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Supporting Information

A DFT Study on the Isomerization Mechanism of Azobenzene Derivatives on Silicon Substrate

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Content

1. Tests of other functionals and basis sets on the isomerization mechanism of azobenzenesulfonamide

This article also tested other functionals and basis sets, this paper explored the isomerization mechanism of azobenzenesulfonamide at the calculation level of B3LYP/6-31G(d) (Scheme S1). Through this study, two conversion pathways were obtained: N1 and N2 conversion, and the free energy barriers were 27.86 and 23.02 kcal/mol, respectively. The ωB97XD functional is also used to calculate the isomerization mechanism of azobenzenesulfonamide at the large basis set 6-311G(d,p) level, the free energy barriers of the two inversion mechanisms are respectively 27.86 and 23.02 kcal/mol (Figure S2). They are consistent with the dominant path obtained by ωB97XD/6-31G(d).

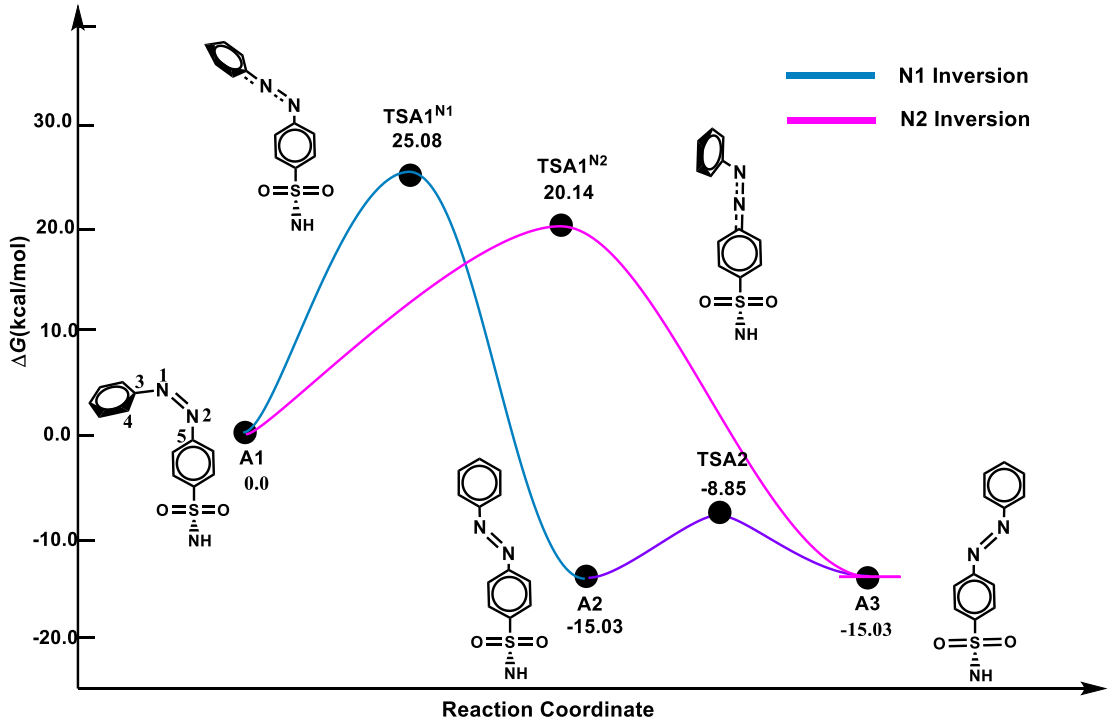

Fig. S1 The Gbbis free energy profiles of the cis-trans isomerization of azobenzenesulfonamide at B3LYP/6-31G(d).

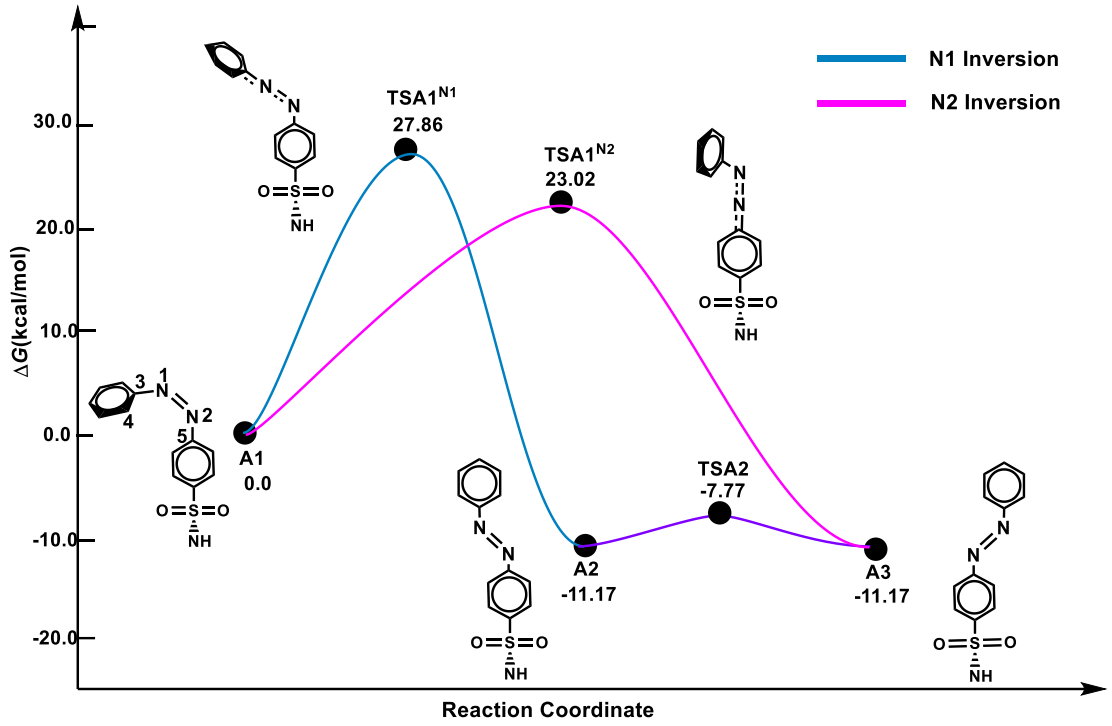

Fig. S2 The Gbbis free energy profiles of the cis-trans isomerization of azobenzenesulfonamide at ωB97XD/6-311+G(d,p).

2. Isomerization mechanism of azobenzenesulfonamides with different substituents

We also discussed the influence of the para-substituents of the benzene ring attached to the N1 atom on the free energy barrier of azobenzenesulfonamide isomerization. Substituents are $N(CH_3)_2$, CH_3, CF_3, CN and NO_2 (Figure S3-S5).

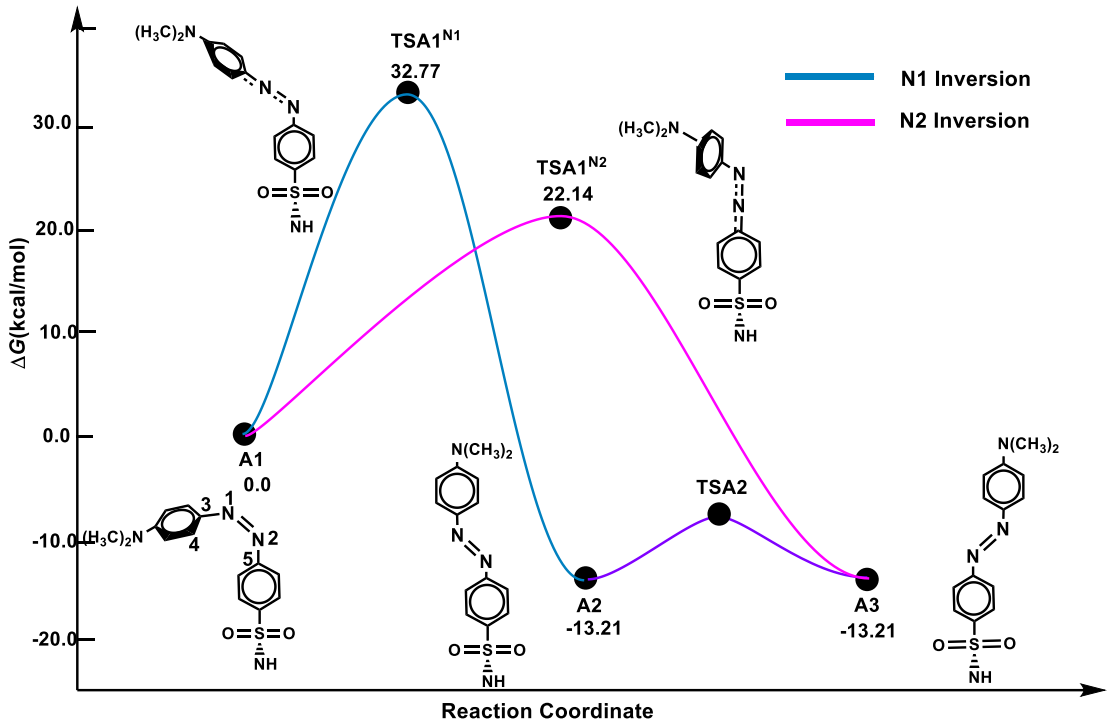

Fig. S3 Isomerization mechanism of $N(CH_3)_2$-substituted azobenzenesulfonamide is at ωB97XD/6-31G(d) level.

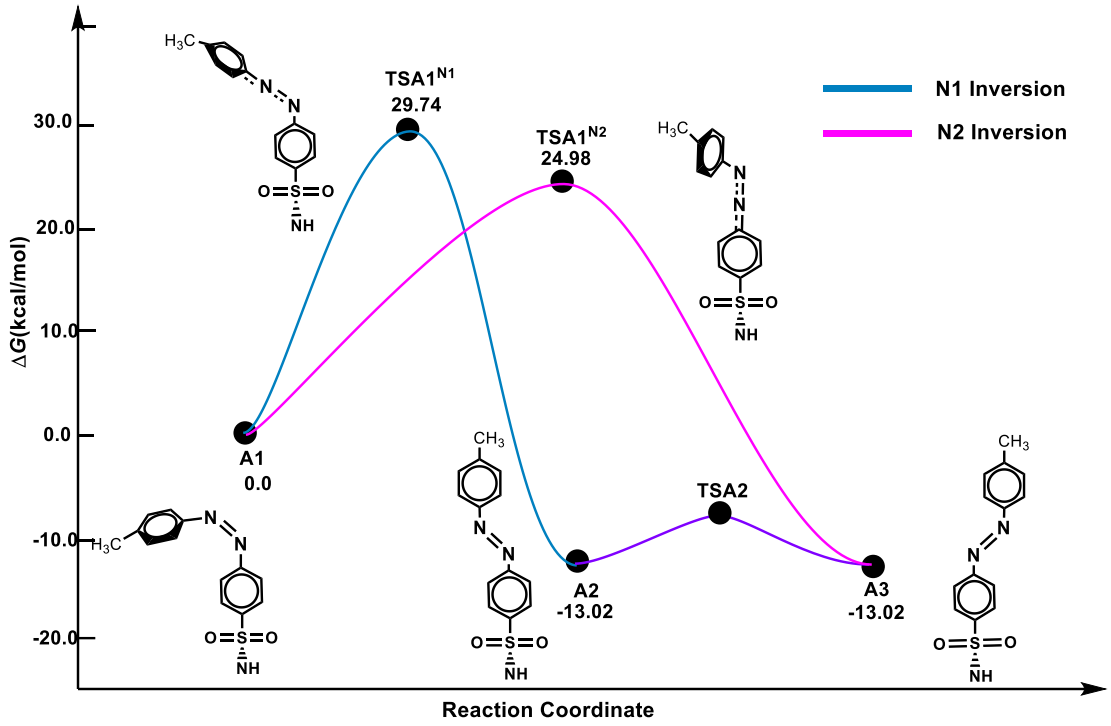

Fig. S4 Isomerization mechanism of CH_3-substituted azobenzenesulfonamide is at ωB97XD/6-31G(d) level.

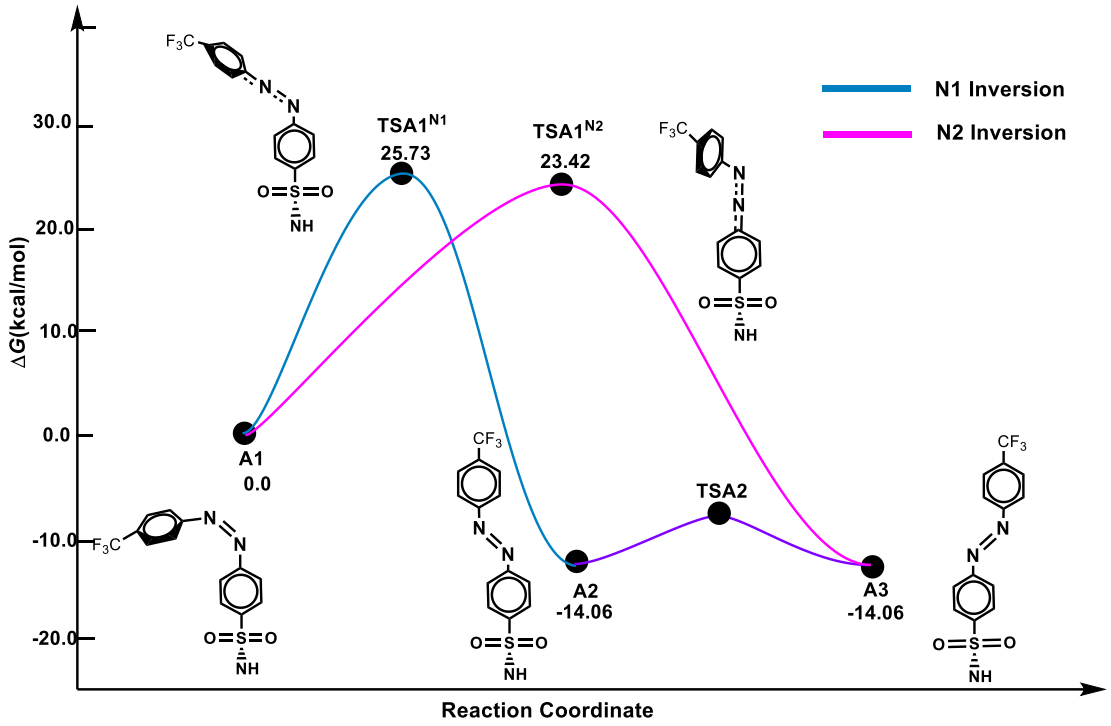

Fig. S5 Isomerization mechanism of CF_3-substituted azobenzenesulfonamide is at ωB97XD/6-31G(d) level.

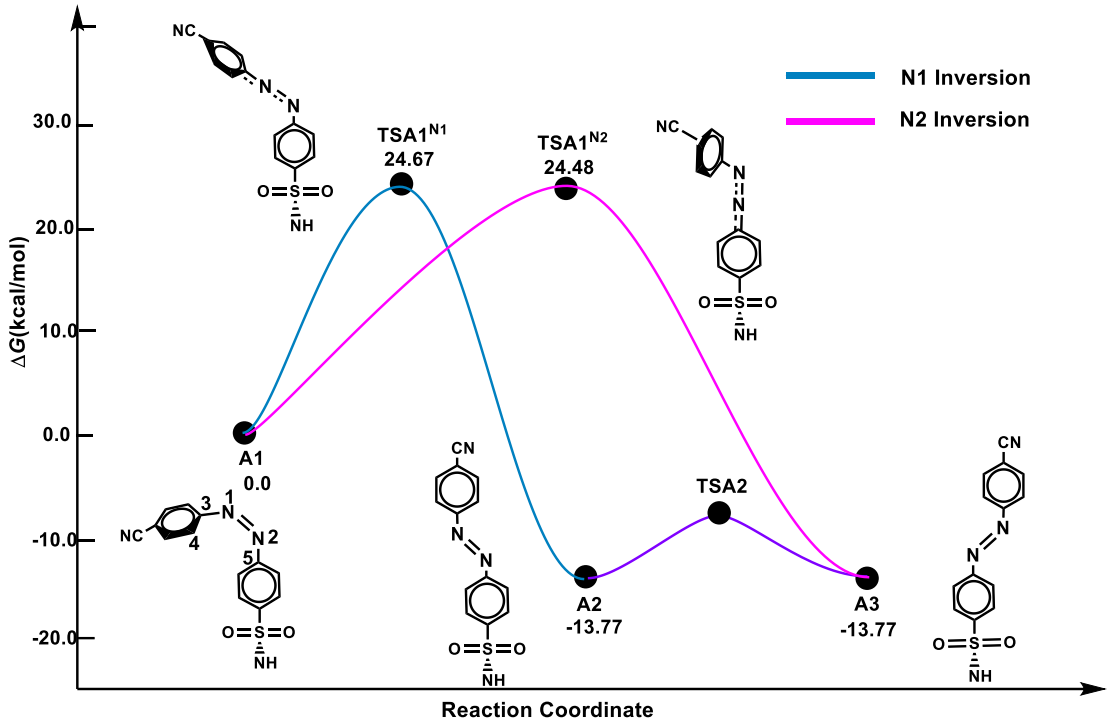

Fig. S6 Isomerization mechanism of CN-substituted azobenzenesulfonamide is at ωB97XD/6-31G(d) level.

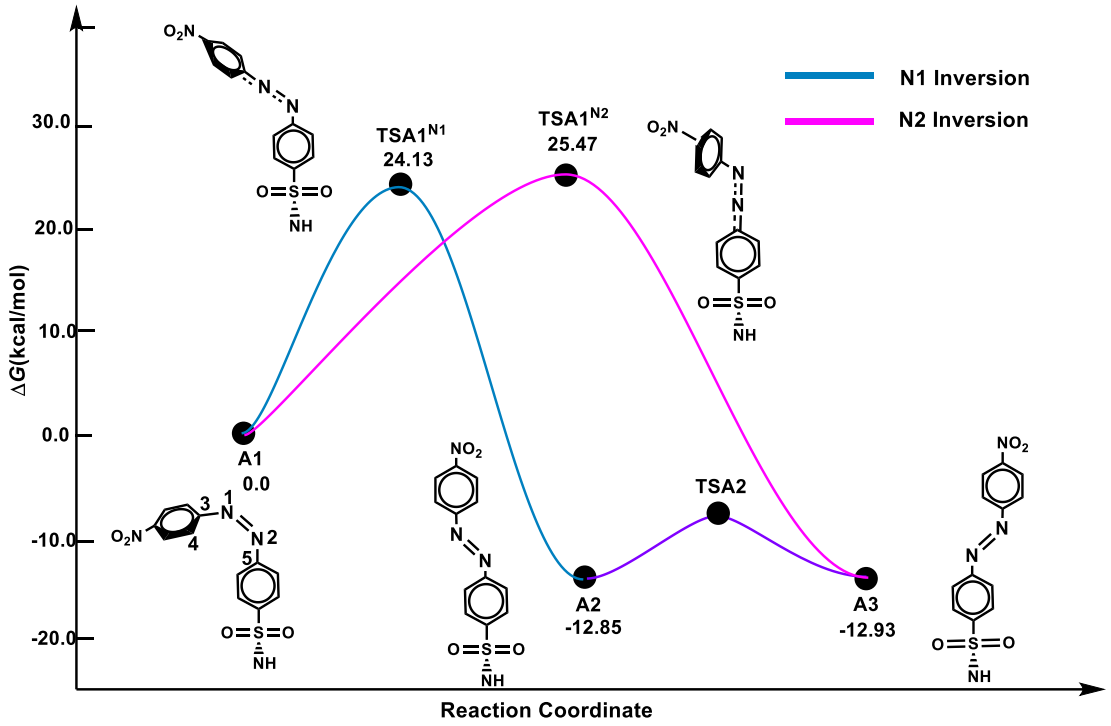

Fig. S7 Isomerization mechanism of NO_2-substituted azobenzenesulfonamide is at ωB97XD/6-31G(d) level.

3. All geometric structures in the cis-trans isomerization of single and bimolecular azobenzenesulfonamides

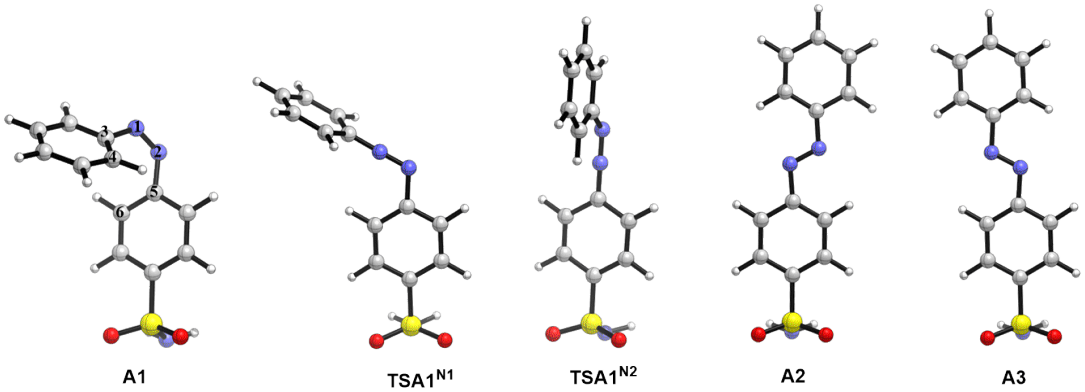

Fig. S8 *cis, trans* and two transition state structures of azobenzenesulfonamide at ωB97XD/6-31G(d) level.

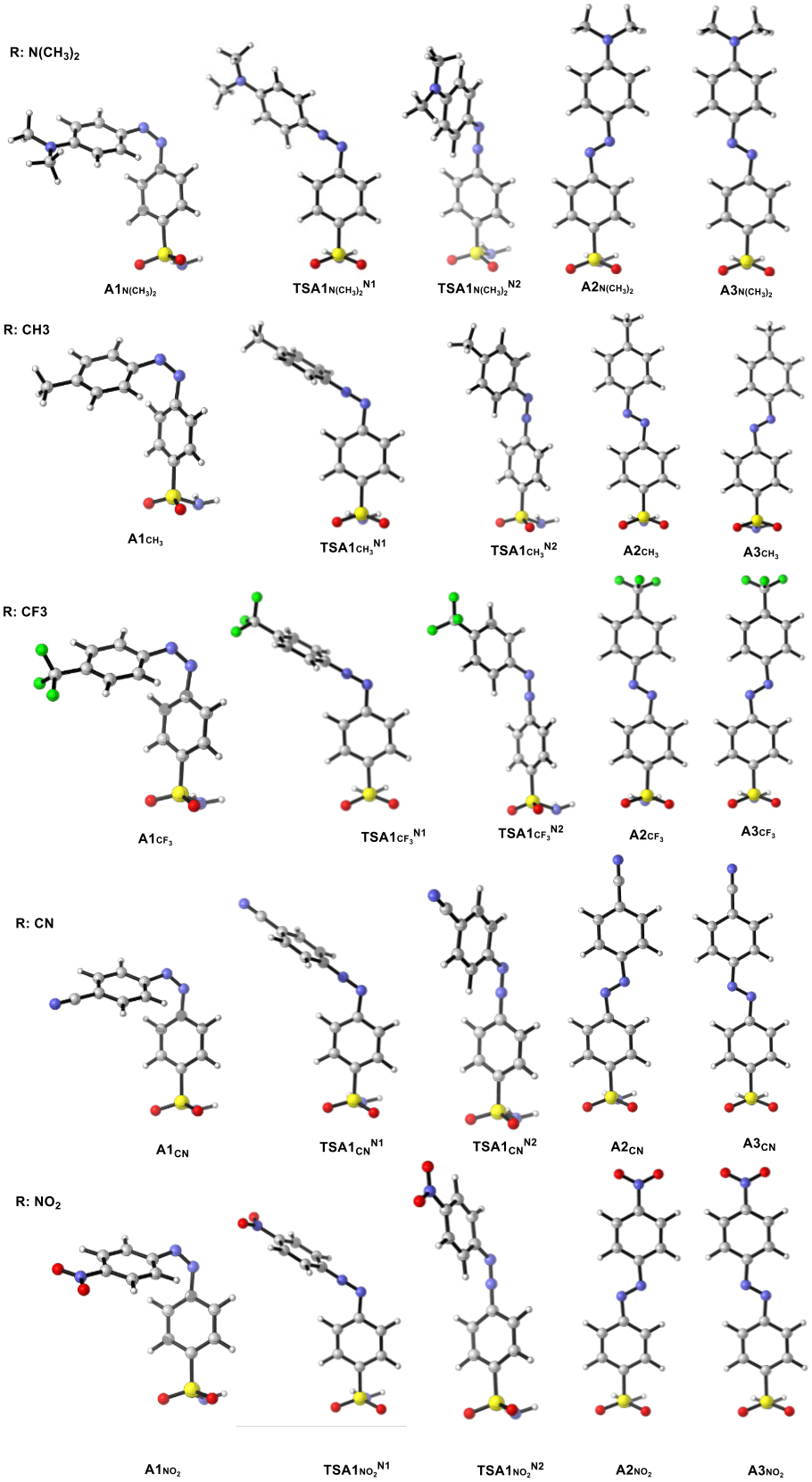

Fig. S9 The best equilibrium geometric configurations of the *cis*, *trans* and transition states of the three 4-azobenzenesulfonamide derivatives at ωB97XD/6-31G(d) level.

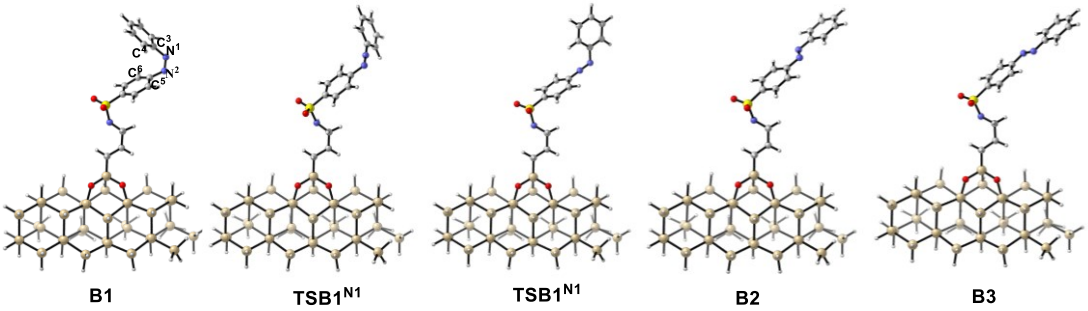

Fig. S10 *cis*, *trans* and two transition state structures of azobenzenesulfonamide assembled on a silicon substrate at ωB97XD/6-31G(d) level.

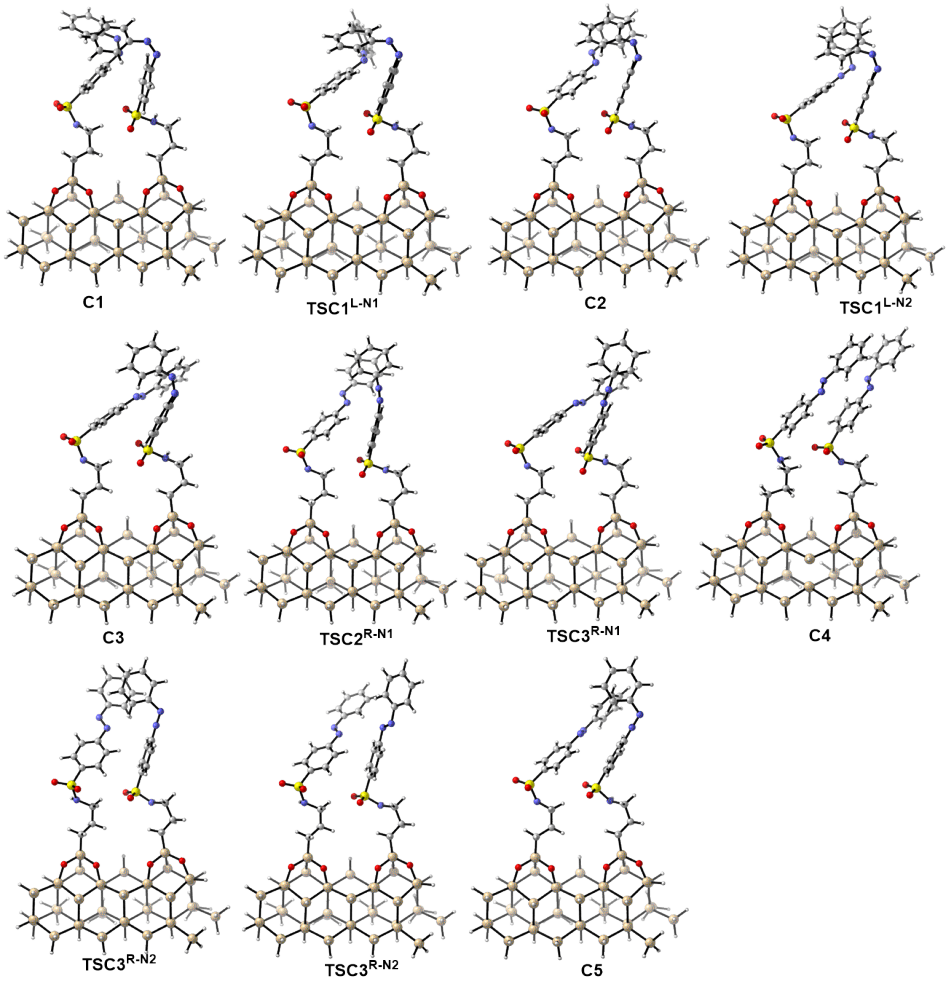

Fig. S11 Geometry of reactants, intermediates, transition states and products of the *cis-trans* isomerism mechanism of bimolecular azobenzenesulfonamide on silicon substrates at ωB97XD/6-31G(d) level.

