400
H	-0.81448000	0.30853000	-1.14267900
C	-2.50031300	-0.37942200	0.02393200
H	-2.67823100	-0.85600400	0.99930700
H	-2.85888000	-1.09059700	-0.73468100
C	-3.32287700	0.91147300	-0.06418400
H	-2.96412100	1.62120300	0.69469400
H	-3.14466100	1.38873200	-1.03834300
C	-4.82480100	0.68200300	0.12293900
H	-5.03948300	0.23958900	1.10394600
H	-5.38485200	1.62207400	0.05244800
H	-5.22046500	0.00079300	-0.64098500
O	1.88914600	-2.59814600	-0.31400900

H	2.83704700	-2.50212700	-0.50750100