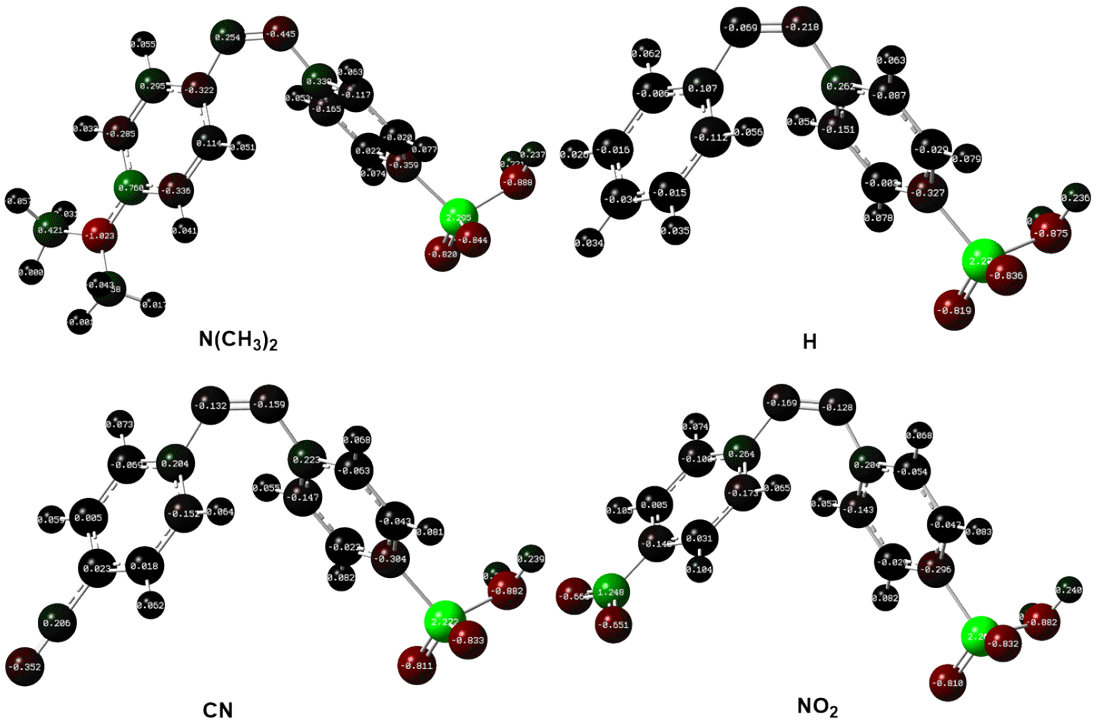

Fig. S12 APT charges with three different substituents and *cis*-structure of azobenzenesulfonamide at ωB97XD/6-31G(d) level.

4. Energies of all the structures

Table S1. Absolute electronic energies (E, in a.u.), thermal free energies (G, in a.u.), and relative Gibbs energies in the calculation process of azobenzenesulfonamide, single- and bi-azobenzenesulfonamide derivative with silicon substrate at ωB97XD/6-31G(d). (Calculated at 298.15 K and 1 atm).

Complex	*E*	*G*	Δ*G*
Azobenzenesulfonamide			
A1	**-1176.387248**	**-1176.210892**	**/**
TSA1^{N1}	**-1176.338873**	**-1176.165633**	**28.40**
A2	**-1176.406068**	**-1176.231193**	**-12.74**
TSA1^{N2}	**-1176.347141**	**-1176.170642**	**25.26**
A3	**-1176.406068**	**-1176.231193**	**-12.74**
TSA2	**-1176.398462**	**-1176.221910**	**-8.14**
Single Molecule Azobenzenesulfonamide Function group on Silicon Substrate			
B1	**-12257.684226**	**-12257.067019**	**/**
TSB1^{N1}	**-12257.636002**	**-12257.021787**	**28.38**
B2	**-12257.703191**	**-12257.089368**	**-14.02**
TSB1^{N2}	**-12257.644125**	**-12257.028901**	**23.91**
B3	**-12257.703134**	**-12257.085899**	**-11.85**
TSB2	**-12257.695718**	**-12257.077471**	**-6.56**
Bimolecule Azobenzenesulfonamide Function group on Silicon Substrate			

C1	**-14064.964170**	**-14064.082578**	**/**
TSC1^{L-N1}	**-14064.912568**	**-14064.033835**	**30.58**
C2	**-14064.982190**	**-14064.099053**	**-10.34**
TSC1^{L-N2}	**-14064.923787**	**-14064.039732**	**26.88**
C3	**-14064.982846**	**-14064.097933**	**-9.63**
TSC2^{R-N1}	**-14064.931012**	**-14064.048002**	**4.36**
TSC3^{R-N1}	**-14064.927198**	**-14064.075626**	**4.36**
C5	**-14064.996674**	**-14064.112051**	**-18.49**
TSC2^{R-N2}	**-14064.943838**	**-14064.061724**	**13.09**
TSC3^{R-N2}	**-14064.943191**	**-14064.061063**	**13.50**
C4	**-14065.008224**	**-14064.122600**	**-25.11**

Table S2. Absolute electronic energies (*E*, in a.u.), thermal free energies (*G*, in a.u.), and relative Gibbs energies (Δ*G*, in kcal/mol) in the calculation process of azobenzenesulfonamide at B3LYP/6-31G(d). (Calculated at 298.15 K and 1 atm).

Complex	***E***	***G***	**Δ*G***
A1	**-1176.657214**	**-1176.484512**	**/**
TSA1^{N1}	**-1176.614332**	**-1176.444539**	**25.08**
A2	**-1176.680917**	**-1176.508469**	**-15.03**
TSA1^{N2}	**-1176.623293**	**-1176.452419**	**20.14**
A3	**-1176.680917**	**-1176.508472**	**-15.03**
TSA2	**-1176.671539**	**-1176.498609**	**-8.84**

Table S3. Absolute electronic energies (*E*, in a.u.), thermal free energies (*G*, in a.u.), and relative Gibbs energies (Δ*G*, in kcal/mol) in the calculation process of azobenzenesulfonamide at ωB97XD/6-311+G(d,p). (Calculated at 298.15 K and 1 atm).

Complex	*E*	*G*	Δ*G*
A1	**-1176.609958**	**-1176.434745**	**/**
TSA1^{N1}	**-1176.562328**	**-1176.390334**	**27.87**
A2	**-1176.628595**	**-1176.452541**	**-11.17**
TSA1^{N2}	**-1176.570624**	**-1176.398055**	**23.02**
A3	**-1176.628595**	**-1176.452541**	**-11.17**
TSA2	**-1176.622238**	**-1176.447136**	**-7.77**

Table S4. Absolute electronic energies (*E*, in a.u.), thermal free energies (*G*, in a.u.), and relative Gibbs energies (Δ*G*, in kcal/mol) in the calculation process of $N(CH_3)_2$-substituted azobenzenesulfonamide at ωB97XD/6-311+G(d,p). (Calculated at 298.15 K and 1 atm).

Complex	*E*	*G*	Δ*G*
A1	**-1310.319591**	**-1310.074686**	**/**
TSA1^{N1}	**-1310.266226**	**-1310.022456**	**32.77**
A2	**-1310.339483**	**-1310.095746**	**-13.21**
TSA1^{N2}	**-1310.282153**	**-1310.039415**	**22.13**

A3	**-1310.339483**	**-1310.095748**	**-13.21**

Table S5. Absolute electronic energies (*E*, in a.u.), thermal free energies (*G*, in a.u.), and relative Gibbs energies (Δ*G*, in kcal/mol) in the calculation process of CH_3-substituted azobenzenesulfonamide at ωB97XD/6-311+G(d,p). (Calculated at 298.15 K and 1 atm).

Complex	***E***	***G***	**Δ*G***
A1	**-1215.695013**	**-1215.492606**	**/**
TSA1^{N1}	**-1215.644854**	**-1215.445215**	**39.78**
A2	**-1215.713773**	**-1215.513359**	**-13.02**
TSA1^{N2}	**-1215.655190**	**-1215.452789**	**24.98**
A3	**-1215.713773**	**-1215.513359**	**-13.02**

Table S6. Absolute electronic energies (*E*, in a.u.), thermal free energies (*G*, in a.u.), and relative Gibbs energies (Δ*G*, in kcal/mol) in the calculation process of CF_3-substituted azobenzenesulfonamide at ωB97XD/6-311+G(d,p). (Calculated at 298.15 K and 1 atm).

Complex	***E***	***G***	**Δ*G***
A1	**-1513.340599**	**-1513.164910**	**/**
TSA1^{N1}	**-1513.296167**	**-1513.123905**	**25.73**
A2	**-1513.359289**	**-1513.187315**	**-14.06**
TSA1^{N2}	**-1513.298908**	**-1513.127586**	**23.42**

A3	**-1513.359289**	**-1513.187315**	**-14.06**

Table S7. Absolute electronic energies (*E*, in a.u.), thermal free energies (*G*, in a.u.), and relative Gibbs energies (Δ*G*, in kcal/mol) in the calculation process of CN-substituted azobenzenesulfonamide at ωB97XD/6-311+G(d,p). (Calculated at 298.15 K and 1 atm).

Complex	***E***	***G***	**Δ*G***
A1	**-1268.593195**	**-1268.420422**	**/**
TSA1^{N1}	**-1268.551164**	**-1268.381103**	**24.67**
A2	**-1268.612218**	**-1268.442369**	**-13.77**
TSA1^{N2}	**-1268.551026**	**-1268.381400**	**24.49**
A3	**-1268.612218**	**-1268.442371**	**-13.77**

Table S8. Absolute electronic energies (*E*, in a.u.), thermal free energies (*G*, in a.u.), and relative Gibbs energies (Δ*G*, in kcal/mol) in the calculation process of NO_2-substituted azobenzenesulfonamide at ωB97XD/6-311+G(d,p). (Calculated at 298.15 K and 1 atm).

Complex	***E***	***G***	**Δ*G***
A1	**-1380.822550**	**-1380.647789**	**/**
TSA1^{N1}	**-1380.782541**	**-1380.609340**	**24.13**
A2	**-1380.841415**	**-1380.668273**	**-12.85**
TSA1^{N2}	**-1380.779868**	**-1380.607189**	**25.48**

A3	**-1380.841415**	**-1380.668391**	**-12.93**

5. Imaginary frequencies of transition states

Table S9. Calculated imaginary frequencies of transition states at ωB97X/6-31G(d) level.

TSA1^{N1}	437.15*i*
TSA1^{N2}	384.16*i*
TSA2	111.74*i*
TSB1^{N1}	440.44*i*
TSB1^{N2}	387.32*i*
TSB2	109.56*i*
TSC1$^{L\text{-}N1}$	440.52*i*
TSC1$^{L\text{-}N2}$	395.27*i*
TSC2$^{R\text{-}N1}$	459.62*i*
TSC3$^{R\text{-}N1}$	431.19*i*
TSC2$^{R\text{-}N2}$	366.83*i*
TSC3$^{R\text{-}N2}$	379.04*i*

Table S10. Calculated imaginary frequencies of transition states at B3LYP/6-31G(d) level.

TSA1^{N1}	432.27*i*
TSA1^{N2}	378.84*i*
TSA2	117.10*i*

Table S11. Calculated imaginary frequencies of transition states at ωB97X/6-311+G(d,p) level.

TSA1^{N1}	434.92*i*
TSA1^{N2}	379.76*i*
TSA2	112.35*i*

Table S12. Azobenzenesulfonamide with different substituents calculated imaginary frequencies of transition states at ωB97X/6-31G(d) level.

$N(CH_3)_2$	**TSA1^{N1}**	493.80*i*
	TSA1^{N2}	371.77*i*
CH_3	**TSA1^{N1}**	450.30*i*
	TSA1^{N2}	381.65*i*
CF_3	**TSA1^{N1}**	412.75*i*
	TSA1^{N2}	394.26*i*
CN	**TSA1^{N1}**	398.42*i*
	TSA1^{N2}	398.13*i*
NO_2	**TSA1^{N1}**	380.70*i*
	TSA1^{N2}	399.15*i*

6. Cartesian coordinates of all the structures

Table S13. During the isomerization of azobenzenesulfonamide, single- and bi-molecular azobenzenesulfonamide derivative atomic cartesian coordinates of intermediates and transition states at at ωB97X/6-31G(d) level.

A1

	Coordinates (Angstroms)		
	X	Y	Z
C	-3.840839000	-2.196863000	0.376539000
C	-4.354793000	-1.489156000	-0.707653000
C	-4.032119000	-0.148360000	-0.881584000
C	-3.147713000	0.467973000	0.002847000
C	-2.644838000	-0.229842000	1.102237000
C	-3.000321000	-1.560590000	1.286860000
H	-4.104728000	-3.239869000	0.520252000
H	-5.023009000	-1.977506000	-1.410132000
H	-4.447437000	0.429117000	-1.701636000
N	-2.904797000	1.867303000	-0.205895000
H	-1.987829000	0.266055000	1.808780000
H	-2.612996000	-2.103209000	2.143402000
C	0.363188000	1.882347000	0.853632000
C	-0.578691000	1.543472000	-0.117809000
C	-0.298372000	0.556036000	-1.064900000
C	0.914699000	-0.115881000	-1.016985000
C	1.835346000	0.201425000	-0.021094000
C	1.565475000	1.191902000	0.920322000
H	0.134294000	2.672716000	1.561277000
N	-1.761418000	2.351547000	-0.197127000
H	-1.032849000	0.307534000	-1.823253000
H	1.138083000	-0.904261000	-1.728338000
H	2.288478000	1.409442000	1.699629000
S	3.405368000	-0.649582000	0.026521000
N	4.452400000	0.237690000	-0.915787000
H	4.197619000	0.249402000	-1.897059000
O	3.230902000	-1.914939000	-0.659670000
O	3.909879000	-0.545669000	1.382005000
H	4.648823000	1.158190000	-0.538752000

TSA1^{N1}

	Coordinates (Angstroms)		
	X	Y	Z
C	5.166183000	-0.926882000	-1.154465000
C	4.038476000	-0.120782000	-1.196145000
C	3.499832000	0.376271000	0.011516000
C	4.111404000	0.038755000	1.238971000
C	5.229574000	-0.781618000	1.236444000
C	5.772494000	-1.272137000	0.051180000
H	5.572849000	-1.296232000	-2.091724000
H	3.569236000	0.140034000	-2.138300000
H	3.699986000	0.425810000	2.164475000
H	5.687889000	-1.033205000	2.188752000
H	6.650653000	-1.908245000	0.066362000
N	2.415294000	1.157660000	-0.007764000
N	1.439083000	1.888219000	-0.025383000
C	-2.236644000	1.513242000	-0.049940000
C	-2.380214000	0.130629000	-0.115704000
C	-1.273130000	-0.717635000	-0.169901000
C	0.001187000	-0.171404000	-0.138442000
C	0.148744000	1.212839000	-0.058573000
C	-0.956755000	2.055541000	-0.021959000
H	-3.114956000	2.150232000	-0.044840000
H	-1.418969000	-1.788991000	-0.260860000
H	0.880857000	-0.806401000	-0.185048000
H	-0.796166000	3.127943000	0.022415000
S	-4.024223000	-0.581364000	-0.100223000
N	-4.399757000	-0.841271000	1.497729000
H	-3.824397000	-1.546973000	1.943099000
O	-3.926518000	-1.895131000	-0.704696000
O	-4.939852000	0.441887000	-0.563920000
H	-4.497694000	0.010651000	2.038178000

A2

	Coordinates (Angstroms)		
	X	Y	Z
C	5.862322000	-1.220945000	0.072223000
C	4.476859000	-1.338736000	0.044468000
C	3.680476000	-0.194306000	0.008846000
C	4.268116000	1.075728000	-0.001699000
C	5.650171000	1.186164000	0.025246000
C	6.448852000	0.040954000	0.062399000
H	6.482043000	-2.111747000	0.100079000
H	3.989951000	-2.308671000	0.049941000

H	3.631392000	1.952631000	-0.031454000
H	6.112934000	2.168276000	0.016031000
H	7.530265000	0.137446000	0.083374000
N	2.280746000	-0.432205000	-0.017836000
N	1.575037000	0.597643000	-0.031390000
C	-2.021675000	1.341715000	-0.056856000
C	-2.575265000	0.067007000	-0.120984000
C	-1.770919000	-1.072732000	-0.173416000
C	-0.392458000	-0.935306000	-0.143834000
C	0.174627000	0.341447000	-0.064796000
C	-0.638696000	1.473526000	-0.029655000
H	-2.667612000	2.213416000	-0.051599000
H	-2.229878000	-2.052167000	-0.261309000
H	0.259790000	-1.799800000	-0.188487000
H	-0.167761000	2.449930000	0.013659000
S	-4.354324000	-0.117334000	-0.098031000
N	-4.781362000	-0.280421000	1.503058000
H	-4.430711000	-1.132283000	1.926683000
O	-4.666878000	-1.388230000	-0.721755000
O	-4.925674000	1.141711000	-0.534636000
H	-4.596214000	0.550257000	2.054239000

TSA1^{N2}

	Coordinates (Angstroms)		
	X	Y	Z
C	1.745705000	-0.204871000	-1.208056000
C	0.422142000	-0.595569000	-1.226103000
C	2.418447000	-0.011113000	-0.000003000
H	-0.105017000	-0.737177000	-2.162422000
C	-0.263954000	-0.800200000	0.000031000
C	1.745631000	-0.204512000	1.208066000
C	0.422066000	-0.595203000	1.226146000
N	-1.534452000	-1.165081000	0.000048000
H	2.262700000	-0.023459000	2.145317000
H	-0.105154000	-0.736516000	2.162476000
N	-2.699507000	-1.523920000	0.000068000
C	-3.692435000	-0.474260000	0.000002000
C	-3.384338000	0.886939000	-0.000178000
C	-5.012450000	-0.914555000	0.000138000
H	-2.346940000	1.208423000	-0.000287000
C	-4.418371000	1.811434000	-0.000211000
C	-6.044165000	0.018485000	0.000110000
H	-5.206965000	-1.982417000	0.000260000

H	-4.194127000	2.873426000	-0.000346000
C	-5.746167000	1.378273000	-0.000065000
H	-7.077154000	-0.314342000	0.000222000
H	-6.549661000	2.108314000	-0.000093000
H	2.262831000	-0.024108000	-2.145333000
S	4.127045000	0.448222000	-0.000011000
O	4.412173000	1.080915000	1.275484000
O	4.412258000	1.080656000	-1.275614000
N	5.022720000	-0.965664000	0.000152000
H	4.878544000	-1.511336000	0.843315000
H	4.878774000	-1.511362000	-0.843034000

A3

	Coordinates (Angstroms)		
	X	Y	Z
C	1.770920000	-1.072737000	-0.173365000
C	0.392460000	-0.935312000	-0.143782000
C	2.575265000	0.067006000	-0.120982000
H	-0.259787000	-1.799808000	-0.188397000
C	-0.174627000	0.341444000	-0.064792000
C	2.021674000	1.341716000	-0.056902000
C	0.638694000	1.473525000	-0.029695000
N	-1.575036000	0.597640000	-0.031383000
H	2.667611000	2.213417000	-0.051679000
H	0.167758000	2.449930000	0.013585000
N	-2.280747000	-0.432207000	-0.017862000
C	-3.680476000	-0.194307000	0.008833000
C	-4.268115000	1.075729000	-0.001660000
C	-4.476862000	-1.338737000	0.044416000
H	-3.631388000	1.952632000	-0.031385000
C	-5.650169000	1.186167000	0.025297000
C	-5.862324000	-1.220944000	0.072182000
H	-3.989955000	-2.308673000	0.049847000
H	-6.112930000	2.168280000	0.016124000
C	-6.448852000	0.040956000	0.062411000
H	-6.482047000	-2.111746000	0.100008000
H	-7.530265000	0.137450000	0.083396000
H	2.229879000	-2.052175000	-0.261221000
S	4.354324000	-0.117333000	-0.098031000
O	4.925666000	1.141705000	-0.534664000
O	4.666882000	-1.388240000	-0.721731000
N	4.781367000	-0.280395000	1.503059000
H	4.596159000	0.550265000	2.054248000

H	4.430769000	-1.132284000	1.926674000

B1

	Coordinates (Angstroms)		
	X	Y	Z
Si	-5.268294000	-4.238910000	1.725146000
Si	-4.075924000	-0.537644000	1.632760000
Si	-2.642231000	3.071624000	1.382032000
Si	-5.503963000	-2.145977000	0.671589000
Si	-4.267828000	1.561025000	0.573928000
H	-6.919717000	-1.694538000	0.822941000
H	-5.618355000	2.113987000	0.889065000
C	14.518623000	-3.325215000	0.835834000
C	14.656266000	-2.331836000	1.802658000
C	14.117375000	-1.068863000	1.586688000
C	13.392089000	-0.818330000	0.422503000
C	13.265252000	-1.804019000	-0.557858000
C	13.836912000	-3.053356000	-0.347912000
H	14.955181000	-4.305707000	0.997765000
H	15.198572000	-2.535348000	2.720810000
H	14.241350000	-0.272184000	2.313668000
N	12.919917000	0.524429000	0.237518000
H	12.733724000	-1.592202000	-1.479534000
H	13.744200000	-3.819136000	-1.111591000
C	10.021948000	-0.281443000	-1.424109000
C	10.745376000	-0.233112000	-0.232902000
C	10.380649000	-1.032946000	0.852783000
C	9.303209000	-1.899083000	0.735587000
C	8.606806000	-1.969569000	-0.469009000
C	8.964425000	-1.171784000	-1.553770000
H	10.305094000	0.371703000	-2.243367000
N	11.757074000	0.777308000	-0.116629000
H	10.942746000	-0.979362000	1.778989000
H	9.015675000	-2.540288000	1.562413000
H	8.420854000	-1.255725000	-2.488810000
S	7.176616000	-3.031880000	-0.591538000
N	5.880881000	-2.099490000	-0.127608000
H	5.861134000	-1.997979000	0.882811000
C	5.578805000	-0.878531000	-0.874194000
H	5.656647000	-1.125996000	-1.936925000
H	6.307626000	-0.083491000	-0.656092000
C	4.165951000	-0.394291000	-0.558793000
H	4.084464000	-0.187016000	0.516628000

H	4.021628000	0.566220000	-1.066487000
C	3.075146000	-1.386251000	-0.986600000
H	3.224461000	-2.350986000	-0.488999000
H	3.147600000	-1.580149000	-2.064263000
Si	1.380066000	-0.750600000	-0.613845000
O	0.193451000	-1.785438000	-1.144317000
O	1.187366000	-0.548253000	1.022490000
O	1.189847000	0.737232000	-1.340475000
O	7.300260000	-4.059398000	0.426976000
O	6.993804000	-3.339231000	-1.998208000
Si	-0.132315000	0.031666000	1.889781000
H	0.229048000	0.004120000	3.330767000
Si	-0.502932000	2.180053000	1.032092000
Si	1.159863000	3.615296000	1.853460000
H	0.983033000	3.798220000	3.321175000
H	2.489973000	2.981602000	1.629497000
Si	1.474141000	5.314648000	-1.526550000
H	1.390177000	6.598949000	-2.276053000
H	2.850724000	4.772189000	-1.699776000
Si	1.057181000	5.678681000	0.754290000
H	2.081142000	6.616184000	1.302958000
Si	-1.910537000	-1.383412000	1.316608000
Si	-1.479383000	-1.583485000	-1.000442000
Si	-1.600515000	-3.480067000	2.318093000
H	-0.188447000	-3.899401000	2.103194000
H	-1.831064000	-3.370373000	3.786198000
Si	-1.136846000	8.680708000	-0.057178000
H	-2.511435000	9.246321000	-0.056430000
H	-0.234758000	9.623653000	0.655961000
H	-0.668470000	8.560367000	-1.461371000
Si	-1.450494000	7.118049000	3.321725000
H	-1.314058000	8.584624000	3.529550000
H	-2.822683000	6.717607000	3.731348000
H	-0.471092000	6.428066000	4.200066000
Si	-2.769993000	3.288896000	3.708419000
H	-4.076858000	3.796173000	4.196581000
H	-2.514361000	1.948200000	4.302563000
H	-1.688443000	4.191157000	4.179213000
Si	-4.719963000	-0.275314000	3.878325000
H	-3.639674000	-0.648766000	4.827277000
H	-5.111450000	1.137000000	4.125182000
H	-5.912028000	-1.119741000	4.150099000
Si	-5.623966000	-4.231209000	4.039978000
H	-6.941086000	-3.643728000	4.396302000

H	-5.584607000	-5.640721000	4.513371000
H	-4.554376000	-3.476658000	4.744669000
Si	-6.793975000	-5.752681000	0.779969000
H	-8.182155000	-5.249718000	0.980977000
H	-6.675125000	-7.056087000	1.492488000
Si	-6.371383000	-6.034283000	-1.507073000
H	-7.354887000	-6.990292000	-2.094131000
Si	-4.192866000	-6.847191000	-1.807621000
H	-3.920523000	-7.042490000	-3.258918000
H	-4.047229000	-8.165039000	-1.129055000
Si	-2.657959000	-5.321623000	-0.902964000
H	-1.264635000	-5.818858000	-1.090664000
Si	-3.083319000	-5.035183000	1.387846000
H	-2.960472000	-6.351419000	2.081922000
Si	-6.580902000	-3.941607000	-2.539001000
H	-7.963562000	-3.419090000	-2.350490000
H	-6.332050000	-4.056697000	-4.003557000
Si	-5.060749000	-2.401435000	-1.626901000
Si	-2.860995000	-3.224366000	-1.937972000
H	-2.619884000	-3.343617000	-3.405856000
Si	-5.463974000	-0.316658000	-2.633302000
H	-5.231717000	-0.399023000	-4.102740000
H	-6.896786000	0.028809000	-2.414704000
Si	-4.033088000	1.308897000	-1.745285000
Si	-1.901571000	0.442422000	-2.091063000
H	-1.683694000	0.241113000	-3.556456000
Si	-0.155476000	1.753481000	-1.255870000
Si	-0.091764000	3.797030000	-2.393936000
H	0.122218000	3.605022000	-3.858156000
Si	-4.000736000	3.354578000	-2.873954000
H	-3.816116000	3.097474000	-4.330047000
H	-5.276170000	4.106672000	-2.703196000
Si	-2.400021000	6.692604000	-3.340161000
H	-3.088786000	6.398677000	-4.625286000
H	-3.185678000	7.725481000	-2.614410000
H	-1.053705000	7.242187000	-3.644203000
Si	-2.253514000	4.712200000	-2.083014000
Si	-2.670911000	5.117198000	0.202080000
H	-4.024150000	5.738609000	0.312152000
Si	-1.073488000	6.619604000	1.055685000

TSB1^{N1}

Coordinates (Angstroms)

	X	Y	Z
Si	-5.369919000	-4.124251000	1.823671000
Si	-4.118708000	-0.443336000	1.676859000
Si	-2.622119000	3.136036000	1.366465000
Si	-5.577892000	-2.041496000	0.744384000
Si	-4.278620000	1.643287000	0.588819000
H	-6.985322000	-1.565194000	0.897613000
H	-5.617005000	2.225835000	0.902300000
C	15.772806000	-1.105898000	2.476726000
C	14.821552000	-0.090960000	2.546322000
C	13.842505000	0.055925000	1.574715000
C	13.809986000	-0.842864000	0.485827000
C	14.770020000	-1.876180000	0.405533000
C	15.730614000	-1.987809000	1.399009000
H	16.532058000	-1.205964000	3.244464000
H	14.835390000	0.611475000	3.375018000
H	13.107132000	0.850611000	1.633640000
N	12.878511000	-0.720790000	-0.464954000
H	14.745350000	-2.565251000	-0.431253000
H	16.463872000	-2.785667000	1.321766000
C	9.909142000	-1.284045000	-2.207153000
C	10.807130000	-1.346970000	-1.147688000
C	10.512988000	-2.068774000	0.008758000
C	9.297488000	-2.729396000	0.105479000
C	8.397468000	-2.663230000	-0.959245000
C	8.693570000	-1.952854000	-2.119268000
H	10.183000000	-0.719715000	-3.092857000
N	12.050283000	-0.617341000	-1.353794000
H	11.237691000	-2.111370000	0.816303000
H	9.047056000	-3.313097000	0.985214000
H	7.990259000	-1.946300000	-2.944839000
S	6.804091000	-3.465875000	-0.805868000
N	5.776146000	-2.319748000	-0.193416000
H	5.902495000	-2.209204000	0.807269000
C	5.511123000	-1.092790000	-0.941990000
H	5.531258000	-1.355105000	-2.003818000
H	6.293104000	-0.340523000	-0.763500000
C	4.135575000	-0.531423000	-0.587036000
H	4.096263000	-0.313514000	0.488333000
H	4.022589000	0.430487000	-1.100355000
C	2.992095000	-1.477871000	-0.975146000
H	3.111386000	-2.440804000	-0.465896000
H	3.033970000	-1.693137000	-2.050679000
Si	1.323610000	-0.783603000	-0.590795000

O	0.114267000	-1.801463000	-1.101715000
O	1.143920000	-0.554799000	1.043159000
O	1.160773000	0.698216000	-1.336215000
O	6.921536000	-4.476918000	0.228900000
O	6.353679000	-3.765742000	-2.152031000
Si	-0.161681000	0.061451000	1.907477000
H	0.206158000	0.048927000	3.346938000
Si	-0.499424000	2.203670000	1.020702000
Si	1.188877000	3.622188000	1.818005000
H	1.021821000	3.826355000	3.284041000
H	2.508311000	2.965073000	1.597030000
Si	1.519842000	5.270555000	-1.584478000
H	1.454829000	6.545842000	-2.351015000
H	2.887515000	4.704300000	-1.753218000
Si	1.115021000	5.672327000	0.692239000
H	2.156358000	6.600659000	1.223841000
Si	-1.968783000	-1.328449000	1.362608000
Si	-1.552999000	-1.567755000	-0.953126000
Si	-1.686678000	-3.416188000	2.390821000
H	-0.282765000	-3.860630000	2.173031000
H	-1.906512000	-3.283174000	3.858630000
Si	-1.019788000	8.693882000	-0.168066000
H	-2.382255000	9.287642000	-0.184609000
H	-0.100920000	9.632210000	0.529533000
H	-0.548063000	8.535618000	-1.567424000
Si	-1.362707000	7.195774000	3.242132000
H	-1.201341000	8.663108000	3.425041000
H	-2.740283000	6.825203000	3.661222000
H	-0.392495000	6.504350000	4.129458000
Si	-2.735987000	3.391621000	3.689641000
H	-4.034428000	3.923002000	4.174552000
H	-2.494363000	2.057501000	4.304029000
H	-1.642027000	4.288244000	4.142152000
Si	-4.741495000	-0.136030000	3.922811000
H	-3.665548000	-0.530013000	4.868407000
H	-5.089343000	1.289980000	4.156654000
H	-5.955603000	-0.942440000	4.212064000
Si	-5.718613000	-4.072912000	4.138986000
H	-7.024106000	-3.455774000	4.488065000
H	-5.702869000	-5.473898000	4.638173000
H	-4.633863000	-3.324385000	4.826723000
Si	-6.919616000	-5.629137000	0.903280000
H	-8.300311000	-5.105358000	1.102774000
H	-6.814943000	-6.924438000	1.632579000

Si	-6.510137000	-5.947102000	-1.381525000
H	-7.511303000	-6.895386000	-1.951196000
Si	-4.345602000	-6.797703000	-1.680334000
H	-4.081400000	-7.013337000	-3.130235000
H	-4.218002000	-8.109574000	-0.986888000
Si	-2.787025000	-5.282950000	-0.799043000
H	-1.400905000	-5.800331000	-0.985393000
Si	-3.198939000	-4.959751000	1.489264000
H	-3.094179000	-6.268211000	2.200624000
Si	-6.694688000	-3.865088000	-2.439668000
H	-8.069808000	-3.322099000	-2.253926000
H	-6.451546000	-4.001640000	-3.903309000
Si	-5.150155000	-2.334569000	-1.552433000
Si	-2.965860000	-3.197382000	-1.861685000
H	-2.733262000	-3.340077000	-3.328834000
Si	-5.521047000	-0.256987000	-2.586335000
H	-5.296786000	-0.364373000	-4.055313000
H	-6.946113000	0.117935000	-2.366484000
Si	-4.058130000	1.356141000	-1.727324000
Si	-1.942525000	0.450226000	-2.069573000
H	-1.736040000	0.224307000	-3.533153000
Si	-0.166370000	1.739460000	-1.262190000
Si	-0.071091000	3.765561000	-2.428794000
H	0.136597000	3.551111000	-3.890847000
Si	-3.994266000	3.384344000	-2.886033000
H	-3.823082000	3.102532000	-4.339206000
H	-5.253614000	4.163648000	-2.719114000
Si	-2.332406000	6.682356000	-3.414125000
H	-3.034263000	6.379776000	-4.690151000
H	-3.092725000	7.743655000	-2.702756000
H	-0.977251000	7.199370000	-3.735585000
Si	-2.217037000	4.720236000	-2.124731000
Si	-2.621179000	5.164129000	0.155637000
H	-3.964427000	5.807835000	0.259518000
Si	-0.998950000	6.653515000	0.984175000

B2

	Coordinates (Angstroms)		
	X	Y	Z
Si	-5.468934000	-3.975429000	1.863828000
Si	-4.104793000	-0.335059000	1.706388000
Si	-2.490798000	3.188876000	1.377472000
Si	-5.636106000	-1.881543000	0.799401000

Si	-4.220707000	1.762507000	0.635054000
H	-7.022996000	-1.360610000	0.991263000
H	-5.527194000	2.392838000	0.988056000
C	16.338480000	0.118383000	1.244783000
C	15.687015000	0.287036000	0.021000000
C	14.436030000	-0.273357000	-0.189237000
C	13.832530000	-1.009679000	0.836215000
C	14.483337000	-1.181948000	2.057443000
C	15.736788000	-0.615477000	2.262644000
H	17.317647000	0.561141000	1.400787000
H	16.162109000	0.857393000	-0.771437000
H	13.914423000	-0.155724000	-1.132347000
N	12.559675000	-1.631285000	0.735724000
H	13.989014000	-1.761113000	2.830912000
H	16.242553000	-0.748053000	3.213856000
C	9.987960000	-1.834132000	-1.609262000
C	10.696282000	-2.075003000	-0.433008000
C	10.162793000	-2.907073000	0.557462000
C	8.917271000	-3.483810000	0.370098000
C	8.212138000	-3.228210000	-0.807050000
C	8.738560000	-2.411391000	-1.803088000
H	10.435637000	-1.196553000	-2.364402000
N	11.966031000	-1.436195000	-0.345071000
H	10.738341000	-3.093197000	1.456711000
H	8.494732000	-4.150486000	1.114721000
H	8.187211000	-2.253810000	-2.723804000
S	6.575918000	-3.918716000	-1.008014000
N	5.530554000	-2.781903000	-0.398356000
H	5.554267000	-2.774405000	0.616556000
C	5.430384000	-1.469674000	-1.034193000
H	5.478565000	-1.636735000	-2.113973000
H	6.271806000	-0.819474000	-0.751970000
C	4.102238000	-0.803973000	-0.676378000
H	4.057233000	-0.638189000	0.408057000
H	4.088799000	0.188933000	-1.140438000
C	2.888307000	-1.622843000	-1.132980000
H	2.925617000	-2.624186000	-0.689024000
H	2.922767000	-1.771371000	-2.219909000
Si	1.269315000	-0.844615000	-0.704698000
O	0.007951000	-1.812910000	-1.186587000
O	1.139334000	-0.619292000	0.934884000
O	1.140974000	0.647716000	-1.435982000
O	6.469254000	-5.061203000	-0.119032000
O	6.317408000	-4.006462000	-2.433408000

Si	-0.118121000	0.038287000	1.839025000
H	0.289781000	0.001794000	3.267289000
Si	-0.406396000	2.195749000	0.973756000
Si	1.348531000	3.552046000	1.734892000
H	1.225673000	3.752967000	3.205689000
H	2.638323000	2.851133000	1.476889000
Si	1.644819000	5.216098000	-1.665171000
H	1.594274000	6.498760000	-2.420523000
H	2.989875000	4.612251000	-1.877214000
Si	1.313554000	5.610918000	0.624126000
H	2.395093000	6.503651000	1.135899000
Si	-1.989911000	-1.281966000	1.337232000
Si	-1.642973000	-1.521114000	-0.989641000
Si	-1.753149000	-3.378841000	2.357253000
H	-0.368791000	-3.868325000	2.112071000
H	-1.939371000	-3.240280000	3.829131000
Si	-0.747906000	8.704371000	-0.151273000
H	-2.089906000	9.342631000	-0.123073000
H	0.220613000	9.605333000	0.528152000
H	-0.321688000	8.545454000	-1.565050000
Si	-1.032663000	7.183814000	3.253352000
H	-0.811679000	8.642658000	3.443911000
H	-2.407542000	6.859793000	3.717436000
H	-0.058857000	6.448711000	4.100971000
Si	-2.525876000	3.429497000	3.704704000
H	-3.783295000	4.012832000	4.236372000
H	-2.323689000	2.080740000	4.301379000
H	-1.378903000	4.272543000	4.128088000
Si	-4.660586000	-0.019373000	3.968682000
H	-3.575020000	-0.455277000	4.884522000
H	-4.952586000	1.416754000	4.218088000
H	-5.893997000	-0.785476000	4.286104000
Si	-5.777518000	-3.921751000	4.184830000
H	-7.052454000	-3.256081000	4.557490000
H	-5.809234000	-5.324417000	4.678666000
H	-4.653559000	-3.219365000	4.858192000
Si	-7.076978000	-5.432290000	0.965772000
H	-8.438611000	-4.872437000	1.196083000
H	-6.992926000	-6.733587000	1.687026000
Si	-6.723167000	-5.750496000	-1.328416000
H	-7.763159000	-6.667572000	-1.879658000
Si	-4.590111000	-6.662959000	-1.669854000
H	-4.358629000	-6.883303000	-3.124521000
H	-4.489524000	-7.979330000	-0.980643000

Si	-2.976014000	-5.193183000	-0.814579000
H	-1.607677000	-5.743855000	-1.033196000
Si	-3.329864000	-4.872707000	1.483598000
H	-3.249649000	-6.188123000	2.185022000
Si	-6.875407000	-3.658873000	-2.373202000
H	-8.233509000	-3.084462000	-2.159535000
H	-6.662326000	-3.793103000	-3.841636000
Si	-5.273975000	-2.174283000	-1.508946000
Si	-3.125240000	-3.101611000	-1.869294000
H	-2.929953000	-3.248509000	-3.341321000
Si	-5.597130000	-0.079212000	-2.524625000
H	-5.403779000	-0.185443000	-3.997971000
H	-7.004779000	0.341038000	-2.276736000
Si	-4.067341000	1.484282000	-1.687696000
Si	-1.989329000	0.515570000	-2.084604000
H	-1.828233000	0.288350000	-3.553572000
Si	-0.145887000	1.734672000	-1.319435000
Si	-0.013131000	3.765389000	-2.474489000
H	0.149127000	3.554654000	-3.942647000
Si	-3.961667000	3.517680000	-2.834012000
H	-3.835959000	3.240907000	-4.292719000
H	-5.187580000	4.340448000	-2.631546000
Si	-2.204279000	6.760593000	-3.382887000
H	-2.936964000	6.487476000	-4.648209000
H	-2.922343000	7.836691000	-2.650125000
H	-0.841685000	7.243747000	-3.725135000
Si	-2.119628000	4.785927000	-2.110214000
Si	-2.452764000	5.225534000	0.182745000
H	-3.770289000	5.913994000	0.324695000
Si	-0.760992000	6.652531000	0.980120000

TSB1^{N2}

	Coordinates (Angstroms)		
	X	Y	Z
Si	-5.430718000	-4.112067000	1.756815000
Si	-4.153418000	-0.440078000	1.639015000
Si	-2.628645000	3.128381000	1.359948000
Si	-5.627612000	-2.018599000	0.696590000
Si	-4.300264000	1.657928000	0.572152000
H	-7.031382000	-1.534223000	0.858642000
H	-5.632713000	2.249106000	0.894887000
C	16.582047000	-1.631454000	0.012044000
C	16.465535000	-0.380474000	0.611467000

C	15.204410000	0.149283000	0.864221000
C	14.072967000	-0.582024000	0.515984000
C	14.180129000	-1.836150000	-0.087032000
C	15.441171000	-2.357275000	-0.337514000
H	17.565254000	-2.047707000	-0.184643000
H	17.354670000	0.180287000	0.881325000
H	15.075182000	1.120687000	1.330820000
N	12.815591000	0.056502000	0.831349000
H	13.283897000	-2.389239000	-0.352200000
H	15.540155000	-3.331235000	-0.806141000
C	10.061154000	-1.089339000	-0.972044000
C	10.699311000	-1.240121000	0.286512000
C	10.145777000	-2.125721000	1.248795000
C	8.993337000	-2.822493000	0.948609000
C	8.367650000	-2.671069000	-0.290705000
C	8.911339000	-1.804475000	-1.241470000
H	10.489009000	-0.421066000	-1.710318000
N	11.806702000	-0.571251000	0.559098000
H	10.641372000	-2.250929000	2.204506000
H	8.581093000	-3.516301000	1.674706000
H	8.435519000	-1.708040000	-2.212243000
S	6.860747000	-3.531709000	-0.628814000
N	5.612666000	-2.528042000	-0.153988000
H	5.562247000	-2.493718000	0.860169000
C	5.473866000	-1.229394000	-0.808968000
H	5.585052000	-1.402947000	-1.883206000
H	6.262194000	-0.528218000	-0.494607000
C	4.097509000	-0.632291000	-0.521611000
H	3.993490000	-0.461542000	0.558174000
H	4.053285000	0.355658000	-0.994385000
C	2.945923000	-1.514026000	-1.024548000
H	3.018165000	-2.511679000	-0.576883000
H	3.030018000	-1.659424000	-2.108965000
Si	1.284534000	-0.802762000	-0.648362000
O	0.061926000	-1.803228000	-1.166190000
O	1.104423000	-0.587540000	0.988608000
O	1.129019000	0.688840000	-1.377311000
O	6.787279000	-4.672080000	0.269533000
O	6.745945000	-3.664614000	-2.071804000
Si	-0.190287000	0.032149000	1.863496000
H	0.180652000	0.001278000	3.302038000
Si	-0.513082000	2.185562000	0.999694000
Si	1.186101000	3.584927000	1.808057000
H	1.021072000	3.777109000	3.275984000

H	2.500738000	2.921483000	1.579590000
Si	1.520064000	5.266358000	-1.578920000
H	1.456651000	6.549960000	-2.331873000
H	2.884828000	4.697159000	-1.758600000
Si	1.124535000	5.646731000	0.703036000
H	2.172259000	6.563585000	1.242073000
Si	-2.010690000	-1.336583000	1.309985000
Si	-1.601293000	-1.557421000	-1.009044000
Si	-1.741968000	-3.433136000	2.323114000
H	-0.341678000	-3.886910000	2.101998000
H	-1.960786000	-3.308655000	3.791919000
Si	-0.993627000	8.691391000	-0.118472000
H	-2.351427000	9.296199000	-0.121711000
H	-0.064694000	9.615202000	0.585434000
H	-0.529699000	8.546406000	-1.521878000
Si	-1.335740000	7.159456000	3.274556000
H	-1.166268000	8.624222000	3.471900000
H	-2.713572000	6.792412000	3.696120000
H	-0.365968000	6.454837000	4.152011000
Si	-2.731096000	3.362188000	3.685894000
H	-4.020763000	3.903878000	4.182988000
H	-2.502226000	2.019669000	4.286759000
H	-1.624603000	4.241777000	4.141711000
Si	-4.765289000	-0.149287000	3.890045000
H	-3.689613000	-0.561515000	4.828229000
H	-5.099851000	1.277390000	4.139232000
H	-5.985407000	-0.947583000	4.177024000
Si	-5.780570000	-4.079205000	4.072265000
H	-7.077404000	-3.446656000	4.426576000
H	-5.786894000	-5.485337000	4.557161000
H	-4.686116000	-3.354385000	4.769923000
Si	-6.991334000	-5.599234000	0.826304000
H	-8.368727000	-5.069581000	1.033703000
H	-6.893069000	-6.901713000	1.543732000
Si	-6.588454000	-5.899298000	-1.462022000
H	-7.597080000	-6.836004000	-2.037979000
Si	-4.429980000	-6.762079000	-1.770052000
H	-4.169661000	-6.970203000	-3.221767000
H	-4.311436000	-8.079667000	-1.085835000
Si	-2.861027000	-5.263427000	-0.880152000
H	-1.478641000	-5.787651000	-1.074240000
Si	-3.265768000	-4.959415000	1.412077000
H	-3.169567000	-6.275324000	2.110757000
Si	-6.763141000	-3.806814000	-2.501237000

H	-8.135217000	-3.258624000	-2.307855000
H	-6.524524000	-3.932187000	-3.966660000
Si	-5.207466000	-2.293380000	-1.603987000
Si	-3.029959000	-3.168526000	-1.925917000
H	-2.804136000	-3.303126000	-3.394890000
Si	-5.564358000	-0.203167000	-2.617461000
H	-5.345002000	-0.298694000	-4.088051000
H	-6.986000000	0.180997000	-2.390957000
Si	-4.086997000	1.391156000	-1.747256000
Si	-1.978188000	0.474646000	-2.103580000
H	-1.778252000	0.261923000	-3.569964000
Si	-0.188063000	1.739697000	-1.288249000
Si	-0.080612000	3.777612000	-2.433503000
H	0.121741000	3.578281000	-3.898347000
Si	-4.010033000	3.430582000	-2.884731000
H	-3.845605000	3.163003000	-4.341379000
H	-5.262105000	4.219176000	-2.706339000
Si	-2.329541000	6.720961000	-3.381473000
H	-3.038100000	6.437645000	-4.658332000
H	-3.082409000	7.777404000	-2.654737000
H	-0.973825000	7.236797000	-3.702591000
Si	-2.219550000	4.743786000	-2.115015000
Si	-2.616618000	5.168182000	0.170279000
H	-3.955057000	5.820658000	0.282904000
Si	-0.982506000	6.638060000	1.010061000

B3

	Coordinates (Angstroms)		
	X	Y	Z
Si	-5.539439000	-3.935615000	1.709510000
Si	-4.148966000	-0.304162000	1.615616000
Si	-2.491518000	3.206963000	1.360167000
Si	-5.662402000	-1.833915000	0.654232000
Si	-4.208213000	1.800257000	0.552408000
H	-7.051987000	-1.307020000	0.806756000
H	-5.519974000	2.441498000	0.864296000
C	16.296682000	0.274974000	0.393869000
C	15.668945000	0.433102000	-0.838017000
C	14.401747000	-0.103083000	-1.040573000
C	13.764712000	-0.795533000	-0.011436000
C	14.394401000	-0.956649000	1.227856000
C	15.657755000	-0.419309000	1.423439000
H	17.285605000	0.693167000	0.556017000

H	16.164903000	0.971012000	-1.639858000
H	13.887144000	0.003088000	-1.990255000
N	12.474942000	-1.299431000	-0.327581000
H	13.882340000	-1.498928000	2.014616000
H	16.151810000	-0.540695000	2.382659000
C	9.997043000	-2.235592000	-0.965912000
C	10.624918000	-2.422359000	0.269946000
C	9.992854000	-3.145821000	1.280943000
C	8.729617000	-3.683574000	1.070766000
C	8.110318000	-3.486676000	-0.159827000
C	8.736563000	-2.770765000	-1.181276000
H	10.512408000	-1.680895000	-1.741445000
N	11.916492000	-1.921776000	0.599464000
H	10.511724000	-3.282907000	2.223868000
H	8.233961000	-4.267479000	1.839061000
H	8.242420000	-2.659547000	-2.140635000
S	6.456709000	-4.115873000	-0.413003000
N	5.432673000	-2.900383000	0.065938000
H	5.385522000	-2.844960000	1.078450000
C	5.443087000	-1.616165000	-0.632490000
H	5.571958000	-1.832250000	-1.696919000
H	6.286286000	-0.988657000	-0.308100000
C	4.118997000	-0.885342000	-0.413002000
H	3.979806000	-0.702609000	0.660590000
H	4.193821000	0.100602000	-0.886109000
C	2.919076000	-1.657650000	-0.975433000
H	2.900605000	-2.669472000	-0.553528000
H	3.024401000	-1.781244000	-2.060577000
Si	1.294266000	-0.855263000	-0.621163000
O	0.040495000	-1.805185000	-1.155919000
O	1.109747000	-0.636425000	1.014392000
O	1.207735000	0.642316000	-1.347730000
O	6.246210000	-5.194230000	0.535744000
O	6.275327000	-4.282087000	-1.843517000
Si	-0.170614000	0.031092000	1.876345000
H	0.184267000	-0.017690000	3.318533000
Si	-0.405585000	2.196005000	1.015321000
Si	1.335872000	3.527797000	1.846382000
H	1.160001000	3.723409000	3.312603000
H	2.625735000	2.811829000	1.633909000
Si	1.765002000	5.210158000	-1.533431000
H	1.747805000	6.498488000	-2.280715000
H	3.111226000	4.597030000	-1.708031000
Si	1.365890000	5.592914000	0.747320000

H	2.439985000	6.468881000	1.301643000
Si	-2.034293000	-1.268817000	1.300310000
Si	-1.613656000	-1.496042000	-1.016123000
Si	-1.834967000	-3.377144000	2.303902000
H	-0.448015000	-3.871398000	2.084618000
H	-2.054766000	-3.253958000	3.772623000
Si	-0.632272000	8.710082000	-0.077942000
H	-1.964920000	9.368096000	-0.090576000
H	0.327444000	9.594785000	0.634647000
H	-0.163861000	8.548164000	-1.478055000
Si	-1.052529000	7.177193000	3.308928000
H	-0.816614000	8.631508000	3.516080000
H	-2.448312000	6.871782000	3.719863000
H	-0.121366000	6.422465000	4.186729000
Si	-2.608479000	3.435658000	3.686002000
H	-3.882929000	4.022629000	4.170939000
H	-2.435260000	2.083833000	4.284447000
H	-1.475333000	4.272252000	4.156522000
Si	-4.770312000	-0.000476000	3.862427000
H	-3.712504000	-0.443222000	4.806905000
H	-5.067896000	1.434478000	4.111685000
H	-6.013338000	-0.766727000	4.138856000
Si	-5.905703000	-3.897718000	4.022244000
H	-7.185880000	-3.227607000	4.368212000
H	-5.957946000	-5.304290000	4.503042000
H	-4.794982000	-3.207411000	4.729198000
Si	-7.139231000	-5.368289000	0.760496000
H	-8.500203000	-4.794833000	0.959080000
H	-7.088600000	-6.676054000	1.472947000
Si	-6.728872000	-5.672494000	-1.525868000
H	-7.762873000	-6.573683000	-2.113255000
Si	-4.596251000	-6.600974000	-1.824374000
H	-4.332151000	-6.805400000	-3.275922000
H	-4.522782000	-7.926589000	-1.149850000
Si	-2.988569000	-5.157503000	-0.913547000
H	-1.621841000	-5.723775000	-1.099863000
Si	-3.400063000	-4.850846000	1.377075000
H	-3.350406000	-6.172219000	2.069843000
Si	-6.828243000	-3.572747000	-2.560797000
H	-8.183930000	-2.981487000	-2.379856000
H	-6.578793000	-3.701983000	-4.024079000
Si	-5.233584000	-2.111920000	-1.644448000
Si	-3.083921000	-3.055436000	-1.952934000
H	-2.848846000	-3.190608000	-3.420388000

Si	-5.511025000	-0.005483000	-2.650141000
H	-5.290404000	-0.102487000	-4.120397000
H	-6.918047000	0.430116000	-2.426087000
Si	-3.983397000	1.535087000	-1.766240000
Si	-1.902076000	0.551164000	-2.107590000
H	-1.696047000	0.335117000	-3.572684000
Si	-0.071081000	1.742495000	-1.270166000
Si	0.120913000	3.779765000	-2.404508000
H	0.327100000	3.579756000	-3.868765000
Si	-3.819554000	3.577482000	-2.889637000
H	-3.653243000	3.312805000	-4.346554000
H	-5.040800000	4.413661000	-2.715994000
Si	-2.011212000	6.799259000	-3.365757000
H	-2.713162000	6.540314000	-4.651337000
H	-2.733933000	7.883104000	-2.649197000
H	-0.633120000	7.264287000	-3.669262000
Si	-1.986542000	4.818515000	-2.099265000
Si	-2.389763000	5.251281000	0.183224000
H	-3.702477000	5.955553000	0.285394000
Si	-0.708413000	6.654319000	1.043458000

TSB2

	Coordinates (Angstroms)		
	X	Y	Z
Si	-5.485064000	-4.032641000	1.768303000
Si	-4.164160000	-0.376585000	1.642255000
Si	-2.586583000	3.168625000	1.353372000
Si	-5.656071000	-1.940044000	0.701777000
Si	-4.278144000	1.719743000	0.567820000
H	-7.054086000	-1.438481000	0.861556000
H	-5.601874000	2.332428000	0.886150000
C	16.667031000	0.027803000	0.655366000
C	15.524179000	0.721035000	1.060259000
C	14.266563000	0.168103000	0.869655000
C	14.156271000	-1.089318000	0.268630000
C	15.294310000	-1.784339000	-0.134859000
C	16.552857000	-1.223779000	0.058216000
H	17.647580000	0.468856000	0.807461000
H	15.619975000	1.696670000	1.526873000
H	13.366337000	0.689535000	1.175772000
N	12.920585000	-1.758129000	0.018138000
H	15.170313000	-2.758026000	-0.597935000
H	17.441249000	-1.762247000	-0.256307000

C	10.026113000	-1.603981000	-1.105950000
C	10.688963000	-1.817214000	0.100593000
C	10.139698000	-2.640229000	1.081628000
C	8.918749000	-3.260658000	0.852688000
C	8.258132000	-3.046627000	-0.354587000
C	8.806687000	-2.227338000	-1.338481000
H	10.475058000	-0.963963000	-1.858226000
N	11.908424000	-1.121778000	0.365546000
H	10.676284000	-2.797536000	2.011378000
H	8.488025000	-3.928287000	1.591630000
H	8.293285000	-2.101932000	-2.285946000
S	6.655497000	-3.786533000	-0.615158000
N	5.543085000	-2.666981000	-0.094135000
H	5.517682000	-2.630183000	0.920194000
C	5.449437000	-1.373302000	-0.767539000
H	5.556666000	-1.565030000	-1.839009000
H	6.261151000	-0.697461000	-0.459402000
C	4.091953000	-0.727538000	-0.494150000
H	3.985109000	-0.548190000	0.583801000
H	4.086015000	0.258774000	-0.972222000
C	2.917776000	-1.573691000	-1.003525000
H	2.958345000	-2.573317000	-0.555871000
H	3.002313000	-1.720992000	-2.087640000
Si	1.271246000	-0.824218000	-0.633812000
O	0.035907000	-1.807769000	-1.151419000
O	1.094165000	-0.600832000	1.001986000
O	1.142860000	0.666720000	-1.368226000
O	6.533640000	-4.906181000	0.301059000
O	6.471044000	-3.921932000	-2.048873000
Si	-0.193691000	0.042048000	1.871571000
H	0.174407000	0.010273000	3.310814000
Si	-0.483259000	2.196563000	0.999683000
Si	1.235263000	3.572799000	1.806656000
H	1.071598000	3.771073000	3.273885000
H	2.539825000	2.887827000	1.582189000
Si	1.599349000	5.240578000	-1.584572000
H	1.553113000	6.522782000	-2.341047000
H	2.956669000	4.652965000	-1.761610000
Si	1.206276000	5.631936000	0.695850000
H	2.265908000	6.535054000	1.234650000
Si	-2.032834000	-1.301730000	1.318641000
Si	-1.623972000	-1.535562000	-0.999158000
Si	-1.788658000	-3.399116000	2.335978000
H	-0.393727000	-3.869079000	2.114066000

H	-2.004083000	-3.269494000	3.804793000
Si	-0.864853000	8.702040000	-0.137745000
H	-2.213079000	9.327612000	-0.147463000
H	0.076460000	9.613821000	0.565273000
H	-0.399084000	8.543840000	-1.539103000
Si	-1.233155000	7.184964000	3.261036000
H	-1.037486000	8.646913000	3.455049000
H	-2.617464000	6.843435000	3.682436000
H	-0.276437000	6.464738000	4.140195000
Si	-2.688209000	3.410669000	3.678502000
H	-3.969556000	3.974709000	4.172217000
H	-2.481596000	2.066457000	4.283633000
H	-1.567904000	4.273462000	4.132583000
Si	-4.774952000	-0.069788000	3.891530000
H	-3.704154000	-0.489769000	4.831797000
H	-5.093989000	1.361608000	4.134343000
H	-6.003742000	-0.853996000	4.180683000
Si	-5.835507000	-3.987609000	4.083430000
H	-7.126121000	-3.340873000	4.434749000
H	-5.855944000	-5.391740000	4.573617000
H	-4.733823000	-3.270975000	4.778198000
Si	-7.062083000	-5.503824000	0.839953000
H	-8.433294000	-4.957480000	1.044650000
H	-6.979296000	-6.805489000	1.560669000
Si	-6.660940000	-5.814567000	-1.447294000
H	-7.680828000	-6.740084000	-2.021458000
Si	-4.513005000	-6.704673000	-1.752321000
H	-4.253772000	-6.916925000	-3.203603000
H	-4.410862000	-8.022738000	-1.066616000
Si	-2.927625000	-5.223193000	-0.863149000
H	-1.551002000	-5.763246000	-1.054810000
Si	-3.330683000	-4.908572000	1.427877000
H	-3.251587000	-6.223798000	2.129780000
Si	-6.810000000	-3.723208000	-2.493012000
H	-8.175693000	-3.158240000	-2.303272000
H	-6.570386000	-3.855371000	-3.957639000
Si	-5.237562000	-2.225707000	-1.597812000
Si	-3.071480000	-3.129576000	-1.914677000
H	-2.844264000	-3.269799000	-3.382889000
Si	-5.563834000	-0.133000000	-2.617018000
H	-5.345680000	-0.235663000	-4.087247000
H	-6.979399000	0.273196000	-2.391476000
Si	-4.064680000	1.443589000	-1.750410000
Si	-1.967353000	0.498319000	-2.100572000

H	-1.767858000	0.277850000	-3.565902000
Si	-0.159134000	1.738171000	-1.286021000
Si	-0.020066000	3.770873000	-2.436638000
H	0.181532000	3.564357000	-3.900604000
Si	-3.955713000	3.479305000	-2.892281000
H	-3.793801000	3.206007000	-4.348120000
H	-5.195502000	4.287439000	-2.716634000
Si	-2.221257000	6.740806000	-3.400203000
H	-2.927885000	6.461732000	-4.678993000
H	-2.960693000	7.812555000	-2.682384000
H	-0.855707000	7.233093000	-3.716843000
Si	-2.146228000	4.767693000	-2.124293000
Si	-2.541698000	5.205239000	0.158827000
H	-3.870298000	5.878154000	0.266765000
Si	-0.887456000	6.652676000	0.997941000

C1

	Coordinates (Angstroms)		
	X	Y	Z
Si	5.356105000	5.962558000	3.607111000
Si	2.663713000	5.441213000	1.024261000
Si	4.980573000	5.600984000	1.324717000
Si	1.650049000	3.513000000	1.885841000
Si	5.930254000	1.845934000	3.761319000
Si	2.909980000	1.639991000	1.235722000
Si	5.236085000	1.736457000	1.518121000
Si	2.004212000	-0.296579000	2.177688000
Si	5.563455000	-2.191573000	3.907105000
Si	2.984702000	-2.206735000	1.247391000
Si	5.298315000	-2.180218000	1.583406000
Si	1.787818000	-4.071241000	2.018641000
Si	5.648212000	-6.346496000	3.841257000
Si	2.827008000	-6.031414000	1.248659000
Si	5.152431000	-6.062327000	1.562638000
Si	5.593548000	7.521523000	0.117632000
Si	2.652112000	7.117515000	-2.435567000
Si	4.987231000	7.348576000	-2.144950000
Si	2.101245000	5.184858000	-1.246357000
Si	6.043261000	3.684371000	0.461452000
Si	3.365371000	3.432191000	-2.146961000
Si	5.670515000	3.587895000	-1.853375000
Si	2.372212000	1.615618000	-1.066208000
Si	6.088021000	-0.223919000	0.522302000

Si	3.146625000	-0.344694000	-2.072291000
Si	5.500556000	-0.270142000	-1.758337000
Si	2.462431000	-2.326698000	-1.047090000
Si	6.164389000	-4.152704000	0.626428000
Si	3.479099000	-4.206059000	-2.044266000
Si	5.791783000	-4.160276000	-1.694756000
Si	2.206560000	-5.896743000	-1.021880000
Si	5.874412000	-8.003611000	0.469955000
Si	6.249644000	5.554379000	-2.992183000
Si	6.510695000	1.601407000	-2.764220000
Si	6.532265000	-2.163701000	-2.674166000
Si	6.895415000	-5.917094000	-2.800354000
H	4.615508000	4.958131000	4.417000000
H	4.843310000	7.312846000	3.960390000
H	6.798219000	5.888344000	3.955623000
H	2.026636000	6.679038000	1.565259000
H	1.347145000	3.553278000	3.339681000
H	4.790604000	1.741529000	4.708922000
H	6.633447000	3.133635000	4.000436000
H	6.895612000	0.752551000	4.049632000
H	2.215224000	-0.303918000	3.653845000
H	0.537440000	-0.319234000	1.925117000
H	4.916288000	-3.421978000	4.436475000
H	4.851360000	-1.027413000	4.494739000
H	6.982501000	-2.167697000	4.343370000
H	1.514823000	-4.053476000	3.479027000
H	5.947127000	-7.780772000	4.100216000
H	4.499842000	-5.947595000	4.695287000
H	6.835874000	-5.543681000	4.234060000
H	7.065726000	7.739329000	0.200569000
H	4.924895000	8.691860000	0.753061000
H	2.352447000	6.982016000	-3.887472000
H	1.982311000	8.344722000	-1.924577000
H	7.506949000	3.795284000	0.733974000
H	3.070735000	3.335904000	-3.609653000
H	7.580022000	-0.196847000	0.595656000
H	2.885962000	-0.349180000	-3.541429000
H	7.631935000	-4.235104000	0.886726000
H	3.197686000	-4.170269000	-3.510697000
H	2.223255000	-7.202424000	-1.729312000
H	5.252339000	-9.182540000	1.129344000
H	7.351762000	-8.157749000	0.508858000
H	5.434057000	-7.986492000	-0.951079000
H	5.982405000	5.344408000	-4.442589000

H	7.695638000	5.875440000	-2.832022000
H	6.248491000	1.587290000	-4.230954000
H	7.982401000	1.485748000	-2.561690000
H	6.262368000	-2.236176000	-4.138429000
H	8.006020000	-2.028848000	-2.495124000
H	5.929563000	-6.921741000	-3.315413000
H	7.855803000	-6.600689000	-1.895054000
H	7.655460000	-5.362669000	-3.952055000
C	-11.574285000	1.052238000	-2.049137000
C	-12.326048000	0.105977000	-1.355810000
C	-12.192696000	-1.246832000	-1.646964000
C	-11.267944000	-1.654449000	-2.605600000
C	-10.504810000	-0.713656000	-3.299801000
C	-10.670245000	0.639889000	-3.024937000
H	-11.699597000	2.109650000	-1.836887000
H	-13.029056000	0.422241000	-0.591483000
H	-12.792809000	-1.989200000	-1.130805000
N	-11.245609000	-3.040607000	-2.988509000
H	-9.805793000	-1.040897000	-4.062738000
H	-10.086443000	1.373227000	-3.572754000
C	-7.852941000	-3.137828000	-2.985859000
C	-9.036555000	-3.222640000	-2.253729000
C	-9.050291000	-2.967638000	-0.881910000
C	-7.874286000	-2.604872000	-0.243752000
C	-6.703778000	-2.476736000	-0.984951000
C	-6.684030000	-2.733795000	-2.354510000
H	-7.861737000	-3.363712000	-4.047415000
N	-10.215018000	-3.725009000	-2.898250000
H	-9.974057000	-3.024158000	-0.317388000
H	-7.886120000	-2.371076000	0.815024000
H	-5.764289000	-2.603072000	-2.914506000
S	-5.206844000	-1.994252000	-0.151907000
N	-4.559233000	-3.361751000	0.510783000
H	-4.950157000	-3.553326000	1.424709000
C	-4.175080000	-4.514496000	-0.306914000
H	-4.397839000	-4.290585000	-1.355681000
H	-4.793551000	-5.374502000	-0.025910000
C	-2.687736000	-4.837044000	-0.158314000
H	-2.466664000	-4.998189000	0.903710000
H	-2.485691000	-5.784852000	-0.671619000
C	-1.801968000	-3.724271000	-0.724424000
H	-2.099243000	-2.760993000	-0.291926000
H	-1.961370000	-3.622426000	-1.805251000
Si	0.005988000	-3.912935000	-0.414034000

O	0.805162000	-2.626073000	-1.091518000
O	0.314577000	-3.949673000	1.216224000
O	0.628027000	-5.311681000	-1.059126000
O	-5.569515000	-1.160978000	0.985005000
O	-4.290021000	-1.527672000	-1.180071000
C	-12.836674000	2.946528000	3.328982000
C	-12.915336000	1.753826000	4.043291000
C	-12.343439000	0.596590000	3.527964000
C	-11.643933000	0.642133000	2.321837000
C	-11.576213000	1.834148000	1.594434000
C	-12.180821000	2.978379000	2.100028000
H	-13.294932000	3.848094000	3.723288000
H	-13.437647000	1.719748000	4.994275000
H	-12.423652000	-0.352041000	4.049549000
N	-11.148905000	-0.624427000	1.860569000
H	-11.059835000	1.865840000	0.642259000
H	-12.128969000	3.903878000	1.535036000
C	-8.609189000	0.552449000	-0.112850000
C	-9.096096000	0.298906000	1.167931000
C	-8.578989000	0.971345000	2.275908000
C	-7.611174000	1.947270000	2.090543000
C	-7.170715000	2.241619000	0.802247000
C	-7.657725000	1.545874000	-0.300244000
H	-9.006255000	-0.005085000	-0.953676000
N	-10.044970000	-0.766306000	1.308944000
H	-8.953891000	0.749877000	3.269724000
H	-7.224702000	2.507018000	2.935601000
H	-7.305218000	1.794392000	-1.295421000
S	-5.952927000	3.530021000	0.568471000
N	-4.462033000	2.833918000	0.722811000
H	-4.251925000	2.645244000	1.697854000
C	-4.024717000	1.795575000	-0.215533000
H	-4.433207000	2.053268000	-1.196773000
H	-4.413698000	0.815001000	0.074595000
C	-2.498914000	1.771066000	-0.281833000
H	-2.105963000	1.588630000	0.727504000
H	-2.197079000	0.910797000	-0.888439000
C	-1.917196000	3.072543000	-0.856839000
H	-2.410325000	3.931095000	-0.383543000
H	-2.132781000	3.144025000	-1.929734000
Si	-0.102673000	3.246301000	-0.574892000
O	0.513290000	4.616128000	-1.293143000
O	0.201261000	3.346255000	1.055915000
O	0.718047000	1.919089000	-1.156787000

O	-6.076013000	4.440750000	1.694207000
O	-6.076332000	3.974801000	-0.808998000
H	5.418740000	8.597194000	-2.840373000
H	2.237750000	-7.247691000	1.884204000

TSC1^{N1}

	Coordinates (Angstroms)		
	X	Y	Z
Si	-5.392603000	-5.516013000	4.057446000
Si	-2.850317000	-5.311909000	1.294641000
Si	-5.149388000	-5.313777000	1.737326000
Si	-1.675749000	-3.407337000	1.986996000
Si	-5.761797000	-1.391122000	3.994296000
Si	-2.871481000	-1.501465000	1.307667000
Si	-5.180915000	-1.443535000	1.717043000
Si	-1.814117000	0.428476000	2.090654000
Si	-5.175383000	2.617069000	3.897590000
Si	-2.744990000	2.338703000	1.110736000
Si	-5.033989000	2.465974000	1.567494000
Si	-1.405961000	4.167022000	1.713660000
Si	-5.050031000	6.770735000	3.586368000
Si	-2.368792000	6.143526000	0.889742000
Si	-4.669768000	6.330246000	1.310253000
Si	-5.949976000	-7.262417000	0.699535000
Si	-3.141852000	-7.189328000	-2.027878000
Si	-5.466583000	-7.257481000	-1.598497000
Si	-2.408786000	-5.215782000	-1.016220000
Si	-6.150543000	-3.392905000	0.813109000
Si	-3.615284000	-3.440969000	-1.949185000
Si	-5.903630000	-3.448036000	-1.521362000
Si	-2.471257000	-1.629649000	-1.017738000
Si	-5.981523000	0.503864000	0.655655000
Si	-3.192291000	0.315756000	-2.090370000
Si	-5.525572000	0.392736000	-1.652681000
Si	-2.348588000	2.307599000	-1.211771000
Si	-5.841782000	4.432639000	0.549259000
Si	-3.313591000	4.191320000	-2.253655000
Si	-5.603510000	4.293379000	-1.784658000
Si	-1.884593000	5.850186000	-1.398744000
Si	-5.319435000	8.247002000	0.131101000
Si	-6.665524000	-5.441961000	-2.491617000
Si	-6.689896000	-1.469938000	-2.495344000
Si	-6.493577000	2.292920000	-2.622240000

Si	-6.688740000	6.046837000	-2.913991000
H	-4.556321000	-4.502307000	4.754842000
H	-4.916637000	-6.866058000	4.460310000
H	-6.803808000	-5.353124000	4.491863000
H	-2.253510000	-6.556130000	1.866619000
H	-1.284132000	-3.386627000	3.419517000
H	-4.570259000	-1.299644000	4.876758000
H	-6.521006000	-2.620836000	4.341236000
H	-6.649809000	-0.229692000	4.263627000
H	-1.942354000	0.522292000	3.572805000
H	-0.364682000	0.358160000	1.760992000
H	-4.445332000	3.841832000	4.321873000
H	-4.488902000	1.453521000	4.516362000
H	-6.569430000	2.688868000	4.404319000
H	-1.054248000	4.209421000	3.156224000
H	-5.254975000	8.231822000	3.777183000
H	-3.893157000	6.348943000	4.417583000
H	-6.265350000	6.062704000	4.067436000
H	-7.424842000	-7.377164000	0.878789000
H	-5.316895000	-8.433449000	1.368955000
H	-2.917965000	-7.184692000	-3.499665000
H	-2.515264000	-8.412615000	-1.455778000
H	-7.601378000	-3.403092000	1.164214000
H	-3.392486000	-3.434763000	-3.427521000
H	-7.466229000	0.559899000	0.813177000
H	-3.007598000	0.229091000	-3.568042000
H	-7.284029000	4.617805000	0.886388000
H	-3.114492000	4.059917000	-3.728003000
H	-1.864968000	7.115489000	-2.176123000
H	-4.570417000	9.411948000	0.672405000
H	-6.775847000	8.517939000	0.246561000
H	-4.972521000	8.105352000	-1.309100000
H	-6.471310000	-5.343456000	-3.964984000
H	-8.116603000	-5.657275000	-2.231532000
H	-6.508716000	-1.547702000	-3.972052000
H	-8.140214000	-1.262643000	-2.222575000
H	-6.281349000	2.275148000	-4.097885000
H	-7.963948000	2.251982000	-2.378746000
H	-5.714037000	6.942888000	-3.587884000
H	-7.511382000	6.855536000	-1.976787000
H	-7.591481000	5.472185000	-3.946659000
C	11.408735000	-1.965562000	-1.721261000
C	11.998093000	-0.882946000	-1.074825000
C	11.936887000	0.390049000	-1.632373000

C	11.256080000	0.577547000	-2.832255000
C	10.662918000	-0.499982000	-3.489953000
C	10.744937000	-1.770986000	-2.929623000
H	11.459874000	-2.956418000	-1.282230000
H	12.511911000	-1.026083000	-0.129237000
H	12.408795000	1.235497000	-1.142289000
N	11.302704000	1.867763000	-3.473110000
H	10.159604000	-0.343397000	-4.438823000
H	10.281072000	-2.611355000	-3.436598000
C	8.014002000	1.819740000	-3.411827000
C	9.132674000	2.284703000	-2.723591000
C	9.069922000	2.556524000	-1.356154000
C	7.886732000	2.331102000	-0.670163000
C	6.778216000	1.839828000	-1.354288000
C	6.832470000	1.581270000	-2.720298000
H	8.076411000	1.637216000	-4.479580000
N	10.322472000	2.626348000	-3.452294000
H	9.949546000	2.912236000	-0.832031000
H	7.845589000	2.492911000	0.402096000
H	5.957050000	1.188842000	-3.225791000
S	5.284862000	1.484706000	-0.449465000
N	4.719938000	2.932737000	0.096530000
H	5.057193000	3.149433000	1.025445000
C	4.434573000	4.050290000	-0.803894000
H	4.627133000	3.722637000	-1.831343000
H	5.132210000	4.869288000	-0.593512000
C	2.983217000	4.513180000	-0.674543000
H	2.783252000	4.749452000	0.377693000
H	2.861020000	5.446298000	-1.237066000
C	2.001495000	3.451922000	-1.179194000
H	2.246496000	2.481482000	-0.729067000
H	2.112397000	3.313104000	-2.261780000
Si	0.225839000	3.771286000	-0.797377000
O	-0.682720000	2.502580000	-1.360450000
O	0.011821000	3.915630000	0.842758000
O	-0.348428000	5.168323000	-1.488093000
O	5.634917000	0.738659000	0.750614000
O	4.334188000	0.959433000	-1.417099000
C	12.098416000	0.407877000	5.932520000
C	10.844205000	0.983518000	5.742430000
C	10.215718000	0.966093000	4.506531000
C	10.865104000	0.358503000	3.408035000
C	12.138636000	-0.226199000	3.590732000
C	12.728002000	-0.193935000	4.845205000

H	12.574719000	0.427353000	6.906413000
H	10.333433000	1.457785000	6.575898000
H	9.237600000	1.413530000	4.367593000
N	10.282156000	0.337984000	2.207834000
H	12.635693000	-0.695450000	2.748751000
H	13.705663000	-0.651326000	4.968921000
C	8.491773000	-0.907228000	-0.509763000
C	8.875170000	-0.772922000	0.818190000
C	8.406460000	-1.645168000	1.800589000
C	7.541373000	-2.665334000	1.441948000
C	7.154504000	-2.795182000	0.106838000
C	7.621606000	-1.927878000	-0.873007000
H	8.894330000	-0.224906000	-1.249675000
N	9.775482000	0.329297000	1.097767000
H	8.723452000	-1.520374000	2.831507000
H	7.180937000	-3.372652000	2.181815000
H	7.319928000	-2.066119000	-1.905322000
S	5.995874000	-4.085925000	-0.336676000
N	4.500175000	-3.517231000	0.082966000
H	4.362445000	-3.590653000	1.086532000
C	4.001490000	-2.273554000	-0.515324000
H	4.244057000	-2.307415000	-1.581035000
H	4.492053000	-1.396337000	-0.078217000
C	2.489050000	-2.178118000	-0.327528000
H	2.264595000	-2.150223000	0.747101000
H	2.164851000	-1.214810000	-0.735809000
C	1.731955000	-3.335196000	-0.997137000
H	2.174777000	-4.290698000	-0.690714000
H	1.847002000	-3.280262000	-2.086829000
Si	-0.066154000	-3.377098000	-0.582584000
O	-0.797249000	-4.744034000	-1.188593000
O	-0.271588000	-3.378283000	1.066246000
O	-0.843139000	-2.033004000	-1.182508000
O	6.247831000	-5.215987000	0.540660000
O	6.030692000	-4.201115000	-1.783675000
H	-6.007241000	-8.514259000	-2.196256000
H	-1.679523000	7.354285000	1.426906000

C2

	Coordinates (Angstroms)		
	X	Y	Z
Si	-5.947616000	-5.209003000	4.036313000
Si	-3.357510000	-5.215453000	1.316071000

Si	-5.657374000	-5.047004000	1.719048000
Si	-2.064029000	-3.397681000	2.028224000
Si	-6.051339000	-1.083424000	3.959576000
Si	-3.109891000	-1.412477000	1.329357000
Si	-5.415235000	-1.183621000	1.698633000
Si	-1.900182000	0.432894000	2.096381000
Si	-5.122425000	2.850640000	3.868061000
Si	-2.689747000	2.404178000	1.114417000
Si	-4.969448000	2.694032000	1.539232000
Si	-1.230589000	4.132781000	1.732771000
Si	-4.696139000	6.974391000	3.557590000
Si	-2.033529000	6.171534000	0.887430000
Si	-4.319453000	6.522040000	1.282993000
Si	-6.580664000	-6.937306000	0.675875000
Si	-3.726859000	-7.075000000	-2.005633000
Si	-6.057324000	-6.974920000	-1.613309000
Si	-2.870815000	-5.155764000	-0.986816000
Si	-6.506414000	-3.060996000	0.779735000
Si	-3.939554000	-3.303892000	-1.938631000
Si	-6.229595000	-3.142861000	-1.549813000
Si	-2.685492000	-1.577005000	-0.989829000
Si	-6.045885000	0.809127000	0.607268000
Si	-3.233668000	0.408348000	-2.088952000
Si	-5.560611000	0.657957000	-1.693733000
Si	-2.264550000	2.336988000	-1.201737000
Si	-5.612891000	4.712289000	0.506769000
Si	-3.070022000	4.282388000	-2.264245000
Si	-5.352117000	4.554214000	-1.823498000
Si	-1.534034000	5.833750000	-1.392142000
Si	-4.840747000	8.481374000	0.111123000
Si	-7.110228000	-5.082335000	-2.530389000
Si	-6.842791000	-1.118310000	-2.552802000
Si	-6.379023000	2.624132000	-2.668875000
Si	-6.307689000	6.376943000	-2.959220000
H	-5.077816000	-4.223560000	4.733573000
H	-5.540039000	-6.572744000	4.467246000
H	-7.356740000	-4.976420000	4.445214000
H	-2.865455000	-6.498573000	1.901055000
H	-1.696909000	-3.403385000	3.467409000
H	-4.884845000	-1.127595000	4.878591000
H	-6.948542000	-2.227231000	4.269996000
H	-6.817483000	0.164820000	4.215071000
H	-1.996716000	0.543686000	3.579623000
H	-0.466323000	0.246624000	1.743973000

H	-4.295632000	4.008278000	4.302873000
H	-4.538824000	1.632350000	4.487886000
H	-6.509813000	3.035600000	4.364039000
H	-0.900945000	4.156607000	3.181059000
H	-4.823470000	8.443326000	3.754846000
H	-3.573269000	6.486035000	4.399082000
H	-5.953588000	6.331657000	4.021829000
H	-8.063098000	-6.944394000	0.829419000
H	-6.045024000	-8.147508000	1.360300000
H	-3.481900000	-7.091689000	-3.473936000
H	-3.198231000	-8.337911000	-1.421373000
H	-7.958805000	-2.966307000	1.112095000
H	-3.695161000	-3.312843000	-3.413574000
H	-7.524319000	0.981890000	0.736147000
H	-3.025726000	0.296098000	-3.561653000
H	-7.043189000	5.003496000	0.819582000
H	-2.862502000	4.130274000	-3.735408000
H	-1.406816000	7.090208000	-2.173455000
H	-4.020377000	9.594441000	0.658120000
H	-6.277240000	8.842213000	0.229283000
H	-4.503754000	8.325149000	-1.329855000
H	-6.881993000	-5.001239000	-4.000087000
H	-8.577051000	-5.197968000	-2.297597000
H	-6.631174000	-1.221993000	-4.023914000
H	-8.279660000	-0.799757000	-2.319024000
H	-6.161116000	2.592302000	-4.143448000
H	-7.849702000	2.691517000	-2.433423000
H	-5.269959000	7.221404000	-3.605223000
H	-7.100561000	7.223928000	-2.029992000
H	-7.221871000	5.865177000	-4.014686000
C	12.537268000	-1.434914000	-0.402464000
C	13.162605000	-0.201923000	-0.233337000
C	12.839614000	0.863732000	-1.063545000
C	11.846202000	0.706559000	-2.028912000
C	11.222995000	-0.528365000	-2.211367000
C	11.580396000	-1.599587000	-1.400063000
H	12.794306000	-2.266850000	0.245548000
H	13.902565000	-0.068204000	0.549706000
H	13.336477000	1.823524000	-0.962929000
N	11.612957000	1.812784000	-2.911535000
H	10.478432000	-0.651690000	-2.991775000
H	11.096368000	-2.561200000	-1.538907000
C	8.188471000	1.473146000	-3.150844000
C	9.313515000	1.829732000	-2.407746000

C	9.234670000	1.951871000	-1.017402000
C	8.032499000	1.704969000	-0.373360000
C	6.918343000	1.327841000	-1.120329000
C	6.989565000	1.200063000	-2.504423000
H	8.264061000	1.412433000	-4.231751000
N	10.475884000	2.257917000	-3.131228000
H	10.118303000	2.221394000	-0.449740000
H	7.972305000	1.758443000	0.709116000
H	6.109509000	0.893758000	-3.059503000
S	5.373984000	1.009776000	-0.287592000
N	4.818739000	2.478511000	0.221815000
H	5.146958000	2.702070000	1.152965000
C	4.622791000	3.593576000	-0.706026000
H	4.795305000	3.226712000	-1.723391000
H	5.374409000	4.367953000	-0.511524000
C	3.205869000	4.157429000	-0.599137000
H	3.010366000	4.421899000	0.447231000
H	3.153624000	5.088202000	-1.176169000
C	2.160739000	3.157575000	-1.102354000
H	2.335161000	2.179318000	-0.635996000
H	2.275165000	2.998246000	-2.181778000
Si	0.406585000	3.606122000	-0.749413000
O	-0.585863000	2.407253000	-1.322338000
O	0.178464000	3.774257000	0.886621000
O	-0.050077000	5.039438000	-1.453382000
O	5.646579000	0.263339000	0.930821000
O	4.455911000	0.509675000	-1.298653000
C	13.411952000	1.745428000	3.285188000
C	12.263264000	2.192038000	2.629542000
C	11.266892000	1.293488000	2.277721000
C	11.418325000	-0.060653000	2.584598000
C	12.547633000	-0.503880000	3.270096000
C	13.551817000	0.398132000	3.607868000
H	14.189581000	2.452729000	3.556880000
H	12.146677000	3.246610000	2.398133000
H	10.366812000	1.616989000	1.768046000
N	10.476062000	-1.062813000	2.229373000
H	12.629888000	-1.559386000	3.509712000
H	14.438989000	0.050955000	4.128247000
C	8.249297000	-1.663005000	-0.348449000
C	8.765327000	-1.729614000	0.944562000
C	8.322192000	-2.708600000	1.837916000
C	7.358099000	-3.617437000	1.432603000
C	6.844667000	-3.540820000	0.138086000

C	7.286237000	-2.574566000	-0.760144000
H	8.622384000	-0.901452000	-1.023053000
N	9.723294000	-0.737518000	1.288054000
H	8.741090000	-2.741735000	2.837257000
H	7.010118000	-4.394019000	2.105870000
H	6.880323000	-2.544499000	-1.765414000
S	5.539190000	-4.663209000	-0.343867000
N	4.127280000	-3.961099000	0.159162000
H	4.021552000	-4.054015000	1.164750000
C	3.719279000	-2.663301000	-0.387809000
H	3.961953000	-2.670983000	-1.453812000
H	4.269702000	-1.839215000	0.081300000
C	2.215269000	-2.472105000	-0.200122000
H	1.987234000	-2.458478000	0.873880000
H	1.955895000	-1.479774000	-0.584959000
C	1.389549000	-3.561319000	-0.901902000
H	1.763037000	-4.550078000	-0.609381000
H	1.523368000	-3.493628000	-1.988782000
Si	-0.412651000	-3.483935000	-0.514082000
O	-1.228496000	-4.796799000	-1.133100000
O	-0.646593000	-3.469006000	1.131152000
O	-1.087029000	-2.090215000	-1.125109000
O	5.684051000	-5.867351000	0.456031000
O	5.514925000	-4.691183000	-1.795222000
H	-6.676067000	-8.192140000	-2.217638000
H	-1.265926000	7.330524000	1.432378000

TSC1^{N2}

	Coordinates (Angstroms)		
	X	Y	Z
Si	-5.898980000	-5.376834000	3.893610000
Si	-3.280684000	-5.276216000	1.201966000
Si	-5.587308000	-5.156750000	1.583785000
Si	-2.025365000	-3.450021000	1.960363000
Si	-6.058828000	-1.245406000	3.898031000
Si	-3.096984000	-1.470883000	1.285951000
Si	-5.408883000	-1.290867000	1.639277000
Si	-1.934657000	0.380509000	2.109352000
Si	-5.215746000	2.718822000	3.887616000
Si	-2.741401000	2.356955000	1.150939000
Si	-5.029968000	2.598509000	1.558993000
Si	-1.321529000	4.101409000	1.814788000
Si	-4.855697000	6.860258000	3.657270000

Si	-2.157475000	6.140074000	1.001811000
Si	-4.453294000	6.442549000	1.380549000
Si	-6.464707000	-7.042228000	0.493669000
Si	-3.583097000	-7.077752000	-2.160856000
Si	-5.918660000	-7.026369000	-1.790398000
Si	-2.771234000	-5.165393000	-1.094073000
Si	-6.460171000	-3.167528000	0.673837000
Si	-3.860483000	-3.314171000	-2.023713000
Si	-6.156420000	-3.200139000	-1.653898000
Si	-2.644966000	-1.584089000	-1.030900000
Si	-6.067604000	0.712606000	0.585807000
Si	-3.222665000	0.413528000	-2.092957000
Si	-5.557860000	0.613804000	-1.712403000
Si	-2.294846000	2.342738000	-1.162696000
Si	-5.705572000	4.623537000	0.559882000
Si	-3.131113000	4.293007000	-2.192965000
Si	-5.421717000	4.514807000	-1.770262000
Si	-1.632931000	5.857205000	-1.279654000
Si	-4.989077000	8.412775000	0.233520000
Si	-6.995695000	-5.134210000	-2.679848000
Si	-6.796143000	-1.167707000	-2.623347000
Si	-6.404016000	2.581547000	-2.659903000
Si	-6.398316000	6.339308000	-2.885048000
H	-5.043403000	-4.403933000	4.625066000
H	-5.486259000	-6.748429000	4.293569000
H	-7.313863000	-5.164719000	4.294035000
H	-2.771845000	-6.561214000	1.768041000
H	-1.674016000	-3.475856000	3.403325000
H	-4.896066000	-1.261878000	4.822765000
H	-6.917327000	-2.423374000	4.188653000
H	-6.869560000	-0.028627000	4.166947000
H	-2.064565000	0.461424000	3.592129000
H	-0.490655000	0.225576000	1.784432000
H	-4.424589000	3.891373000	4.348082000
H	-4.611810000	1.508402000	4.503071000
H	-6.614223000	2.865292000	4.365339000
H	-1.003897000	4.103350000	3.266026000
H	-4.998465000	8.325578000	3.871292000
H	-3.735609000	6.372620000	4.502869000
H	-6.111158000	6.200704000	4.102940000
H	-7.948123000	-7.080921000	0.631825000
H	-5.912847000	-8.255459000	1.159801000
H	-3.324486000	-7.059520000	-3.626855000
H	-3.038491000	-8.343664000	-1.598171000

H	-7.917710000	-3.103815000	0.990898000
H	-3.603133000	-3.293205000	-3.496285000
H	-7.549667000	0.857699000	0.705571000
H	-3.004616000	0.335570000	-3.566659000
H	-7.143885000	4.880105000	0.866933000
H	-2.908263000	4.173922000	-3.665080000
H	-1.525716000	7.130936000	-2.035884000
H	-4.199277000	9.529950000	0.816088000
H	-6.433649000	8.747238000	0.329160000
H	-4.620565000	8.290329000	-1.202895000
H	-6.757308000	-5.020002000	-4.145744000
H	-8.462261000	-5.278969000	-2.461879000
H	-6.564845000	-1.236294000	-4.093744000
H	-8.241694000	-0.880850000	-2.401485000
H	-6.173212000	2.580781000	-4.132934000
H	-7.877845000	2.616915000	-2.436342000
H	-5.369546000	7.204307000	-3.518319000
H	-7.203785000	7.165503000	-1.947997000
H	-7.303818000	5.829496000	-3.948955000
C	12.407549000	-1.497657000	-0.863536000
C	13.113877000	-0.319290000	-0.632389000
C	12.791713000	0.835936000	-1.332258000
C	11.727739000	0.821948000	-2.233959000
C	11.028292000	-0.359211000	-2.484125000
C	11.377172000	-1.518812000	-1.798743000
H	12.668207000	-2.401396000	-0.322109000
H	13.916914000	-0.301615000	0.097587000
H	13.348353000	1.756178000	-1.184958000
N	11.509513000	2.016670000	-2.997775000
H	10.231377000	-0.374963000	-3.220485000
H	10.833967000	-2.438777000	-1.990251000
C	8.099328000	1.726400000	-3.121156000
C	9.237341000	2.075023000	-2.394671000
C	9.191488000	2.163071000	-1.000799000
C	8.004527000	1.893431000	-0.335547000
C	6.880691000	1.512393000	-1.064526000
C	6.921766000	1.417780000	-2.452711000
H	8.148412000	1.693532000	-4.204926000
N	10.386547000	2.528344000	-3.123297000
H	10.078901000	2.433790000	-0.438788000
H	7.970432000	1.944532000	0.747995000
H	6.034087000	1.109936000	-2.994449000
S	5.352312000	1.177183000	-0.208246000
N	4.792365000	2.641589000	0.311856000

H	5.141614000	2.869517000	1.234185000
C	4.562622000	3.754405000	-0.610621000
H	4.746600000	3.400494000	-1.630677000
H	5.291494000	4.548717000	-0.410751000
C	3.130286000	4.277865000	-0.501399000
H	2.927859000	4.530550000	0.546553000
H	3.052073000	5.210169000	-1.073072000
C	2.112515000	3.252803000	-1.010355000
H	2.310016000	2.277944000	-0.546318000
H	2.234735000	3.098828000	-2.089721000
Si	0.346726000	3.656759000	-0.663586000
O	-0.617428000	2.449880000	-1.268171000
O	0.100802000	3.788972000	0.973141000
O	-0.133811000	5.094104000	-1.344121000
O	5.645335000	0.433250000	1.006231000
O	4.423166000	0.674815000	-1.207963000
C	14.126233000	-0.289169000	3.076345000
C	13.769889000	1.030775000	2.809908000
C	12.475921000	1.325523000	2.391657000
C	11.558082000	0.294560000	2.226801000
C	11.903583000	-1.029133000	2.496967000
C	13.191894000	-1.316270000	2.925060000
H	15.133108000	-0.520563000	3.410266000
H	14.496956000	1.827197000	2.932623000
H	12.164019000	2.343633000	2.179957000
N	10.246167000	0.698646000	1.774706000
H	11.166974000	-1.816217000	2.365753000
H	13.472008000	-2.342131000	3.143297000
C	8.306643000	-1.457025000	-0.202068000
C	8.625022000	-1.163442000	1.144016000
C	8.014619000	-1.901002000	2.188525000
C	7.104761000	-2.889872000	1.877661000
C	6.801936000	-3.185972000	0.548135000
C	7.406340000	-2.467361000	-0.481593000
H	8.771284000	-0.883189000	-0.993578000
N	9.489722000	-0.200280000	1.444784000
H	8.263273000	-1.674936000	3.219258000
H	6.648428000	-3.466520000	2.676492000
H	7.163131000	-2.706468000	-1.511703000
S	5.607834000	-4.442435000	0.185340000
N	4.107919000	-3.761994000	0.417845000
H	3.908669000	-3.702604000	1.412294000
C	3.753000000	-2.555348000	-0.334582000
H	4.072319000	-2.713436000	-1.368718000

H	4.272625000	-1.670936000	0.052628000
C	2.241070000	-2.345302000	-0.281823000
H	1.939797000	-2.217453000	0.766691000
H	2.012102000	-1.400137000	-0.785349000
C	1.463264000	-3.506611000	-0.921600000
H	1.857944000	-4.457776000	-0.543059000
H	1.622407000	-3.517611000	-2.006831000
Si	-0.345314000	-3.462172000	-0.566091000
O	-1.134271000	-4.776905000	-1.216529000
O	-0.599583000	-3.478959000	1.076381000
O	-1.037718000	-2.069424000	-1.161134000
O	5.716325000	-5.471327000	1.208309000
O	5.721488000	-4.744756000	-1.232238000
H	-6.510922000	-8.241956000	-2.423925000
H	-1.417013000	7.303133000	1.575335000

C3

	Coordinates (Angstroms)		
	X	Y	Z
Si	-6.340445000	-4.906256000	3.979069000
Si	-3.716033000	-5.104971000	1.301256000
Si	-6.002605000	-4.763604000	1.667067000
Si	-2.303501000	-3.384383000	2.028112000
Si	-6.116030000	-0.771483000	3.886281000
Si	-3.177973000	-1.329060000	1.296880000
Si	-5.464755000	-0.925544000	1.632955000
Si	-1.850273000	0.426930000	2.081228000
Si	-4.898348000	3.085336000	3.785134000
Si	-2.466326000	2.446160000	1.071573000
Si	-4.724832000	2.910752000	1.459128000
Si	-0.888539000	4.065836000	1.698355000
Si	-4.151053000	7.138006000	3.470805000
Si	-1.526016000	6.151522000	0.825522000
Si	-3.782928000	6.671046000	1.197382000
Si	-7.048548000	-6.579498000	0.605319000
Si	-4.174261000	-6.945294000	-2.030405000
Si	-6.495767000	-6.665726000	-1.676099000
Si	-3.189100000	-5.098963000	-0.993021000
Si	-6.685521000	-2.721242000	0.712835000
Si	-4.104085000	-3.175523000	-1.964220000
Si	-6.381237000	-2.835819000	-1.610440000
Si	-2.728208000	-1.545585000	-1.014016000
Si	-5.924221000	1.104178000	0.523674000

Si	-3.107179000	0.470690000	-2.128331000
Si	-5.413464000	0.900430000	-1.767215000
Si	-2.007345000	2.324252000	-1.235118000
Si	-5.196676000	4.964121000	0.401501000
Si	-2.650600000	4.311235000	-2.327985000
Si	-4.910585000	4.763541000	-1.922756000
Si	-1.023208000	5.758144000	-1.444500000
Si	-4.159141000	8.674686000	0.044939000
Si	-7.392507000	-4.701319000	-2.607059000
Si	-6.816307000	-0.776402000	-2.635334000
Si	-6.073507000	2.913066000	-2.768948000
Si	-5.654503000	6.656341000	-3.101126000
H	-5.399110000	-4.002169000	4.693236000
H	-6.059688000	-6.301688000	4.409119000
H	-7.729984000	-4.553551000	4.368053000
H	-3.329584000	-6.415662000	1.903770000
H	-1.964024000	-3.409948000	3.473973000
H	-4.962185000	-0.870460000	4.816848000
H	-7.074446000	-1.864494000	4.197195000
H	-6.818682000	0.516809000	4.125625000
H	-1.970542000	0.553996000	3.561298000
H	-0.426384000	0.133838000	1.762362000
H	-3.981134000	4.167053000	4.233329000
H	-4.429692000	1.822331000	4.412007000
H	-6.271968000	3.386898000	4.261549000
H	-0.579746000	4.077445000	3.151496000
H	-4.178240000	8.611716000	3.673399000
H	-3.073275000	6.569641000	4.320952000
H	-5.454781000	6.582109000	3.918853000
H	-8.529320000	-6.472320000	0.733523000
H	-6.619630000	-7.826055000	1.299594000
H	-3.905098000	-6.976460000	-3.494192000
H	-3.756890000	-8.247680000	-1.443040000
H	-8.130899000	-2.515180000	1.025477000
H	-3.846507000	-3.212773000	-3.436742000
H	-7.387912000	1.387746000	0.624658000
H	-2.888344000	0.336755000	-3.597717000
H	-6.605498000	5.365803000	0.686986000
H	-2.434282000	4.131843000	-3.794863000
H	-0.793976000	6.996163000	-2.232026000
H	-3.294738000	9.731707000	0.633869000
H	-5.576626000	9.111439000	0.133802000
H	-3.793156000	8.526836000	-1.389570000
H	-7.140985000	-4.635666000	-4.073739000

H	-8.866826000	-4.706870000	-2.391894000
H	-6.590154000	-0.908541000	-4.102055000
H	-8.226836000	-0.343838000	-2.427051000
H	-5.843299000	2.852529000	-4.240537000
H	-7.537427000	3.089845000	-2.549141000
H	-4.514607000	7.403295000	-3.693247000
H	-6.414722000	7.574223000	-2.212669000
H	-6.555813000	6.222538000	-4.201583000
C	13.016785000	-1.821555000	-0.322724000
C	13.749699000	-0.664553000	-0.581538000
C	13.281565000	0.261815000	-1.504930000
C	12.054424000	0.055224000	-2.139772000
C	11.330757000	-1.115068000	-1.900393000
C	11.816649000	-2.048697000	-0.991557000
H	13.384443000	-2.550127000	0.392609000
H	14.693773000	-0.492298000	-0.074348000
H	13.852700000	1.151328000	-1.752458000
N	11.720524000	1.025309000	-3.141652000
H	10.406733000	-1.305477000	-2.434246000
H	11.248337000	-2.953480000	-0.800766000
C	8.313857000	0.588145000	-3.177791000
C	9.437927000	1.106005000	-2.533425000
C	9.377490000	1.473108000	-1.186762000
C	8.195744000	1.297448000	-0.481959000
C	7.083570000	0.757946000	-1.124701000
C	7.136520000	0.395203000	-2.467751000
H	8.371749000	0.348092000	-4.234576000
N	10.568066000	1.434139000	-3.350489000
H	10.248992000	1.891940000	-0.695478000
H	8.151375000	1.563764000	0.569712000
H	6.254545000	-0.017171000	-2.945103000
S	5.552364000	0.557401000	-0.229818000
N	5.103747000	2.077779000	0.226324000
H	5.449968000	2.315052000	1.147213000
C	4.951727000	3.164183000	-0.741403000
H	5.095750000	2.749966000	-1.745116000
H	5.742507000	3.907532000	-0.584153000
C	3.565938000	3.801369000	-0.642230000
H	3.399061000	4.121566000	0.393606000
H	3.550556000	4.707476000	-1.259500000
C	2.465202000	2.834530000	-1.088293000
H	2.592358000	1.870916000	-0.578775000
H	2.561517000	2.620228000	-2.160082000
Si	0.741795000	3.400953000	-0.754354000

O	-0.325705000	2.269003000	-1.329314000
O	0.502710000	3.597923000	0.876840000
O	0.399438000	4.856847000	-1.476770000
O	5.805213000	-0.150405000	1.015095000
O	4.579056000	0.065650000	-1.192981000
C	12.229285000	2.673649000	2.903301000
C	11.243280000	2.441557000	3.858459000
C	10.332587000	1.404384000	3.679069000
C	10.404717000	0.608099000	2.537046000
C	11.398992000	0.834216000	1.579835000
C	12.306773000	1.865609000	1.767208000
H	12.944870000	3.477861000	3.046219000
H	11.186432000	3.064191000	4.745957000
H	9.558044000	1.196880000	4.410795000
N	9.425728000	-0.418991000	2.425562000
H	11.445986000	0.189781000	0.710416000
H	13.083424000	2.034256000	1.026760000
C	8.124753000	-2.336823000	-0.152547000
C	8.429681000	-1.986308000	1.160858000
C	7.798999000	-2.621363000	2.233658000
C	6.843641000	-3.591113000	1.982568000
C	6.516937000	-3.908683000	0.663507000
C	7.148622000	-3.290770000	-0.409505000
H	8.639864000	-1.825981000	-0.959092000
N	9.402523000	-0.965311000	1.302964000
H	8.064382000	-2.342703000	3.246817000
H	6.357552000	-4.114167000	2.800002000
H	6.883941000	-3.568930000	-1.423679000
S	5.207912000	-5.086690000	0.357516000
N	3.796226000	-4.245836000	0.571903000
H	3.599482000	-4.137438000	1.562444000
C	3.538434000	-3.047309000	-0.233947000
H	3.850582000	-3.271679000	-1.257885000
H	4.123787000	-2.190725000	0.121424000
C	2.047058000	-2.719677000	-0.203649000
H	1.748566000	-2.535698000	0.837249000
H	1.897421000	-1.775159000	-0.737312000
C	1.183050000	-3.834188000	-0.815358000
H	1.488593000	-4.801781000	-0.398262000
H	1.353399000	-3.897067000	-1.897006000
Si	-0.619197000	-3.618962000	-0.484344000
O	-1.521497000	-4.870752000	-1.110676000
O	-0.881076000	-3.568750000	1.155937000
O	-1.174507000	-2.184548000	-1.121829000

O	5.241139000	-6.072307000	1.424491000
O	5.286902000	-5.455487000	-1.044783000
H	-7.195792000	-7.836377000	-2.283401000
H	-0.678974000	7.253290000	1.371494000

TSC2$^{R\text{-}N1}$

	Coordinates (Angstroms)		
	X	Y	Z
Si	-5.753555000	-5.348875000	4.072185000
Si	-3.198901000	-5.236660000	1.318091000
Si	-5.498384000	-5.167234000	1.751961000
Si	-1.971564000	-3.367432000	2.014374000
Si	-6.017529000	-1.223770000	3.998805000
Si	-3.109011000	-1.428201000	1.329137000
Si	-5.417198000	-1.297663000	1.727210000
Si	-1.980453000	0.467841000	2.095174000
Si	-5.288380000	2.759783000	3.897649000
Si	-2.857198000	2.403907000	1.116549000
Si	-5.141755000	2.601168000	1.568368000
Si	-1.461929000	4.190923000	1.715232000
Si	-5.021843000	6.904911000	3.576204000
Si	-2.358564000	6.194792000	0.882400000
Si	-4.653029000	6.452988000	1.300421000
Si	-6.352470000	-7.094931000	0.718311000
Si	-3.530356000	-7.110782000	-1.999241000
Si	-5.857704000	-7.109835000	-1.577280000
Si	-2.744295000	-5.156117000	-0.990933000
Si	-6.439209000	-3.219392000	0.820895000
Si	-3.896850000	-3.349629000	-1.931133000
Si	-6.186016000	-3.287846000	-1.512342000
Si	-2.704486000	-1.572867000	-0.994529000
Si	-6.149347000	0.670002000	0.653572000
Si	-3.361266000	0.386924000	-2.081484000
Si	-5.691892000	0.538327000	-1.653885000
Si	-2.463673000	2.355225000	-1.206082000
Si	-5.883681000	4.590669000	0.544571000
Si	-3.361402000	4.267108000	-2.255496000
Si	-5.647643000	4.442203000	-1.788935000
Si	-1.876610000	5.878750000	-1.403696000
Si	-5.251561000	8.385370000	0.120130000
Si	-7.000132000	-5.262650000	-2.479942000
Si	-6.912952000	-1.289935000	-2.492471000
Si	-6.597177000	2.468421000	-2.624961000

Si	-6.688700000	6.222806000	-2.917093000
H	-4.900694000	-4.345494000	4.764621000
H	-5.304410000	-6.704300000	4.487866000
H	-7.162739000	-5.156167000	4.501195000
H	-2.643378000	-6.497946000	1.894169000
H	-1.586876000	-3.356560000	3.448896000
H	-4.833153000	-1.182211000	4.894670000
H	-6.830262000	-2.421670000	4.335575000
H	-6.859813000	-0.027043000	4.260082000
H	-2.085763000	0.574068000	3.578220000
H	-0.539088000	0.345892000	1.746183000
H	-4.515099000	3.956704000	4.324562000
H	-4.649896000	1.572130000	4.522367000
H	-6.681663000	2.884713000	4.396297000
H	-1.111327000	4.228321000	3.158203000
H	-5.186293000	8.370943000	3.767879000
H	-3.878403000	6.450756000	4.409029000
H	-6.257173000	6.231004000	4.055361000
H	-7.830965000	-7.166449000	0.891012000
H	-5.756393000	-8.281371000	1.394581000
H	-3.303411000	-7.118015000	-3.470496000
H	-2.941623000	-8.349894000	-1.421156000
H	-7.890938000	-3.185994000	1.167268000
H	-3.668565000	-3.349227000	-3.408601000
H	-7.631687000	0.776717000	0.806176000
H	-3.170569000	0.288075000	-3.557521000
H	-7.319731000	4.823333000	0.879256000
H	-3.165185000	4.123443000	-3.729092000
H	-1.812408000	7.140119000	-2.184992000
H	-4.465559000	9.529260000	0.653854000
H	-6.698691000	8.698826000	0.244568000
H	-4.918442000	8.230353000	-1.322008000
H	-6.796877000	-5.173858000	-3.952789000
H	-8.457798000	-5.436364000	-2.225833000
H	-6.734467000	-1.376185000	-3.968997000
H	-8.356443000	-1.038310000	-2.220373000
H	-6.384896000	2.443950000	-4.100544000
H	-8.068458000	2.475047000	-2.382862000
H	-5.693261000	7.095646000	-3.591273000
H	-7.490352000	7.050862000	-1.978486000
H	-7.606363000	5.671578000	-3.949410000
C	14.743042000	0.610451000	-0.090496000
C	14.475453000	1.919940000	-0.480532000
C	13.345073000	2.240010000	-1.218973000

C	12.430141000	1.219829000	-1.552313000
C	12.677275000	-0.106866000	-1.135458000
C	13.836962000	-0.390539000	-0.431360000
H	15.633852000	0.375496000	0.481209000
H	15.168353000	2.715388000	-0.220510000
H	13.155937000	3.256760000	-1.545187000
N	11.330576000	1.487391000	-2.268883000
H	11.956459000	-0.881873000	-1.369421000
H	14.017067000	-1.415809000	-0.122105000
C	7.950321000	1.315330000	-3.012855000
C	9.072197000	1.592018000	-2.240939000
C	8.975930000	1.782085000	-0.863378000
C	7.743092000	1.660129000	-0.244807000
C	6.622926000	1.351331000	-1.018078000
C	6.710746000	1.179299000	-2.395499000
H	8.068557000	1.179363000	-4.083039000
N	10.336220000	1.623271000	-2.963362000
H	9.874516000	1.987967000	-0.292904000
H	7.653569000	1.760835000	0.832042000
H	5.821924000	0.924524000	-2.962175000
S	5.036676000	1.168892000	-0.215324000
N	4.563557000	2.684730000	0.217381000
H	4.862753000	2.930697000	1.152151000
C	4.377578000	3.765575000	-0.750604000
H	4.559012000	3.361616000	-1.752336000
H	5.130467000	4.542726000	-0.574042000
C	2.960968000	4.337530000	-0.674345000
H	2.756688000	4.626767000	0.363736000
H	2.918245000	5.255157000	-1.272784000
C	1.919513000	3.329242000	-1.166633000
H	2.107902000	2.352205000	-0.702922000
H	2.024126000	3.169386000	-2.246873000
Si	0.159409000	3.732685000	-0.791166000
O	-0.792651000	2.496895000	-1.352967000
O	-0.051066000	3.891611000	0.847943000
O	-0.361914000	5.147564000	-1.487147000
O	5.242108000	0.460728000	1.037714000
O	4.118027000	0.681023000	-1.230982000
C	13.798221000	1.183624000	3.231069000
C	12.739305000	1.728161000	2.502876000
C	11.726575000	0.910076000	2.029628000
C	11.770676000	-0.462873000	2.286679000
C	12.817805000	-1.005721000	3.029738000
C	13.838038000	-0.182135000	3.493609000

H	14.590567000	1.830167000	3.596231000
H	12.712438000	2.793676000	2.297894000
H	10.892253000	1.310195000	1.467324000
N	10.783264000	-1.385259000	1.857899000
H	12.816696000	-2.073497000	3.224798000
H	14.659250000	-0.605138000	4.063771000
C	8.385581000	-1.699847000	-0.629844000
C	8.995174000	-1.888616000	0.609281000
C	8.569893000	-2.916842000	1.456737000
C	7.537775000	-3.750947000	1.059304000
C	6.932779000	-3.552074000	-0.181961000
C	7.351465000	-2.535247000	-1.033679000
H	8.738408000	-0.903994000	-1.275553000
N	10.020399000	-0.964764000	0.961651000
H	9.058220000	-3.045493000	2.415836000
H	7.206681000	-4.564855000	1.696055000
H	6.880269000	-2.411810000	-2.002610000
S	5.553861000	-4.589973000	-0.651653000
N	4.205348000	-3.897513000	0.010913000
H	4.157381000	-4.082128000	1.007871000
C	3.784430000	-2.554481000	-0.397252000
H	4.009009000	-2.452639000	-1.462285000
H	4.339913000	-1.781024000	0.145943000
C	2.283101000	-2.384816000	-0.168699000
H	2.071235000	-2.478032000	0.904211000
H	2.020316000	-1.359192000	-0.450414000
C	1.449632000	-3.403499000	-0.960450000
H	1.831808000	-4.413649000	-0.769188000
H	1.568314000	-3.232934000	-2.037824000
Si	-0.349092000	-3.384378000	-0.548056000
O	-1.120991000	-4.728356000	-1.157297000
O	-0.563948000	-3.380624000	1.099928000
O	-1.087378000	-2.018754000	-1.149450000
O	5.716200000	-5.860494000	0.033780000
O	5.422776000	-4.493390000	-2.094680000
H	-6.433370000	-8.351264000	-2.174783000
H	-1.633594000	7.385117000	1.418329000

TSC3$^{R\text{-}N1}$

	Coordinates (Angstroms)		
	X	Y	Z
Si	-7.141424000	-4.836074000	3.757754000
Si	-4.155865000	-5.049738000	1.322810000

Si	-6.471282000	-4.609000000	1.501272000
Si	-2.661917000	-3.399338000	2.130766000
Si	-6.472695000	-0.559315000	3.736408000
Si	-3.355417000	-1.270599000	1.347318000
Si	-5.665562000	-0.746781000	1.511927000
Si	-2.026644000	0.461317000	2.254477000
Si	-5.278343000	3.387362000	3.661836000
Si	-2.434118000	2.533899000	1.187526000
Si	-4.716357000	3.125747000	1.381907000
Si	-0.815772000	4.119828000	1.882106000
Si	-4.049455000	7.481530000	3.426902000
Si	-1.329324000	6.245887000	0.956264000
Si	-3.594860000	6.902213000	1.173343000
Si	-7.527831000	-6.365365000	0.305121000
Si	-4.469923000	-6.890083000	-2.100485000
Si	-6.811058000	-6.480047000	-1.945049000
Si	-3.471214000	-5.092358000	-0.952067000
Si	-6.933385000	-2.497162000	0.493995000
Si	-4.175140000	-3.098213000	-1.999977000
Si	-6.468871000	-2.628530000	-1.828856000
Si	-2.751026000	-1.537635000	-0.948034000
Si	-5.928638000	1.331543000	0.364887000
Si	-2.931499000	0.531600000	-2.078584000
Si	-5.266735000	1.084692000	-1.905250000
Si	-1.820245000	2.379103000	-1.112877000
Si	-5.020545000	5.216027000	0.265859000
Si	-2.315665000	4.398729000	-2.276982000
Si	-4.592607000	4.975791000	-2.060619000
Si	-0.690492000	5.808052000	-1.288586000
Si	-3.835614000	8.948457000	0.013177000
Si	-7.518536000	-4.443320000	-2.927023000
Si	-6.707906000	-0.530265000	-2.880975000
Si	-5.767913000	3.136515000	-2.967465000
Si	-5.184000000	6.861865000	-3.371390000
H	-6.229144000	-4.092346000	4.666131000
H	-7.084192000	-6.279080000	4.109826000
H	-8.528407000	-4.344355000	3.962255000
H	-3.866040000	-6.371186000	1.955219000
H	-2.411142000	-3.450796000	3.594158000
H	-5.371014000	-0.560771000	4.733369000
H	-7.380386000	-1.700003000	4.027753000
H	-7.255441000	0.695149000	3.887529000
H	-2.300740000	0.604562000	3.712910000
H	-0.590635000	0.104817000	2.091830000

H	-4.506818000	4.526238000	4.225407000
H	-4.910758000	2.165397000	4.423507000
H	-6.728753000	3.653875000	3.839220000
H	-0.578936000	4.143231000	3.348729000
H	-3.774477000	8.933243000	3.599991000
H	-3.187048000	6.724842000	4.370705000
H	-5.473716000	7.227663000	3.766769000
H	-9.005399000	-6.170236000	0.327406000
H	-7.226287000	-7.638108000	1.018870000
H	-4.066997000	-6.922830000	-3.532227000
H	-4.176431000	-8.215455000	-1.490795000
H	-8.380376000	-2.189779000	0.698051000
H	-3.800511000	-3.172107000	-3.445233000
H	-7.380262000	1.685302000	0.361380000
H	-2.607832000	0.390501000	-3.528071000
H	-6.431857000	5.662883000	0.457395000
H	-1.988476000	4.188559000	-3.719212000
H	-0.360733000	7.026214000	-2.071190000
H	-2.899975000	9.941276000	0.603404000
H	-5.223279000	9.468031000	0.130406000
H	-3.505515000	8.794284000	-1.429479000
H	-7.156968000	-4.380544000	-4.369882000
H	-9.001320000	-4.358837000	-2.817987000
H	-6.388910000	-0.678191000	-4.328573000
H	-8.100946000	-0.013495000	-2.769488000
H	-5.431451000	3.053373000	-4.416974000
H	-7.236671000	3.366990000	-2.859791000
H	-3.978065000	7.612023000	-3.807877000
H	-6.067972000	7.781892000	-2.608464000
H	-5.915380000	6.395247000	-4.578228000
C	15.179708000	0.832795000	-1.013341000
C	14.475667000	1.913463000	-1.542013000
C	13.218855000	1.757247000	-2.107379000
C	12.639679000	0.469621000	-2.162829000
C	13.341473000	-0.632228000	-1.620316000
C	14.593571000	-0.431425000	-1.059460000
H	16.161832000	0.971739000	-0.575354000
H	14.910893000	2.908526000	-1.516533000
H	12.682930000	2.603043000	-2.523158000
N	11.453371000	0.282241000	-2.744016000
H	12.896265000	-1.620102000	-1.662621000
H	15.118519000	-1.289610000	-0.649867000
C	8.025186000	-0.300995000	-2.977375000
C	9.208798000	0.148684000	-2.401681000

C	9.240422000	0.641279000	-1.097996000
C	8.068857000	0.664138000	-0.358178000
C	6.887358000	0.193468000	-0.930336000
C	6.849829000	-0.286863000	-2.234821000
H	8.045160000	-0.665003000	-3.999611000
N	10.373909000	0.065163000	-3.266953000
H	10.174194000	0.986233000	-0.664555000
H	8.082739000	1.022611000	0.666675000
H	5.913730000	-0.641516000	-2.650652000
S	5.389065000	0.155643000	0.047134000
N	5.191019000	1.688720000	0.609792000
H	5.549336000	1.806086000	1.548074000
C	5.125579000	2.859352000	-0.264742000
H	5.290549000	2.528297000	-1.296295000
H	5.951321000	3.534390000	-0.011762000
C	3.778894000	3.576782000	-0.161202000
H	3.595681000	3.833319000	0.889273000
H	3.846770000	4.522863000	-0.711601000
C	2.634878000	2.720874000	-0.708472000
H	2.653646000	1.731846000	-0.234321000
H	2.780175000	2.534177000	-1.780180000
Si	0.930869000	3.385089000	-0.469519000
O	-0.140290000	2.285852000	-1.098400000
O	0.601944000	3.602253000	1.142650000
O	0.693093000	4.848527000	-1.217265000
O	5.612899000	-0.658608000	1.230948000
O	4.313926000	-0.150668000	-0.882602000
C	12.370735000	2.030648000	2.588562000
C	11.303640000	1.963606000	3.480206000
C	10.368884000	0.939436000	3.365318000
C	10.498214000	-0.007764000	2.349655000
C	11.579165000	0.049671000	1.463089000
C	12.510866000	1.070745000	1.584120000
H	13.104313000	2.826279000	2.678836000
H	11.201328000	2.705539000	4.266237000
H	9.528885000	0.857836000	4.048329000
N	9.465362000	-0.982789000	2.286154000
H	11.676454000	-0.705237000	0.690709000
H	13.349697000	1.113915000	0.896825000
C	8.027261000	-2.954955000	-0.155153000
C	8.393204000	-2.579466000	1.135239000
C	7.744970000	-3.120671000	2.248370000
C	6.716088000	-4.027620000	2.061399000
C	6.329983000	-4.369880000	0.765001000

C	6.973568000	-3.839900000	-0.347253000
H	8.563180000	-2.527260000	-0.996588000
N	9.447086000	-1.632352000	1.219592000
H	8.059316000	-2.823511000	3.242155000
H	6.220885000	-4.484152000	2.912456000
H	6.661662000	-4.139513000	-1.341735000
S	4.949537000	-5.483251000	0.537795000
N	3.589588000	-4.577554000	0.815240000
H	3.449308000	-4.451053000	1.813027000
C	3.341117000	-3.378513000	0.008639000
H	3.620649000	-3.618225000	-1.021437000
H	3.957959000	-2.537077000	0.345414000
C	1.860627000	-3.008666000	0.068940000
H	1.587257000	-2.808160000	1.113693000
H	1.728252000	-2.064285000	-0.469793000
C	0.952575000	-4.101297000	-0.515459000
H	1.190285000	-5.065427000	-0.049975000
H	1.150094000	-4.222226000	-1.588011000
Si	-0.845803000	-3.766472000	-0.274380000
O	-1.788172000	-4.961112000	-0.947609000
O	-1.207956000	-3.685808000	1.345567000
O	-1.249923000	-2.297444000	-0.949256000
O	4.989375000	-6.461819000	1.610852000
O	4.939067000	-5.864745000	-0.863595000
H	-7.528960000	-7.604913000	-2.613550000
H	-0.455245000	7.300676000	1.550593000

C5

	Coordinates (Angstroms)		
	X	Y	Z
Si	-5.965130000	-5.199923000	4.014985000
Si	-3.467132000	-5.179712000	1.204323000
Si	-5.749928000	-5.003335000	1.692060000
Si	-2.132480000	-3.384182000	1.897072000
Si	-6.024627000	-1.068370000	4.007147000
Si	-3.186313000	-1.379246000	1.269303000
Si	-5.475443000	-1.141473000	1.722465000
Si	-1.943361000	0.448363000	2.025448000
Si	-5.064770000	2.861520000	3.943555000
Si	-2.753844000	2.438285000	1.098134000
Si	-5.014741000	2.737643000	1.608440000
Si	-1.265064000	4.147471000	1.696678000
Si	-4.652468000	6.986450000	3.682219000

Si	-2.083823000	6.204843000	0.914891000
Si	-4.353445000	6.565264000	1.390168000
Si	-6.726630000	-6.866430000	0.647866000
Si	-3.969245000	-6.981595000	-2.132554000
Si	-6.283475000	-6.871203000	-1.658427000
Si	-3.064789000	-5.085105000	-1.113754000
Si	-6.615283000	-2.995704000	0.815353000
Si	-4.149397000	-3.208459000	-1.995199000
Si	-6.422723000	-3.039383000	-1.523541000
Si	-2.845042000	-1.508408000	-1.065687000
Si	-6.134430000	0.872880000	0.688422000
Si	-3.420427000	0.497274000	-2.113068000
Si	-5.730357000	0.756582000	-1.630349000
Si	-2.409306000	2.407620000	-1.232263000
Si	-5.684453000	4.775529000	0.631441000
Si	-3.238756000	4.376088000	-2.230887000
Si	-5.502846000	4.653792000	-1.708744000
Si	-1.664568000	5.904509000	-1.385888000
Si	-4.893285000	8.543339000	0.259331000
Si	-7.349837000	-4.955029000	-2.507880000
Si	-7.063470000	-0.993965000	-2.464175000
Si	-6.564493000	2.741953000	-2.552298000
Si	-6.479991000	6.497511000	-2.790710000
H	-5.061687000	-4.235131000	4.698181000
H	-5.559190000	-6.574519000	4.411441000
H	-7.357049000	-4.958373000	4.474639000
H	-2.963180000	-6.475430000	1.750324000
H	-1.712869000	-3.416795000	3.321510000
H	-4.823324000	-1.137568000	4.878343000
H	-6.921501000	-2.207002000	4.337188000
H	-6.766340000	0.184326000	4.309899000
H	-1.995291000	0.538742000	3.512460000
H	-0.521780000	0.262700000	1.627073000
H	-4.209578000	4.007640000	4.354602000
H	-4.460000000	1.631163000	4.517459000
H	-6.425163000	3.048479000	4.508424000
H	-0.882037000	4.143501000	3.131877000
H	-4.780555000	8.451923000	3.903912000
H	-3.497533000	6.493363000	4.476087000
H	-5.888916000	6.330500000	4.183034000
H	-8.203024000	-6.861949000	0.853123000
H	-6.180353000	-8.093448000	1.293161000
H	-3.773866000	-6.977300000	-3.608214000
H	-3.430420000	-8.256601000	-1.585091000

H	-8.053538000	-2.893640000	1.202241000
H	-3.956497000	-3.196520000	-3.477723000
H	-7.606650000	1.049253000	0.872896000
H	-3.267968000	0.407871000	-3.593920000
H	-7.101259000	5.067856000	0.998670000
H	-3.083574000	4.250649000	-3.710779000
H	-1.558807000	7.174073000	-2.149025000
H	-4.048381000	9.643407000	0.795313000
H	-6.322902000	8.914146000	0.422460000
H	-4.598979000	8.401923000	-1.192581000
H	-7.166504000	-4.849496000	-3.982129000
H	-8.809769000	-5.063870000	-2.232082000
H	-6.920509000	-1.072423000	-3.944879000
H	-8.485135000	-0.669045000	-2.158738000
H	-6.384037000	2.730359000	-4.032228000
H	-8.028299000	2.814142000	-2.278963000
H	-5.455617000	7.343385000	-3.455938000
H	-7.240025000	7.337940000	-1.828629000
H	-7.427640000	6.005711000	-3.825911000
C	15.511459000	2.601863000	-2.104649000
C	14.617110000	3.380098000	-2.834348000
C	13.248379000	3.206813000	-2.661116000
C	12.776831000	2.271809000	-1.739994000
C	13.672979000	1.478391000	-1.015775000
C	15.037172000	1.648144000	-1.202564000
H	16.580422000	2.728523000	-2.246347000
H	14.984420000	4.114830000	-3.543808000
H	12.528350000	3.792657000	-3.223547000
N	11.364706000	2.174812000	-1.633022000
H	13.293371000	0.727246000	-0.332934000
H	15.735626000	1.028278000	-0.648688000
C	8.715792000	1.506986000	-1.660214000
C	9.545861000	1.454727000	-0.536390000
C	9.015812000	1.179917000	0.724875000
C	7.651847000	0.973920000	0.874697000
C	6.832932000	1.027594000	-0.249991000
C	7.353005000	1.288471000	-1.517224000
H	9.155170000	1.696401000	-2.632914000
N	10.959652000	1.603828000	-0.599388000
H	9.686645000	1.112643000	1.574329000
H	7.229159000	0.730827000	1.843535000
H	6.696166000	1.283983000	-2.380636000
S	5.079095000	0.762903000	-0.059873000
N	4.413800000	2.228272000	0.303386000

H	4.479585000	2.441565000	1.291742000
C	4.463897000	3.357830000	-0.623479000
H	4.684659000	2.959059000	-1.618109000
H	5.273518000	4.045656000	-0.348606000
C	3.111088000	4.072349000	-0.649273000
H	2.850999000	4.362561000	0.376450000
H	3.210220000	5.001708000	-1.221259000
C	2.019847000	3.180663000	-1.252188000
H	2.139456000	2.159257000	-0.866410000
H	2.139506000	3.107495000	-2.339694000
Si	0.282778000	3.657104000	-0.851733000
O	-0.736115000	2.474831000	-1.412421000
O	0.110932000	3.797337000	0.793945000
O	-0.187069000	5.105532000	-1.513871000
O	4.878428000	-0.052108000	1.127571000
O	4.567164000	0.367516000	-1.361596000
C	13.754680000	-0.289004000	3.772840000
C	13.193235000	0.196495000	2.589801000
C	12.120176000	-0.457721000	2.001235000
C	11.598111000	-1.604946000	2.609695000
C	12.156413000	-2.089565000	3.791705000
C	13.236556000	-1.433122000	4.372399000
H	14.596175000	0.227190000	4.225310000
H	13.594796000	1.092136000	2.123612000
H	11.678415000	-0.089073000	1.081283000
N	10.494279000	-2.350159000	2.114094000
H	11.728506000	-2.981315000	4.238562000
H	13.671851000	-1.813686000	5.291134000
C	8.266446000	-2.143276000	-0.560442000
C	8.890621000	-2.660561000	0.573370000
C	8.434261000	-3.849352000	1.152773000
C	7.355518000	-4.512363000	0.591779000
C	6.731502000	-3.980987000	-0.537933000
C	7.173990000	-2.796577000	-1.118770000
H	8.655267000	-1.230662000	-0.998760000
N	9.998272000	-1.908234000	1.057033000
H	8.941158000	-4.241462000	2.026705000
H	7.004977000	-5.452282000	1.005090000
H	6.683772000	-2.407256000	-2.004626000
S	5.321222000	-4.839472000	-1.227246000
N	3.984665000	-4.223445000	-0.471247000
H	3.928297000	-4.554000000	0.487077000
C	3.604500000	-2.822523000	-0.672597000
H	3.783875000	-2.587829000	-1.724753000

H	4.215576000	-2.149300000	-0.060699000
C	2.125309000	-2.629972000	-0.340629000
H	1.966791000	-2.812543000	0.729771000
H	1.885670000	-1.574503000	-0.512302000
C	1.209400000	-3.541993000	-1.170336000
H	1.533941000	-4.583590000	-1.060453000
H	1.308048000	-3.306764000	-2.237591000
Si	-0.573707000	-3.441624000	-0.704950000
O	-1.427427000	-4.735478000	-1.314731000
O	-0.750005000	-3.454815000	0.947800000
O	-1.256882000	-2.030894000	-1.266057000
O	5.412203000	-6.223614000	-0.795184000
O	5.233408000	-4.463969000	-2.626730000
H	-6.933733000	-8.073572000	-2.259238000
H	-1.290822000	7.349824000	1.453113000

TSC2$^{R\text{-}N2}$

	Coordinates (Angstroms)		
	X	Y	Z
Si	-5.685275000	-5.377275000	4.163522000
Si	-3.149943000	-5.246136000	1.392814000
Si	-5.447809000	-5.226962000	1.839227000
Si	-1.965700000	-3.336637000	2.052148000
Si	-6.056143000	-1.266669000	4.021607000
Si	-3.154828000	-1.437413000	1.340522000
Si	-5.463725000	-1.358498000	1.748629000
Si	-2.068583000	0.499081000	2.065630000
Si	-5.407957000	2.724215000	3.851744000
Si	-2.997265000	2.394244000	1.054929000
Si	-5.282566000	2.542769000	1.523049000
Si	-1.642215000	4.223876000	1.615505000
Si	-5.255308000	6.867321000	3.468908000
Si	-2.596209000	6.191746000	0.761594000
Si	-4.892916000	6.398404000	1.195526000
Si	-6.260234000	-7.191872000	0.842671000
Si	-3.451069000	-7.182983000	-1.888990000
Si	-5.775867000	-7.232704000	-1.454775000
Si	-2.706918000	-5.192164000	-0.919321000
Si	-6.441409000	-3.319905000	0.879249000
Si	-3.908834000	-3.431569000	-1.883944000
Si	-6.196652000	-3.420903000	-1.453607000
Si	-2.758222000	-1.609960000	-0.982518000
Si	-6.248566000	0.573187000	0.647487000

Si	-3.469782000	0.313185000	-2.101712000
Si	-5.800754000	0.414353000	-1.660005000
Si	-2.615703000	2.319121000	-1.269023000
Si	-6.083703000	4.496239000	0.475815000
Si	-3.574012000	4.189931000	-2.338967000
Si	-5.860216000	4.313502000	-1.856447000
Si	-2.126196000	5.853244000	-1.523726000
Si	-5.545138000	8.304011000	-0.000103000
Si	-6.967862000	-5.430391000	-2.383826000
Si	-6.982041000	-1.457631000	-2.457874000
Si	-6.763350000	2.303277000	-2.657381000
Si	-6.945585000	6.055619000	-3.002653000
H	-4.856985000	-4.339585000	4.834936000
H	-5.196418000	-6.712870000	4.598300000
H	-7.096750000	-5.216803000	4.598389000
H	-2.560957000	-6.484514000	1.985880000
H	-1.576133000	-3.292098000	3.484790000
H	-4.869778000	-1.186385000	4.912104000
H	-6.839475000	-2.478608000	4.378091000
H	-6.925385000	-0.087005000	4.272012000
H	-2.169980000	0.631796000	3.546805000
H	-0.626729000	0.405319000	1.711079000
H	-4.659874000	3.943760000	4.259268000
H	-4.732398000	1.558102000	4.478155000
H	-6.797640000	2.818455000	4.367112000
H	-1.281095000	4.291812000	3.054981000
H	-5.455237000	8.330955000	3.645668000
H	-4.094460000	6.451669000	4.297771000
H	-6.469372000	6.168567000	3.966804000
H	-7.735815000	-7.295868000	1.023749000
H	-5.633903000	-8.353264000	1.535035000
H	-3.232039000	-7.211865000	-3.361146000
H	-2.830480000	-8.398151000	-1.293049000
H	-7.892079000	-3.317222000	1.231658000
H	-3.688322000	-3.450912000	-3.362363000
H	-7.732424000	0.646540000	0.806872000
H	-3.287925000	0.189396000	-3.576833000
H	-7.522482000	4.698543000	0.818272000
H	-3.387522000	4.029967000	-3.812112000
H	-2.103510000	7.104145000	-2.323988000
H	-4.790510000	9.473067000	0.524536000
H	-7.000138000	8.580037000	0.122619000
H	-5.208463000	8.148018000	-1.441210000
H	-6.773562000	-5.363022000	-3.859075000

H	-8.419944000	-5.634690000	-2.119798000
H	-6.816778000	-1.562782000	-3.934647000
H	-8.428843000	-1.238957000	-2.174627000
H	-6.556750000	2.261654000	-4.133307000
H	-8.233215000	2.273709000	-2.408570000
H	-5.972908000	6.940320000	-3.694435000
H	-7.759265000	6.879530000	-2.070604000
H	-7.857695000	5.472352000	-4.022239000
C	14.788960000	0.212549000	-1.207511000
C	15.126783000	1.548280000	-1.003576000
C	14.123239000	2.498208000	-0.855930000
C	12.791196000	2.094987000	-0.897471000
C	12.443145000	0.761175000	-1.111384000
C	13.450766000	-0.177859000	-1.270091000
H	15.571138000	-0.532414000	-1.315359000
H	16.169223000	1.846461000	-0.957035000
H	14.347096000	3.547565000	-0.692003000
N	11.834890000	3.145778000	-0.672004000
H	11.400064000	0.458690000	-1.109617000
H	13.194202000	-1.221824000	-1.417839000
C	8.566064000	2.364721000	-1.565013000
C	9.405084000	2.464100000	-0.421113000
C	8.863555000	2.183281000	0.863940000
C	7.541548000	1.814651000	0.982175000
C	6.721619000	1.719901000	-0.146235000
C	7.243892000	2.000072000	-1.411271000
H	8.979668000	2.565626000	-2.546302000
N	10.669495000	2.807626000	-0.551571000
H	9.502627000	2.250707000	1.736541000
H	7.140103000	1.567070000	1.959724000
H	6.611736000	1.896315000	-2.287479000
S	5.033018000	1.251199000	0.033859000
N	4.147073000	2.622523000	0.333252000
H	4.189089000	2.873835000	1.314675000
C	4.158646000	3.738509000	-0.610827000
H	4.417114000	3.334662000	-1.594443000
H	4.924729000	4.476330000	-0.338442000
C	2.768829000	4.374922000	-0.673885000
H	2.475399000	4.674619000	0.340175000
H	2.822140000	5.294022000	-1.268241000
C	1.742051000	3.404925000	-1.269359000
H	1.923664000	2.401620000	-0.860907000
H	1.877766000	3.317961000	-2.354029000
Si	-0.026204000	3.771404000	-0.898047000

O	-0.951452000	2.502638000	-1.433630000
O	-0.232241000	3.946994000	0.740901000
O	-0.594403000	5.161233000	-1.608624000
O	4.906435000	0.461324000	1.251424000
O	4.589018000	0.743132000	-1.257293000
C	14.614892000	0.228829000	2.580811000
C	13.411336000	0.911030000	2.400570000
C	12.276272000	0.226856000	1.992812000
C	12.345988000	-1.149771000	1.763150000
C	13.537645000	-1.839835000	1.977983000
C	14.676498000	-1.146561000	2.373429000
H	15.502479000	0.770787000	2.892897000
H	13.363267000	1.982279000	2.571198000
H	11.331876000	0.734895000	1.830750000
N	11.251589000	-1.925289000	1.299520000
H	13.556200000	-2.912109000	1.809845000
H	15.610541000	-1.678818000	2.524277000
C	8.322690000	-1.332413000	-0.496945000
C	9.244695000	-2.023190000	0.287813000
C	9.045944000	-3.372787000	0.593934000
C	7.927069000	-4.024858000	0.101217000
C	7.013508000	-3.327356000	-0.690405000
C	7.199279000	-1.981165000	-0.995213000
H	8.504984000	-0.286691000	-0.716334000
N	10.358601000	-1.258628000	0.733863000
H	9.773817000	-3.892566000	1.206242000
H	7.757487000	-5.076316000	0.305992000
H	6.484982000	-1.446657000	-1.613752000
S	5.574310000	-4.197636000	-1.307498000
N	4.298290000	-3.744696000	-0.362501000
H	4.361445000	-4.152969000	0.564235000
C	3.758449000	-2.384064000	-0.429788000
H	3.884363000	-2.037651000	-1.458324000
H	4.309616000	-1.701911000	0.227069000
C	2.274714000	-2.380881000	-0.063425000
H	2.154798000	-2.655324000	0.992022000
H	1.921446000	-1.347058000	-0.154158000
C	1.442214000	-3.323256000	-0.945899000
H	1.838723000	-4.342504000	-0.870340000
H	1.543321000	-3.038839000	-2.001018000
Si	-0.353407000	-3.355185000	-0.516952000
O	-1.095335000	-4.728518000	-1.099922000
O	-0.562526000	-3.333415000	1.131823000
O	-1.131898000	-2.019197000	-1.134902000

O	5.789136000	-5.608327000	-1.032538000
O	5.314094000	-3.697552000	-2.644990000
H	-6.322576000	-8.498199000	-2.028569000
H	-1.897813000	7.408392000	1.273227000

TSC3$^{R\text{-}N2}$

	Coordinates (Angstroms)		
	X	Y	Z
Si	-6.597288000	-4.788793000	4.021067000
Si	-4.019227000	-5.042864000	1.302351000
Si	-6.291247000	-4.645194000	1.704637000
Si	-2.550782000	-3.360063000	2.007211000
Si	-6.266486000	-0.651270000	3.929149000
Si	-3.391338000	-1.284173000	1.292670000
Si	-5.661410000	-0.821473000	1.664278000
Si	-2.017460000	0.438074000	2.070043000
Si	-4.978557000	3.189602000	3.802371000
Si	-2.591429000	2.471328000	1.064540000
Si	-4.831040000	3.000062000	1.475791000
Si	-0.960717000	4.041569000	1.676647000
Si	-4.101854000	7.216869000	3.468930000
Si	-1.535575000	6.144385000	0.802863000
Si	-3.773624000	6.729585000	1.193921000
Si	-7.391790000	-6.435336000	0.653250000
Si	-4.569242000	-6.867050000	-2.027295000
Si	-6.877245000	-6.531460000	-1.636845000
Si	-3.527741000	-5.046838000	-0.999414000
Si	-6.942879000	-2.585520000	0.765475000
Si	-4.415449000	-3.101460000	-1.952474000
Si	-6.677607000	-2.705153000	-1.562498000
Si	-2.983978000	-1.507504000	-1.024861000
Si	-6.089650000	1.221675000	0.564715000
Si	-3.330370000	0.517890000	-2.128791000
Si	-5.618610000	1.006731000	-1.733130000
Si	-2.159899000	2.332501000	-1.246553000
Si	-5.247650000	5.065299000	0.415884000
Si	-2.745012000	4.337173000	-2.337809000
Si	-4.987868000	4.852893000	-1.910697000
Si	-1.061172000	5.728201000	-1.469214000
Si	-4.105929000	8.740051000	0.039913000
Si	-7.742399000	-4.544927000	-2.551471000
Si	-7.075419000	-0.634419000	-2.581562000
Si	-6.222080000	3.037505000	-2.733902000

Si	-5.690122000	6.761996000	-3.088509000
H	-5.619405000	-3.915534000	4.724281000
H	-6.350120000	-6.193798000	4.440854000
H	-7.969812000	-4.398162000	4.434423000
H	-3.659230000	-6.364439000	1.897699000
H	-2.188783000	-3.395773000	3.447272000
H	-5.095071000	-0.760624000	4.836258000
H	-7.231667000	-1.730909000	4.264776000
H	-6.948529000	0.646344000	4.177629000
H	-2.130386000	0.567628000	3.550573000
H	-0.601616000	0.114188000	1.746468000
H	-4.029782000	4.248412000	4.238948000
H	-4.539734000	1.917291000	4.431696000
H	-6.339805000	3.530231000	4.288340000
H	-0.641022000	4.046319000	3.127529000
H	-4.069791000	8.691344000	3.665731000
H	-3.038259000	6.611423000	4.311254000
H	-5.421734000	6.713931000	3.932122000
H	-8.867999000	-6.297653000	0.804639000
H	-6.979082000	-7.692003000	1.339318000
H	-4.322324000	-6.899949000	-3.494941000
H	-4.175590000	-8.181139000	-1.449640000
H	-8.377468000	-2.346239000	1.102721000
H	-4.184325000	-3.142687000	-3.429333000
H	-7.544651000	1.538291000	0.689967000
H	-3.137154000	0.383651000	-3.601663000
H	-6.639788000	5.514672000	0.712281000
H	-2.548525000	4.148965000	-3.806268000
H	-0.794562000	6.955955000	-2.260922000
H	-3.202486000	9.773312000	0.612337000
H	-5.508679000	9.219011000	0.147423000
H	-3.766288000	8.577704000	-1.399661000
H	-7.505023000	-4.479698000	-4.020571000
H	-9.214237000	-4.520020000	-2.321068000
H	-6.873054000	-0.772566000	-4.051129000
H	-8.471790000	-0.166762000	-2.354022000
H	-6.010930000	2.961022000	-4.207581000
H	-7.676360000	3.269093000	-2.499710000
H	-4.534669000	7.478450000	-3.688286000
H	-6.422703000	7.700925000	-2.198848000
H	-6.607625000	6.348552000	-4.183526000
C	15.298850000	-0.384229000	-1.833487000
C	15.606341000	0.949018000	-1.573521000
C	14.581735000	1.876536000	-1.410562000

C	13.259758000	1.451021000	-1.485148000
C	12.941330000	0.121007000	-1.760580000
C	13.967965000	-0.795490000	-1.936586000
H	16.097068000	-1.108273000	-1.964474000
H	16.641860000	1.265656000	-1.500899000
H	14.784683000	2.923629000	-1.209527000
N	12.266581000	2.474082000	-1.255459000
H	11.900946000	-0.185802000	-1.819790000
H	13.735592000	-1.834085000	-2.149806000
C	9.033265000	1.395343000	-1.930282000
C	9.895304000	1.670840000	-0.836681000
C	9.422182000	1.497425000	0.490432000
C	8.141860000	1.031453000	0.696827000
C	7.295715000	0.759388000	-0.382168000
C	7.747779000	0.955702000	-1.687723000
H	9.395805000	1.531858000	-2.942736000
N	11.133073000	2.075191000	-1.054606000
H	10.089591000	1.693624000	1.321137000
H	7.801566000	0.847969000	1.711803000
H	7.087334000	0.729577000	-2.518730000
S	5.637529000	0.230219000	-0.101017000
N	4.755552000	1.590141000	0.287891000
H	4.859184000	1.804211000	1.274410000
C	4.800516000	2.749312000	-0.603819000
H	4.961787000	2.373356000	-1.618923000
H	5.643433000	3.408082000	-0.353863000
C	3.473264000	3.505778000	-0.548764000
H	3.265512000	3.784452000	0.492297000
H	3.578027000	4.442742000	-1.107592000
C	2.323878000	2.666593000	-1.116384000
H	2.365455000	1.661236000	-0.677180000
H	2.449564000	2.530449000	-2.197687000
Si	0.628151000	3.312945000	-0.786030000
O	-0.482447000	2.218582000	-1.353679000
O	0.406680000	3.521930000	0.846521000
O	0.329242000	4.778525000	-1.508710000
O	5.594093000	-0.592860000	1.099490000
O	5.121096000	-0.253638000	-1.373647000
C	13.232105000	0.872818000	2.881402000
C	12.167815000	0.781248000	3.775807000
C	11.096091000	-0.060806000	3.496159000
C	11.075420000	-0.783657000	2.303898000
C	12.147395000	-0.703507000	1.412270000
C	13.225375000	0.120153000	1.706544000

H	14.074449000	1.520314000	3.105743000
H	12.177506000	1.357101000	4.696148000
H	10.258729000	-0.158793000	4.180142000
N	9.919988000	-1.577772000	2.075167000
H	12.120367000	-1.291821000	0.502773000
H	14.063532000	0.173807000	1.017729000
C	8.016339000	-2.566046000	-0.639170000
C	8.567480000	-2.638161000	0.638370000
C	8.027020000	-3.493191000	1.602313000
C	6.929596000	-4.274042000	1.281418000
C	6.369290000	-4.178956000	0.007522000
C	6.895160000	-3.323686000	-0.955280000
H	8.466612000	-1.897590000	-1.365583000
N	9.710593000	-1.826264000	0.869317000
H	8.486682000	-3.545446000	2.582482000
H	6.519664000	-4.976254000	1.999779000
H	6.443078000	-3.269561000	-1.938909000
S	4.934137000	-5.175181000	-0.376461000
N	3.613577000	-4.314214000	0.126317000
H	3.560382000	-4.299032000	1.140173000
C	3.260313000	-3.052083000	-0.529693000
H	3.476068000	-3.171949000	-1.594493000
H	3.867123000	-2.222558000	-0.151161000
C	1.771942000	-2.768068000	-0.330039000
H	1.569993000	-2.647378000	0.742561000
H	1.547900000	-1.801874000	-0.796054000
C	0.874495000	-3.869895000	-0.915745000
H	1.187471000	-4.844394000	-0.522246000
H	1.004893000	-3.923803000	-2.003840000
Si	-0.913424000	-3.628402000	-0.533213000
O	-1.858384000	-4.857583000	-1.142465000
O	-1.147333000	-3.574551000	1.111555000
O	-1.449211000	-2.181271000	-1.159589000
O	4.986243000	-6.345848000	0.483050000
O	4.853394000	-5.276781000	-1.822961000
H	-7.616345000	-7.683846000	-2.232581000
H	-0.652336000	7.221828000	1.340182000

C4

	Coordinates (Angstroms)		
	X	Y	Z
Si	-5.965130000	-5.199923000	4.014985000
Si	-3.467132000	-5.179712000	1.204323000

Si	-5.749928000	-5.003335000	1.692060000
Si	-2.132480000	-3.384182000	1.897072000
Si	-6.024627000	-1.068370000	4.007147000
Si	-3.186313000	-1.379246000	1.269303000
Si	-5.475443000	-1.141473000	1.722465000
Si	-1.943361000	0.448363000	2.025448000
Si	-5.064770000	2.861520000	3.943555000
Si	-2.753844000	2.438285000	1.098134000
Si	-5.014741000	2.737643000	1.608440000
Si	-1.265064000	4.147471000	1.696678000
Si	-4.652468000	6.986450000	3.682219000
Si	-2.083823000	6.204843000	0.914891000
Si	-4.353445000	6.565264000	1.390168000
Si	-6.726630000	-6.866430000	0.647866000
Si	-3.969245000	-6.981595000	-2.132554000
Si	-6.283475000	-6.871203000	-1.658427000
Si	-3.064789000	-5.085105000	-1.113754000
Si	-6.615283000	-2.995704000	0.815353000
Si	-4.149397000	-3.208459000	-1.995199000
Si	-6.422723000	-3.039383000	-1.523541000
Si	-2.845042000	-1.508408000	-1.065687000
Si	-6.134430000	0.872880000	0.688422000
Si	-3.420427000	0.497274000	-2.113068000
Si	-5.730357000	0.756582000	-1.630349000
Si	-2.409306000	2.407620000	-1.232263000
Si	-5.684453000	4.775529000	0.631441000
Si	-3.238756000	4.376088000	-2.230887000
Si	-5.502846000	4.653792000	-1.708744000
Si	-1.664568000	5.904509000	-1.385888000
Si	-4.893285000	8.543339000	0.259331000
Si	-7.349837000	-4.955029000	-2.507880000
Si	-7.063470000	-0.993965000	-2.464175000
Si	-6.564493000	2.741953000	-2.552298000
Si	-6.479991000	6.497511000	-2.790710000
H	-5.061687000	-4.235131000	4.698181000
H	-5.559190000	-6.574519000	4.411441000
H	-7.357049000	-4.958373000	4.474639000
H	-2.963180000	-6.475430000	1.750324000
H	-1.712869000	-3.416795000	3.321510000
H	-4.823324000	-1.137568000	4.878343000
H	-6.921501000	-2.207002000	4.337188000
H	-6.766340000	0.184326000	4.309899000
H	-1.995291000	0.538742000	3.512460000
H	-0.521780000	0.262700000	1.627073000

H	-4.209578000	4.007640000	4.354602000
H	-4.460000000	1.631163000	4.517459000
H	-6.425163000	3.048479000	4.508424000
H	-0.882037000	4.143501000	3.131877000
H	-4.780555000	8.451923000	3.903912000
H	-3.497533000	6.493363000	4.476087000
H	-5.888916000	6.330500000	4.183034000
H	-8.203024000	-6.861949000	0.853123000
H	-6.180353000	-8.093448000	1.293161000
H	-3.773866000	-6.977300000	-3.608214000
H	-3.430420000	-8.256601000	-1.585091000
H	-8.053538000	-2.893640000	1.202241000
H	-3.956497000	-3.196520000	-3.477723000
H	-7.606650000	1.049253000	0.872896000
H	-3.267968000	0.407871000	-3.593920000
H	-7.101259000	5.067856000	0.998670000
H	-3.083574000	4.250649000	-3.710779000
H	-1.558807000	7.174073000	-2.149025000
H	-4.048381000	9.643407000	0.795313000
H	-6.322902000	8.914146000	0.422460000
H	-4.598979000	8.401923000	-1.192581000
H	-7.166504000	-4.849496000	-3.982129000
H	-8.809769000	-5.063870000	-2.232082000
H	-6.920509000	-1.072423000	-3.944879000
H	-8.485135000	-0.669045000	-2.158738000
H	-6.384037000	2.730359000	-4.032228000
H	-8.028299000	2.814142000	-2.278963000
H	-5.455617000	7.343385000	-3.455938000
H	-7.240025000	7.337940000	-1.828629000
H	-7.427640000	6.005711000	-3.825911000
C	15.511459000	2.601863000	-2.104649000
C	14.617110000	3.380098000	-2.834348000
C	13.248379000	3.206813000	-2.661116000
C	12.776831000	2.271809000	-1.739994000
C	13.672979000	1.478391000	-1.015775000
C	15.037172000	1.648144000	-1.202564000
H	16.580422000	2.728523000	-2.246347000
H	14.984420000	4.114830000	-3.543808000
H	12.528350000	3.792657000	-3.223547000
N	11.364706000	2.174812000	-1.633022000
H	13.293371000	0.727246000	-0.332934000
H	15.735626000	1.028278000	-0.648688000
C	8.715792000	1.506986000	-1.660214000
C	9.545861000	1.454727000	-0.536390000

C	9.015812000	1.179917000	0.724875000
C	7.651847000	0.973920000	0.874697000
C	6.832932000	1.027594000	-0.249991000
C	7.353005000	1.288471000	-1.517224000
H	9.155170000	1.696401000	-2.632914000
N	10.959652000	1.603828000	-0.599388000
H	9.686645000	1.112643000	1.574329000
H	7.229159000	0.730827000	1.843535000
H	6.696166000	1.283983000	-2.380636000
S	5.079095000	0.762903000	-0.059873000
N	4.413800000	2.228272000	0.303386000
H	4.479585000	2.441565000	1.291742000
C	4.463897000	3.357830000	-0.623479000
H	4.684659000	2.959059000	-1.618109000
H	5.273518000	4.045656000	-0.348606000
C	3.111088000	4.072349000	-0.649273000
H	2.850999000	4.362561000	0.376450000
H	3.210220000	5.001708000	-1.221259000
C	2.019847000	3.180663000	-1.252188000
H	2.139456000	2.159257000	-0.866410000
H	2.139506000	3.107495000	-2.339694000
Si	0.282778000	3.657104000	-0.851733000
O	-0.736115000	2.474831000	-1.412421000
O	0.110932000	3.797337000	0.793945000
O	-0.187069000	5.105532000	-1.513871000
O	4.878428000	-0.052108000	1.127571000
O	4.567164000	0.367516000	-1.361596000
C	13.754680000	-0.289004000	3.772840000
C	13.193235000	0.196495000	2.589801000
C	12.120176000	-0.457721000	2.001235000
C	11.598111000	-1.604946000	2.609695000
C	12.156413000	-2.089565000	3.791705000
C	13.236556000	-1.433122000	4.372399000
H	14.596175000	0.227190000	4.225310000
H	13.594796000	1.092136000	2.123612000
H	11.678415000	-0.089073000	1.081283000
N	10.494279000	-2.350159000	2.114094000
H	11.728506000	-2.981315000	4.238562000
H	13.671851000	-1.813686000	5.291134000
C	8.266446000	-2.143276000	-0.560442000
C	8.890621000	-2.660561000	0.573370000
C	8.434261000	-3.849352000	1.152773000
C	7.355518000	-4.512363000	0.591779000
C	6.731502000	-3.980987000	-0.537933000

C	7.173990000	-2.796577000	-1.118770000
H	8.655267000	-1.230662000	-0.998760000
N	9.998272000	-1.908234000	1.057033000
H	8.941158000	-4.241462000	2.026705000
H	7.004977000	-5.452282000	1.005090000
H	6.683772000	-2.407256000	-2.004626000
S	5.321222000	-4.839472000	-1.227246000
N	3.984665000	-4.223445000	-0.471247000
H	3.928297000	-4.554000000	0.487077000
C	3.604500000	-2.822523000	-0.672597000
H	3.783875000	-2.587829000	-1.724753000
H	4.215576000	-2.149300000	-0.060699000
C	2.125309000	-2.629972000	-0.340629000
H	1.966791000	-2.812543000	0.729771000
H	1.885670000	-1.574503000	-0.512302000
C	1.209400000	-3.541993000	-1.170336000
H	1.533941000	-4.583590000	-1.060453000
H	1.308048000	-3.306764000	-2.237591000
Si	-0.573707000	-3.441624000	-0.704950000
O	-1.427427000	-4.735478000	-1.314731000
O	-0.750005000	-3.454815000	0.947800000
O	-1.256882000	-2.030894000	-1.266057000
O	5.412203000	-6.223614000	-0.795184000
O	5.233408000	-4.463969000	-2.626730000
H	-6.933733000	-8.073572000	-2.259238000
H	-1.290822000	7.349824000	1.453113000

Table S14. During the isomerization of azobenzenesulfonamide atomic cartesian coordinates of intermediates and transition states at B3LYP/6-31G(d) level.

A1

	Coordinates (Angstroms)		
	X	Y	Z
C	-4.205309000	-2.090826000	0.366229000
C	-4.690180000	-1.311052000	-0.687186000
C	-4.218911000	-0.013198000	-0.868394000
C	-3.211717000	0.488937000	-0.032510000
C	-2.734988000	-0.286120000	1.035602000
C	-3.242281000	-1.568605000	1.233746000
H	-4.588800000	-3.095153000	0.521832000
H	-5.451907000	-1.706255000	-1.353341000

H	-4.611116000	0.624729000	-1.654814000
N	-2.858591000	1.863219000	-0.238617000
H	-1.992218000	0.118650000	1.714295000
H	-2.881200000	-2.163494000	2.067984000
C	0.441530000	1.842817000	0.879257000
C	-0.522653000	1.476868000	-0.070870000
C	-0.238982000	0.473266000	-1.010243000
C	0.991104000	-0.176485000	-0.979636000
C	1.931161000	0.170985000	-0.005217000
C	1.658598000	1.171211000	0.932994000
H	0.217462000	2.645039000	1.575851000
N	-1.691361000	2.301327000	-0.166562000
H	-0.979083000	0.206883000	-1.757364000
H	1.215100000	-0.968685000	-1.686697000
H	2.392053000	1.412106000	1.695656000
S	3.526507000	-0.659096000	0.022111000
N	4.572069000	0.237971000	-0.947920000
H	4.289361000	0.248512000	-1.924589000
O	3.361043000	-1.939725000	-0.662846000
O	4.054081000	-0.539173000	1.379958000
H	4.746182000	1.169969000	-0.580422000

TSA1^{N1}

	Coordinates (Angstroms)		
	X	Y	Z
C	5.492008000	-0.358808000	-1.154385000
C	4.374518000	0.459580000	-1.050554000
C	3.529891000	0.350866000	0.086736000
C	3.868263000	-0.573780000	1.111780000
C	5.029067000	-1.329267000	0.997757000
C	5.843850000	-1.248473000	-0.134752000
H	6.113219000	-0.277772000	-2.042936000
H	4.121069000	1.167575000	-1.832217000
H	3.231285000	-0.654044000	1.986528000
H	5.285570000	-2.011577000	1.804503000
H	6.734150000	-1.863084000	-0.220330000
N	2.440971000	1.118691000	0.197732000
N	1.447312000	1.830673000	0.315394000
C	-2.237689000	1.509789000	0.175372000
C	-2.399901000	0.148810000	-0.091809000
C	-1.298003000	-0.702086000	-0.248563000
C	-0.014423000	-0.185399000	-0.115184000
C	0.154236000	1.175534000	0.168588000

C	-0.948170000	2.021877000	0.305346000
H	-3.108003000	2.152514000	0.255997000
H	-1.455625000	-1.747385000	-0.494423000
H	0.857253000	-0.821551000	-0.235929000
H	-0.772930000	3.074615000	0.505436000
S	-4.065383000	-0.530949000	-0.230189000
N	-4.507060000	-1.057148000	1.304734000
H	-3.940346000	-1.831001000	1.641242000
O	-3.971707000	-1.737774000	-1.048089000
O	-4.960682000	0.581548000	-0.538209000
H	-4.590835000	-0.300667000	1.978524000

A2

	Coordinates (Angstroms)		
	X	Y	Z
C	5.889377000	1.221729000	-0.051265000
C	4.501345000	1.341848000	-0.023696000
C	3.695356000	0.195156000	-0.006793000
C	4.287069000	-1.080744000	-0.016206000
C	5.671518000	-1.192798000	-0.043248000
C	6.475676000	-0.045147000	-0.061070000
H	6.511460000	2.112100000	-0.064339000
H	4.015289000	2.312643000	-0.014584000
H	3.647448000	-1.955978000	-0.001317000
H	6.133129000	-2.176541000	-0.049910000
H	7.557692000	-0.142971000	-0.081763000
N	2.300743000	0.437847000	0.020960000
N	1.579164000	-0.596038000	0.026834000
C	-2.022524000	-1.343484000	0.071069000
C	-2.581090000	-0.064494000	0.109983000
C	-1.773754000	1.080503000	0.140896000
C	-0.392323000	0.944586000	0.112689000
C	0.183597000	-0.337205000	0.058211000
C	-0.636386000	-1.473531000	0.044455000
H	-2.667252000	-2.215912000	0.084332000
H	-2.234351000	2.060895000	0.210163000
H	0.258383000	1.811026000	0.140850000
H	-0.163652000	-2.450304000	0.019849000
S	-4.372816000	0.116531000	0.104392000
N	-4.844711000	0.261670000	-1.506712000
H	-4.487211000	1.105638000	-1.946987000
O	-4.683440000	1.404997000	0.720153000
O	-4.939995000	-1.148979000	0.565531000

H	-4.651934000	-0.576107000	-2.049769000

TSA1^{N2}

	Coordinates (Angstroms)		
	X	Y	Z
C	-1.760624000	-0.198117000	1.211612000
C	-0.430462000	-0.576538000	1.229640000
C	-2.440206000	-0.012106000	-0.000018000
H	0.097895000	-0.712795000	2.166739000
C	0.264992000	-0.778550000	0.000108000
C	-1.761129000	-0.200324000	-1.211592000
C	-0.430997000	-0.578851000	-1.229496000
N	1.535893000	-1.151256000	0.000212000
H	-2.279910000	-0.023879000	-2.148915000
H	0.096949000	-0.716869000	-2.166569000
N	2.709435000	-1.502656000	0.000590000
C	3.716456000	-0.466070000	0.000133000
C	3.438380000	0.907386000	-0.000948000
C	5.033435000	-0.933799000	0.000870000
H	2.408058000	1.250410000	-0.001536000
C	4.494889000	1.811120000	-0.001258000
C	6.087509000	-0.021442000	0.000576000
H	5.203482000	-2.006179000	0.001678000
H	4.293537000	2.878537000	-0.002100000
C	5.817633000	1.348544000	-0.000490000
H	7.113934000	-0.376151000	0.001171000
H	6.637235000	2.061683000	-0.000736000
H	-2.279015000	-0.019960000	2.148825000
S	-4.159966000	0.443381000	-0.000071000
O	-4.451093000	1.077602000	-1.287002000
O	-4.450579000	1.079481000	1.286042000
N	-5.081502000	-0.979623000	0.001086000
H	-4.923300000	-1.529384000	-0.840467000
H	-4.922071000	-1.528950000	0.842683000

A3

	Coordinates (Angstroms)		
	X	Y	Z
C	1.773697000	1.080514000	0.140183000
C	0.392293000	0.944551000	0.112020000
C	2.581082000	-0.064500000	0.110037000
H	-0.258486000	1.810949000	0.139543000

C	-0.183593000	-0.337322000	0.058407000
C	2.022548000	-1.343494000	0.071955000
C	0.636390000	-1.473621000	0.045411000
N	-1.579161000	-0.596158000	0.027172000
H	2.667331000	-2.215874000	0.085715000
H	0.163739000	-2.450445000	0.021449000
N	-2.300732000	0.437726000	0.021109000
C	-3.695366000	0.195019000	-0.006673000
C	-4.287140000	-1.080837000	-0.017009000
C	-4.501244000	1.341800000	-0.022950000
H	-3.647573000	-1.956119000	-0.002698000
C	-5.671580000	-1.192701000	-0.044194000
C	-5.889305000	1.221862000	-0.050623000
H	-4.014990000	2.312484000	-0.013191000
H	-6.133369000	-2.176359000	-0.051544000
C	-6.475663000	-0.044953000	-0.061278000
H	-6.511313000	2.112291000	-0.063176000
H	-7.557677000	-0.142786000	-0.082092000
H	2.234243000	2.060973000	0.208902000
S	4.372802000	0.116602000	0.104287000
O	4.940169000	-1.148926000	0.565192000
O	4.683361000	1.405022000	0.720182000
N	4.844559000	0.261825000	-1.506741000
H	4.653165000	-0.576435000	-2.049510000
H	4.486466000	1.105269000	-1.947498000

TSA2

	Coordinates (Angstroms)		
	X	Y	Z
C	5.899147000	-1.208150000	0.000450000
C	4.510326000	-1.332359000	0.000565000
C	3.705451000	-0.187518000	0.000125000
C	4.289082000	1.089698000	-0.000412000
C	5.673974000	1.206406000	-0.000510000
C	6.480704000	0.060498000	-0.000085000
H	6.524202000	-2.096426000	0.000779000
H	4.025376000	-2.303690000	0.000980000
H	3.646413000	1.963364000	-0.000739000
H	6.133112000	2.191250000	-0.000917000
H	7.562629000	0.161661000	-0.000168000
N	2.302299000	-0.439815000	0.000275000
N	1.581381000	0.586329000	-0.000303000
C	-1.891271000	0.038942000	-1.215780000

C	-2.575191000	-0.040509000	0.000053000
C	-1.891259000	0.040158000	1.215794000
C	-0.510682000	0.222779000	1.214201000
C	0.178279000	0.309945000	-0.000139000
C	-0.510702000	0.221589000	-1.214386000
H	-2.434799000	-0.067183000	-2.149059000
H	-2.434798000	-0.065009000	2.149174000
H	0.040807000	0.284771000	2.147086000
H	0.040777000	0.282667000	-2.147336000
S	-4.362611000	-0.232805000	0.000158000
N	-5.028375000	1.317470000	-0.001195000
H	-4.803692000	1.837356000	0.843509000
O	-4.739344000	-0.816192000	1.286535000
O	-4.739268000	-0.818374000	-1.285250000
H	-4.803646000	1.835872000	-0.846797000

Table S15. During the isomerization of azobenzenesulfonamide atomic cartesian coordinates of intermediates and transition states at ωB97XD/6-311+G(d) level.

A1

	Coordinates (Angstroms)		
	X	Y	Z
C	-3.738766000	-2.225538000	0.376676000
C	-4.255818000	-1.538811000	-0.716773000
C	-3.977513000	-0.189647000	-0.888188000
C	-3.133210000	0.455818000	0.009742000
C	-2.630682000	-0.219062000	1.120029000
C	-2.941497000	-1.559217000	1.300976000
H	-3.967354000	-3.275581000	0.516691000
H	-4.891861000	-2.051342000	-1.429259000
H	-4.396518000	0.369660000	-1.716948000
N	-2.919024000	1.860361000	-0.196945000
H	-2.006491000	0.300374000	1.836899000
H	-2.553711000	-2.085537000	2.165330000
C	0.335779000	1.888144000	0.853085000
C	-0.596495000	1.561764000	-0.127524000
C	-0.310567000	0.591229000	-1.086079000
C	0.898683000	-0.083123000	-1.037717000
C	1.806448000	0.217033000	-0.028818000
C	1.534067000	1.195018000	0.920774000
H	0.103068000	2.667731000	1.569052000

N	-1.787590000	2.358236000	-0.199466000
H	-1.037828000	0.354591000	-1.852896000
H	1.127342000	-0.859907000	-1.757755000
H	2.250692000	1.400073000	1.707343000
S	3.372439000	-0.645132000	0.026880000
N	4.441884000	0.242246000	-0.884261000
H	4.206973000	0.270065000	-1.867863000
O	3.201410000	-1.895823000	-0.675652000
O	3.857601000	-0.567708000	1.385606000
H	4.645131000	1.152675000	-0.492701000

TSA1^{N1}

	Coordinates (Angstroms)		
	X	Y	Z
C	5.211285000	-0.759497000	-1.211968000
C	4.092473000	0.056149000	-1.194403000
C	3.492142000	0.376453000	0.041952000
C	4.037160000	-0.141726000	1.235965000
C	5.156758000	-0.954258000	1.172356000
C	5.757221000	-1.274875000	-0.040707000
H	5.664677000	-0.992998000	-2.169256000
H	3.675826000	0.455522000	-2.110396000
H	3.578330000	0.105631000	2.184960000
H	5.566753000	-1.342880000	2.098358000
H	6.632413000	-1.911216000	-0.072427000
N	2.415025000	1.162602000	0.081509000
N	1.441559000	1.884741000	0.117627000
C	-2.229944000	1.512572000	-0.018414000
C	-2.367584000	0.133592000	-0.106413000
C	-1.261940000	-0.712847000	-0.141184000
C	0.008324000	-0.166258000	-0.068317000
C	0.150212000	1.214619000	0.034583000
C	-0.954082000	2.054854000	0.056370000
H	-3.108209000	2.147022000	-0.028828000
H	-1.404608000	-1.781744000	-0.246972000
H	0.887559000	-0.800244000	-0.099061000
H	-0.797931000	3.125260000	0.123472000
S	-4.012894000	-0.580067000	-0.148565000
N	-4.443671000	-0.852529000	1.429697000
H	-3.888671000	-1.561541000	1.890184000
O	-3.897922000	-1.884394000	-0.757604000
O	-4.911799000	0.440663000	-0.633268000
H	-4.564595000	-0.008245000	1.973236000

A2

	Coordinates (Angstroms)		
	X	Y	Z
C	5.855953000	-1.221174000	0.114035000
C	4.472002000	-1.336812000	0.089837000
C	3.680498000	-0.193789000	0.013771000
C	4.269568000	1.071845000	-0.043867000
C	5.650031000	1.178897000	-0.021406000
C	6.444878000	0.035737000	0.057641000
H	6.472564000	-2.110400000	0.174172000
H	3.985264000	-2.304367000	0.130572000
H	3.638285000	1.948970000	-0.106413000
H	6.114763000	2.157129000	-0.068482000
H	7.524846000	0.130057000	0.074358000
N	2.279297000	-0.425880000	-0.007095000
N	1.573827000	0.594281000	-0.030671000
C	-2.018893000	1.343222000	-0.005951000
C	-2.570722000	0.074734000	-0.120902000
C	-1.770499000	-1.060933000	-0.225074000
C	-0.393862000	-0.926471000	-0.193613000
C	0.172333000	0.344024000	-0.064352000
C	-0.637434000	1.473028000	0.018715000
H	-2.663946000	2.212500000	0.039341000
H	-2.230189000	-2.034078000	-0.352114000
H	0.254251000	-1.789094000	-0.278014000
H	-0.168183000	2.446363000	0.097889000
S	-4.351795000	-0.110873000	-0.097562000
N	-4.773928000	-0.364917000	1.489336000
H	-4.428624000	-1.239439000	1.862580000
O	-4.669623000	-1.338777000	-0.788680000
O	-4.925214000	1.164856000	-0.458171000
H	-4.589100000	0.429462000	2.087920000

TSA1^{N2}

	Coordinates (Angstroms)		
	X	Y	Z
C	-1.760624000	-0.198117000	1.211612000
C	-0.430462000	-0.576538000	1.229640000
C	-2.440206000	-0.012106000	-0.000018000
H	0.097895000	-0.712795000	2.166739000
C	0.264992000	-0.778550000	0.000108000

C	-1.761129000	-0.200324000	-1.211592000
C	-0.430997000	-0.578851000	-1.229496000
N	1.535893000	-1.151256000	0.000212000
H	-2.279910000	-0.023879000	-2.148915000
H	0.096949000	-0.716869000	-2.166569000
N	2.709435000	-1.502656000	0.000590000
C	3.716456000	-0.466070000	0.000133000
C	3.438380000	0.907386000	-0.000948000
C	5.033435000	-0.933799000	0.000870000
H	2.408058000	1.250410000	-0.001536000
C	4.494889000	1.811120000	-0.001258000
C	6.087509000	-0.021442000	0.000576000
H	5.203482000	-2.006179000	0.001678000
H	4.293537000	2.878537000	-0.002100000
C	5.817633000	1.348544000	-0.000490000
H	7.113934000	-0.376151000	0.001171000
H	6.637235000	2.061683000	-0.000736000
H	-2.279015000	-0.019960000	2.148825000
S	-4.159966000	0.443381000	-0.000071000
O	-4.451093000	1.077602000	-1.287002000
O	-4.450579000	1.079481000	1.286042000
N	-5.081502000	-0.979623000	0.001086000
H	-4.923300000	-1.529384000	-0.840467000
H	-4.922071000	-1.528950000	0.842683000

A3

	Coordinates (Angstroms)		
	X	Y	Z
C	1.770499000	-1.060933000	-0.225075000
C	0.393862000	-0.926471000	-0.193613000
C	2.570722000	0.074734000	-0.120902000
H	-0.254251000	-1.789094000	-0.278015000
C	-0.172333000	0.344024000	-0.064351000
C	2.018893000	1.343222000	-0.005950000
C	0.637434000	1.473028000	0.018716000
N	-1.573827000	0.594281000	-0.030670000
H	2.663946000	2.212500000	0.039343000
H	0.168183000	2.446363000	0.097892000
N	-2.279297000	-0.425880000	-0.007095000
C	-3.680498000	-0.193789000	0.013771000
C	-4.269568000	1.071845000	-0.043869000
C	-4.472002000	-1.336812000	0.089838000
H	-3.638285000	1.948970000	-0.106417000

C	-5.650031000	1.178897000	-0.021408000
C	-5.855953000	-1.221174000	0.114036000
H	-3.985264000	-2.304367000	0.130574000
H	-6.114763000	2.157129000	-0.068485000
C	-6.444878000	0.035737000	0.057641000
H	-6.472564000	-2.110399000	0.174175000
H	-7.524846000	0.130057000	0.074358000
H	2.230189000	-2.034078000	-0.352116000
S	4.351795000	-0.110873000	-0.097562000
O	4.925214000	1.164856000	-0.458169000
O	4.669623000	-1.338775000	-0.788682000
N	4.773928000	-0.364920000	1.489335000
H	4.589103000	0.429460000	2.087921000
H	4.428623000	-1.239441000	1.862578000

TSA2

	Coordinates (Angstroms)		
	X	Y	Z
C	5.847356000	-1.223992000	0.054688000
C	4.462088000	-1.331321000	0.073086000
C	3.679640000	-0.182752000	0.019220000
C	4.271089000	1.079578000	-0.051018000
C	5.652445000	1.178527000	-0.067887000
C	6.441313000	0.029528000	-0.016430000
H	6.460205000	-2.116873000	0.094898000
H	3.968908000	-2.294839000	0.128420000
H	3.642911000	1.960720000	-0.091111000
H	6.122040000	2.153948000	-0.123091000
H	7.521885000	0.117196000	-0.031605000
N	2.270564000	-0.409151000	0.038256000
N	1.572914000	0.609466000	-0.030409000
C	-1.878190000	-0.027392000	-1.207026000
C	-2.555408000	-0.043065000	0.006471000
C	-1.882379000	0.124130000	1.210383000
C	-0.509614000	0.323482000	1.199090000
C	0.170850000	0.343471000	-0.013323000
C	-0.506275000	0.173931000	-1.216388000
H	-2.418168000	-0.195210000	-2.131506000
H	-2.427208000	0.073992000	2.145713000
H	0.037218000	0.450845000	2.125672000
H	0.044158000	0.186540000	-2.149516000
S	-4.332086000	-0.241070000	0.015052000
N	-4.981865000	1.283216000	-0.130179000

H	-4.780560000	1.881335000	0.660642000
O	-4.710312000	-0.704117000	1.330323000
O	-4.697624000	-0.936946000	-1.197400000
H	-4.783298000	1.718498000	-1.021598000

Table S16. During the isomerization of $N(CH_3)_2$-substituted azobenzenesulfonamide atomic cartesian coordinates of intermediates and transition states at ωB97XD/6-31G(d) level.

A1

	Coordinates (Angstroms)		
	X	Y	Z
C	-3.643432000	-0.578758000	0.061030000
C	-3.972963000	0.528925000	-0.750569000
C	-3.201860000	1.676924000	-0.726303000
C	-2.044774000	1.757025000	0.051370000
C	-1.728678000	0.680652000	0.888078000
C	-2.516023000	-0.455871000	0.904144000
H	-4.848184000	0.505047000	-1.388123000
H	-3.481030000	2.535312000	-1.329869000
N	-1.364183000	3.007632000	0.005189000
H	-0.876231000	0.733474000	1.555829000
H	-2.247186000	-1.255772000	1.582942000
C	1.717597000	1.914550000	1.097734000
C	0.764943000	2.004679000	0.081747000
C	0.803250000	1.121275000	-1.001761000
C	1.770755000	0.129513000	-1.048411000
C	2.696916000	0.024408000	-0.011839000
C	2.673626000	0.908293000	1.064259000
H	1.688717000	2.628877000	1.914258000
N	-0.126900000	3.122267000	0.093430000
H	0.062385000	1.204424000	-1.789867000
H	1.794193000	-0.582010000	-1.867450000
H	3.393587000	0.799864000	1.868943000
S	3.963919000	-1.228575000	-0.091971000
N	5.255139000	-0.545781000	-0.895000000
H	5.046003000	-0.319221000	-1.861120000
O	3.476566000	-2.285671000	-0.957406000
O	4.425030000	-1.466465000	1.262628000
H	5.674129000	0.225583000	-0.387071000
N	-4.399040000	-1.727227000	0.045219000
C	-5.619474000	-1.773000000	-0.731642000
H	-6.075112000	-2.758466000	-0.627435000
H	-6.351449000	-1.022050000	-0.401322000
H	-5.418750000	-1.611232000	-1.797848000
C	-4.107702000	-2.794523000	0.979434000

H	-4.802815000	-3.618014000	0.810988000
H	-3.092142000	-3.182829000	0.836013000
H	-4.209799000	-2.471487000	2.025406000

TSA1^{N1}

	Coordinates (Angstroms)		
	X	Y	Z
C	4.636754000	0.996506000	-0.465760000
C	3.431751000	1.660243000	-0.366103000
C	2.277001000	1.021899000	0.141969000
C	2.423001000	-0.308586000	0.599094000
C	3.648688000	-0.943243000	0.591161000
C	4.788882000	-0.318174000	0.034783000
H	5.479816000	1.514740000	-0.906455000
H	3.340835000	2.683846000	-0.714547000
H	1.553900000	-0.818666000	1.003427000
H	3.715678000	-1.946720000	0.993924000
N	1.103313000	1.668190000	0.197808000
N	0.025504000	2.272989000	0.271919000
C	-3.570560000	1.410147000	0.290868000
C	-3.551809000	0.082359000	-0.130902000
C	-2.354582000	-0.561806000	-0.443271000
C	-1.157772000	0.126331000	-0.306390000
C	-1.164196000	1.450475000	0.134725000
C	-2.368025000	2.093965000	0.413623000
H	-4.517257000	1.901027000	0.491462000
H	-2.373167000	-1.581655000	-0.814396000
H	-0.214200000	-0.346429000	-0.560129000
H	-2.337988000	3.134781000	0.720669000
S	-5.086889000	-0.823196000	-0.243972000
N	-5.324414000	-1.523008000	1.251295000
H	-4.618262000	-2.213974000	1.480283000
O	-4.878541000	-1.924541000	-1.164446000
O	-6.155832000	0.144483000	-0.399313000
N	6.000080000	-0.962536000	-0.016084000
C	7.138677000	-0.313432000	-0.631645000
H	7.387795000	0.625066000	-0.121211000
H	8.007212000	-0.969352000	-0.562736000
H	6.962625000	-0.092716000	-1.693757000
C	6.103277000	-2.343404000	0.406895000
H	5.444622000	-3.000811000	-0.177094000
H	7.129204000	-2.686299000	0.268377000
H	5.853119000	-2.459942000	1.469178000

H	-5.466641000	-0.840407000	1.987780000

A2

	Coordinates (Angstroms)		
	X	Y	Z
C	4.571752000	-1.304155000	0.049351000
C	3.191540000	-1.388433000	0.022516000
C	2.396123000	-0.241461000	-0.008178000
C	3.022457000	1.012362000	-0.018474000
C	4.397665000	1.110934000	0.006960000
C	5.214535000	-0.046743000	0.049481000
H	5.149607000	-2.219796000	0.067831000
H	2.700396000	-2.356698000	0.023059000
H	2.408284000	1.905680000	-0.049600000
H	4.847996000	2.095954000	-0.008430000
N	1.007284000	-0.451224000	-0.032795000
N	0.307960000	0.588905000	-0.043924000
C	-3.286761000	1.347477000	-0.044951000
C	-3.847537000	0.076333000	-0.124255000
C	-3.046757000	-1.064894000	-0.195448000
C	-1.667697000	-0.933120000	-0.170122000
C	-1.091549000	0.339322000	-0.075578000
C	-1.903543000	1.472855000	-0.022428000
H	-3.928397000	2.222230000	-0.024140000
H	-3.509343000	-2.041728000	-0.294046000
H	-1.019475000	-1.799754000	-0.229066000
H	-1.428910000	2.446968000	0.032225000
S	-5.624348000	-0.101639000	-0.088372000
N	-6.038248000	-0.287816000	1.516413000
H	-5.675378000	-1.144401000	1.920395000
O	-5.951516000	-1.361923000	-0.727033000
O	-6.199113000	1.164917000	-0.499470000
H	-5.832105000	0.533223000	2.075012000
N	6.583604000	0.054241000	0.091396000
C	7.219078000	1.351217000	-0.014723000
H	8.300716000	1.226220000	0.047914000
H	6.987665000	1.849507000	-0.966516000
H	6.913671000	2.014129000	0.804042000
C	7.395395000	-1.143912000	0.045210000
H	8.448830000	-0.868781000	0.109269000
H	7.173259000	-1.807340000	0.889979000
H	7.245380000	-1.708580000	-0.885752000

TSA1^{N2}

	Coordinates (Angstroms)		
	X	Y	Z
C	2.884585000	-0.216170000	-1.200648000
C	1.626440000	-0.780382000	-1.198030000
C	3.541102000	0.077885000	-0.002671000
H	1.111344000	-0.999498000	-2.126274000
C	0.983150000	-1.066656000	0.038628000
C	2.913645000	-0.194464000	1.215744000
C	1.655542000	-0.758274000	1.253802000
N	-0.221613000	-1.598619000	0.053799000
H	3.414306000	0.061583000	2.144532000
H	1.162963000	-0.959387000	2.198201000
N	-1.331282000	-2.112727000	0.031101000
C	-2.451742000	-1.234198000	0.031232000
C	-2.368573000	0.160796000	0.093670000
C	-3.703692000	-1.843522000	-0.039317000
H	-1.395987000	0.641026000	0.152328000
C	-3.513866000	0.927755000	0.085067000
C	-4.859829000	-1.086146000	-0.054205000
H	-3.752270000	-2.927094000	-0.088432000
H	-3.417559000	2.005082000	0.138238000
C	-4.796004000	0.325070000	0.010633000
H	-5.815401000	-1.591099000	-0.118395000
H	3.363467000	0.021334000	-2.145628000
S	5.173518000	0.750031000	-0.029438000
O	5.393172000	1.435182000	1.232563000
O	5.367895000	1.393386000	-1.317455000
N	6.244892000	-0.539409000	-0.018577000
H	6.170312000	-1.084837000	0.834009000
H	6.150844000	-1.115645000	-0.848689000
N	-5.932740000	1.088473000	0.004093000
C	-5.838036000	2.534695000	0.015696000
H	-5.288343000	2.914035000	-0.855737000
H	-6.841205000	2.961088000	-0.009485000
H	-5.341869000	2.899259000	0.923853000
C	-7.230569000	0.454092000	-0.106442000
H	-7.407938000	-0.242998000	0.721997000
H	-8.008003000	1.217630000	-0.071375000
H	-7.337187000	-0.096432000	-1.050873000

A3

	Coordinates (Angstroms)		
	X	Y	Z
C	-4.397667000	1.110932000	0.006940000
C	-3.022459000	1.012361000	-0.018490000
C	-2.396122000	-0.241461000	-0.008165000
C	-3.191538000	-1.388434000	0.022556000
C	-4.571751000	-1.304158000	0.049391000
C	-5.214535000	-0.046745000	0.049487000
H	-4.848001000	2.095950000	-0.008473000
H	-2.408288000	1.905680000	-0.049635000
H	-2.700393000	-2.356698000	0.023124000
H	-5.149604000	-2.219799000	0.067899000
N	-1.007284000	-0.451222000	-0.032777000
N	-0.307962000	0.588908000	-0.043914000
C	3.046756000	-1.064881000	-0.195496000
C	3.847536000	0.076344000	-0.124254000
C	3.286759000	1.347484000	-0.044898000
C	1.903541000	1.472860000	-0.022375000
C	1.091547000	0.339329000	-0.075572000
C	1.667696000	-0.933110000	-0.170165000
H	3.509342000	-2.041712000	-0.294135000
H	3.928396000	2.222235000	-0.024048000
H	1.428907000	2.446970000	0.032316000
H	1.019475000	-1.799742000	-0.229147000
S	5.624347000	-0.101630000	-0.088378000
N	6.038241000	-0.287950000	1.516392000
H	5.832099000	0.533041000	2.075063000
O	6.199116000	1.164962000	-0.499359000
O	5.951523000	-1.361857000	-0.727149000
H	5.675367000	-1.144569000	1.920299000
N	-6.583603000	0.054239000	0.091397000
C	-7.395393000	-1.143915000	0.045209000
H	-8.448831000	-0.868783000	0.109210000
H	-7.245336000	-1.708610000	-0.885731000
H	-7.173295000	-1.807320000	0.890006000
C	-7.219071000	1.351215000	-0.014767000
H	-8.300710000	1.226227000	0.047873000
H	-6.913662000	2.014151000	0.803978000
H	-6.987653000	1.849474000	-0.966574000

Table S17. During the isomerization of CH_3-substituted azobenzenesulfonamide atomic cartesian coordinates of intermediates and transition states at ωB97XD/6-31G(d)

level.

A1

	Coordinates (Angstroms)		
	X	Y	Z
C	3.875920000	1.553877000	0.177802000
C	4.302906000	0.670936000	-0.819972000
C	3.797847000	-0.618585000	-0.898342000
C	2.806543000	-1.032075000	-0.007547000
C	2.382714000	-0.173247000	1.006199000
C	2.923751000	1.103869000	1.094174000
H	5.055244000	0.994538000	-1.534775000
H	4.152652000	-1.315629000	-1.651251000
N	2.379455000	-2.395894000	-0.123354000
H	1.642720000	-0.499916000	1.728821000
H	2.591529000	1.766029000	1.889071000
C	-0.847642000	-1.938202000	0.971437000
C	0.111271000	-1.781492000	-0.029719000
C	-0.066334000	-0.833594000	-1.040249000
C	-1.190115000	-0.020089000	-1.028827000
C	-2.125411000	-0.157311000	-0.005695000
C	-1.958718000	-1.106676000	0.999820000
H	-0.703061000	-2.701090000	1.729764000
N	1.184588000	-2.731250000	-0.069282000
H	0.681010000	-0.727296000	-1.819310000
H	-1.330517000	0.739691000	-1.790706000
H	-2.689879000	-1.183087000	1.797989000
S	-3.585485000	0.871862000	-0.008409000
N	-4.747352000	0.041840000	-0.864977000
H	-4.514190000	-0.078045000	-1.844478000
O	-3.280182000	2.050693000	-0.796116000
O	-4.071421000	0.934781000	1.356373000
H	-5.041406000	-0.816921000	-0.413035000
C	4.453137000	2.943527000	0.265790000
H	5.528404000	2.909446000	0.474319000
H	4.320779000	3.483888000	-0.677814000
H	3.975249000	3.526298000	1.057963000

TSA1^{N1}

	Coordinates (Angstroms)		
	X	Y	Z

C	4.778931000	-0.564886000	-1.152079000
C	3.597547000	0.160156000	-1.200515000
C	3.064081000	0.694722000	-0.009218000
C	3.740218000	0.469003000	1.208189000
C	4.903764000	-0.285094000	1.210608000
C	5.455433000	-0.816478000	0.042808000
H	5.180215000	-0.955403000	-2.084534000
H	3.090027000	0.336299000	-2.142608000
H	3.342762000	0.886806000	2.126435000
H	5.405243000	-0.451124000	2.161484000
N	1.931794000	1.408371000	-0.033956000
N	0.911964000	2.077461000	-0.055934000
C	-2.734248000	1.475406000	-0.058559000
C	-2.792344000	0.086048000	-0.115735000
C	-1.635291000	-0.692366000	-0.173168000
C	-0.396816000	-0.068698000	-0.153165000
C	-0.334579000	1.322514000	-0.081142000
C	-1.489996000	2.095184000	-0.041974000
H	-3.650621000	2.056229000	-0.050974000
H	-1.715884000	-1.771193000	-0.257479000
H	0.520473000	-0.647739000	-0.202832000
H	-1.394608000	3.175663000	-0.004283000
S	-4.388763000	-0.725712000	-0.082781000
N	-4.736066000	-0.996611000	1.520093000
H	-4.112990000	-1.660535000	1.965582000
O	-4.216131000	-2.035817000	-0.678916000
O	-5.369148000	0.235916000	-0.546491000
H	-4.881596000	-0.147826000	2.054801000
C	6.713869000	-1.647161000	0.074498000
H	7.402278000	-1.300695000	0.852442000
H	6.496399000	-2.703334000	0.277446000
H	7.243497000	-1.601195000	-0.882427000

A2

	Coordinates (Angstroms)		
	X	Y	Z
C	5.399438000	-1.253802000	0.082120000
C	4.014410000	-1.365542000	0.054999000
C	3.221159000	-0.220949000	0.000669000
C	3.823178000	1.042407000	-0.030007000
C	5.203806000	1.140787000	-0.004392000
C	6.015061000	-0.001837000	0.050119000
H	6.010114000	-2.151549000	0.128138000

H	3.526683000	-2.334873000	0.079559000
H	3.196771000	1.926378000	-0.071053000
H	5.670801000	2.122239000	-0.027008000
N	1.822380000	-0.448094000	-0.020610000
N	1.122458000	0.586559000	-0.038243000
C	-2.471834000	1.345315000	-0.036348000
C	-3.030889000	0.074171000	-0.120952000
C	-2.230936000	-1.067392000	-0.196624000
C	-0.851892000	-0.935769000	-0.169408000
C	-0.279013000	0.337037000	-0.069750000
C	-1.088238000	1.471255000	-0.012855000
H	-3.114286000	2.219297000	-0.013072000
H	-2.693696000	-2.043500000	-0.300594000
H	-0.203040000	-1.801741000	-0.231583000
H	-0.613518000	2.445070000	0.045247000
S	-4.810007000	-0.104230000	-0.093523000
N	-5.229383000	-0.306371000	1.505606000
H	-4.877057000	-1.169037000	1.905356000
O	-5.131202000	-1.357794000	-0.747305000
O	-5.379824000	1.167199000	-0.494855000
H	-5.036574000	0.509593000	2.075872000
C	7.516332000	0.126962000	0.049901000
H	7.893118000	0.282161000	-0.968155000
H	7.842173000	0.980747000	0.652387000
H	7.995173000	-0.772876000	0.446447000

TSA1^{N2}

	Coordinates (Angstroms)		
	X	Y	Z
C	2.155899000	-0.201952000	-1.204921000
C	0.857237000	-0.668052000	-1.216595000
C	2.819671000	0.038133000	-0.000001000
H	0.337060000	-0.847155000	-2.150422000
C	0.186812000	-0.906368000	0.012831000
C	2.160847000	-0.183018000	1.211196000
C	0.862114000	-0.648786000	1.235556000
N	-1.054201000	-1.358696000	0.017788000
H	2.669408000	0.033839000	2.145526000
H	0.345927000	-0.813350000	2.174265000
N	-2.194226000	-1.791997000	0.015603000
C	-3.255553000	-0.818178000	0.008083000
C	-3.055434000	0.564111000	0.018747000
C	-4.540520000	-1.348293000	-0.012660000

H	-2.047575000	0.968632000	0.034282000
C	-4.155583000	1.404341000	0.008163000
C	-5.636899000	-0.493314000	-0.024414000
H	-4.662014000	-2.426907000	-0.021968000
H	-4.007147000	2.481031000	0.015433000
C	-5.461481000	0.891094000	-0.012746000
H	-6.640930000	-0.907607000	-0.043577000
H	2.660642000	0.000087000	-2.144611000
S	4.503641000	0.578338000	-0.007980000
O	4.762640000	1.234053000	1.261608000
O	4.756767000	1.213011000	-1.289453000
N	5.464611000	-0.792667000	0.001233000
H	5.346165000	-1.336920000	0.849384000
H	5.340882000	-1.352157000	-0.836178000
C	-6.641654000	1.827319000	-0.007822000
H	-6.733402000	2.330402000	0.961605000
H	-6.530776000	2.605742000	-0.769865000
H	-7.577777000	1.295741000	-0.198311000

A3

	Coordinates (Angstroms)		
	X	Y	Z
C	2.230937000	-1.067393000	-0.196617000
C	0.851892000	-0.935770000	-0.169401000
C	3.030889000	0.074170000	-0.120952000
H	0.203040000	-1.801742000	-0.231572000
C	0.279013000	0.337036000	-0.069749000
C	2.471834000	1.345315000	-0.036354000
C	1.088237000	1.471255000	-0.012860000
N	-1.122458000	0.586559000	-0.038242000
H	3.114286000	2.219297000	-0.013083000
H	0.613518000	2.445070000	0.045238000
N	-1.822380000	-0.448094000	-0.020612000
C	-3.221159000	-0.220949000	0.000668000
C	-3.823177000	1.042407000	-0.030002000
C	-4.014411000	-1.365542000	0.054993000
H	-3.196771000	1.926378000	-0.071044000
C	-5.203806000	1.140787000	-0.004386000
C	-5.399438000	-1.253802000	0.082114000
H	-3.526684000	-2.334873000	0.079549000
H	-5.670800000	2.122239000	-0.026998000
C	-6.015061000	-0.001837000	0.050119000
H	-6.010115000	-2.151549000	0.128129000

H	2.693696000	-2.043502000	-0.300583000
S	4.810007000	-0.104230000	-0.093523000
O	5.379824000	1.167198000	-0.494862000
O	5.131202000	-1.357796000	-0.747300000
N	5.229384000	-0.306365000	1.505606000
H	5.036572000	0.509600000	2.075870000
H	4.877062000	-1.169031000	1.905358000
C	-7.516332000	0.126963000	0.049902000
H	-7.842173000	0.980750000	0.652384000
H	-7.893119000	0.282158000	-0.968155000
H	-7.995172000	-0.772874000	0.446451000

Table S18. During the isomerization of CH_3-substituted azobenzenesulfonamide atomic cartesian coordinates of intermediates and transition states at ωB97XD/6-31G(d) level.

A1

	Coordinates (Angstroms)		
	X	Y	Z
C	-3.317512000	-0.310935000	0.077537000
C	-3.484842000	0.608843000	-0.958018000
C	-2.714566000	1.760602000	-0.990530000
C	-1.738549000	1.967207000	-0.014760000
C	-1.583236000	1.060330000	1.032615000
C	-2.379855000	-0.077285000	1.078053000
H	-4.226353000	0.428052000	-1.729413000
H	-2.849560000	2.502470000	-1.770973000
N	-1.024164000	3.210390000	-0.074442000
H	-0.845043000	1.240382000	1.806594000
H	-2.260636000	-0.788283000	1.887400000
C	2.028733000	2.034437000	0.980369000
C	1.046097000	2.102592000	-0.007078000
C	0.984005000	1.139762000	-1.016671000
C	1.886577000	0.085600000	-1.014355000
C	2.840084000	0.001668000	-0.002540000
C	2.914458000	0.965790000	0.999604000
H	2.076363000	2.812776000	1.735035000
N	0.213903000	3.271375000	-0.013169000
H	0.227818000	1.209136000	-1.791060000
H	1.834760000	-0.686938000	-1.774490000
H	3.653940000	0.871484000	1.787929000
S	4.011647000	-1.349236000	-0.008777000
N	5.313954000	-0.841749000	-0.909673000
H	5.099675000	-0.700617000	-1.890343000
O	3.409531000	-2.434599000	-0.757684000
O	4.501269000	-1.494958000	1.347918000
H	5.824425000	-0.073834000	-0.488542000
C	-4.195926000	-1.532855000	0.108479000
F	-3.800977000	-2.419165000	1.033711000
F	-5.472894000	-1.210361000	0.379290000
F	-4.197994000	-2.159923000	-1.080647000

TSA1^{N1}

	Coordinates (Angstroms)		
	X	Y	Z
C	3.813903000	0.166722000	-1.182081000
C	2.590410000	0.807867000	-1.206164000
C	1.949324000	1.126707000	0.015355000
C	2.571868000	0.782968000	1.238556000
C	3.795501000	0.139632000	1.220688000
C	4.429845000	-0.179565000	0.021196000
H	4.295727000	-0.075581000	-2.123975000
H	2.115091000	1.069105000	-2.144497000
H	2.083045000	1.025930000	2.174807000
H	4.262665000	-0.121613000	2.164332000
N	0.768314000	1.736368000	0.013025000
N	-0.304998000	2.313233000	0.021477000
C	-3.883369000	1.408527000	0.020191000
C	-3.823963000	0.024276000	-0.109748000
C	-2.606437000	-0.649105000	-0.217782000
C	-1.424902000	0.075066000	-0.174210000
C	-1.480787000	1.461185000	-0.029481000
C	-2.696210000	2.131096000	0.058957000
H	-4.845101000	1.908320000	0.066025000
H	-2.595605000	-1.724922000	-0.358712000
H	-0.464186000	-0.422756000	-0.263279000
H	-2.693390000	3.212285000	0.152119000
S	-5.347400000	-0.921656000	-0.117379000
N	-5.663857000	-1.301119000	1.467106000
H	-4.996464000	-1.941419000	1.881112000
O	-5.064599000	-2.178302000	-0.780822000
O	-6.404285000	-0.021179000	-0.531494000
H	-5.890248000	-0.501958000	2.047530000
C	5.778562000	-0.826203000	0.014318000
F	5.911598000	-1.695459000	-1.005961000
F	6.776502000	0.071214000	-0.119012000
F	6.018484000	-1.502362000	1.152874000

A2

	Coordinates (Angstroms)		
	X	Y	Z
C	-4.256780000	1.319905000	0.072163000
C	-2.871448000	1.425049000	0.046458000
C	-2.083913000	0.276482000	0.001319000

C	-2.680744000	-0.988583000	-0.021064000
C	-4.061179000	-1.091543000	0.003812000
C	-4.848976000	0.061465000	0.051027000
H	-4.872165000	2.211529000	0.112017000
H	-2.380919000	2.392490000	0.063544000
H	-2.052884000	-1.871185000	-0.055613000
H	-4.534057000	-2.067678000	-0.008797000
N	-0.680195000	0.503633000	-0.021896000
N	0.010946000	-0.535399000	-0.027249000
C	3.592626000	-1.341249000	-0.045219000
C	4.167302000	-0.076385000	-0.114815000
C	3.383059000	1.077098000	-0.172798000
C	2.002462000	0.963929000	-0.143381000
C	1.414800000	-0.303122000	-0.059507000
C	2.207474000	-1.449460000	-0.018293000
H	4.223527000	-2.223816000	-0.036190000
H	3.858849000	2.047965000	-0.265319000
H	1.365967000	1.839803000	-0.192514000
H	1.720265000	-2.417618000	0.029009000
S	5.950673000	0.078147000	-0.097805000
N	6.385379000	0.242106000	1.499450000
H	6.057957000	1.103500000	1.921932000
O	6.279839000	1.340351000	-0.729858000
O	6.496811000	-1.193077000	-0.530386000
H	6.196705000	-0.582971000	2.057461000
C	-6.348952000	-0.069982000	0.020954000
F	-6.764618000	-1.145349000	0.710522000
F	-6.957914000	1.006305000	0.542669000
F	-6.801301000	-0.211464000	-1.237055000

TSA1^{N2}

	Coordinates (Angstroms)		
	X	Y	Z
C	-3.172507000	0.168869000	-1.211365000
C	-1.929876000	0.769446000	-1.250022000
C	-3.808523000	-0.080401000	0.005762000
H	-1.428805000	0.955317000	-2.192895000
C	-1.293546000	1.133495000	-0.035768000
C	-3.181520000	0.270077000	1.202409000
C	-1.939471000	0.872869000	1.199798000
N	-0.096930000	1.701187000	-0.053125000
H	-3.666948000	0.047463000	2.147456000
H	-1.445017000	1.137617000	2.127139000

N	0.994366000	2.242789000	-0.056433000
C	2.142692000	1.359155000	-0.032253000
C	2.051632000	-0.033252000	-0.072068000
C	3.374270000	1.998206000	0.030972000
H	1.080146000	-0.514867000	-0.124130000
C	3.213962000	-0.784370000	-0.046447000
C	4.540969000	1.240863000	0.059945000
H	3.402715000	3.082538000	0.059619000
H	3.163450000	-1.867923000	-0.076185000
C	4.455960000	-0.145945000	0.020620000
H	5.508144000	1.726200000	0.115056000
H	-3.649614000	-0.134681000	-2.138054000
S	-5.417674000	-0.819194000	0.030790000
O	-5.605207000	-1.412434000	1.342634000
O	-5.574990000	-1.565685000	-1.204310000
N	-6.536270000	0.419956000	-0.058695000
H	-6.501789000	1.034046000	0.747943000
H	-6.485707000	0.925022000	-0.936964000
C	5.700356000	-0.997291000	0.021349000
F	5.860377000	-1.617177000	-1.159502000
F	6.806887000	-0.277314000	0.253002000
F	5.631983000	-1.954011000	0.961160000

A3

	Coordinates (Angstroms)		
	X	Y	Z
C	-3.383059000	1.077097000	-0.172803000
C	-2.002461000	0.963928000	-0.143386000
C	-4.167301000	-0.076385000	-0.114815000
H	-1.365966000	1.839801000	-0.192523000
C	-1.414800000	-0.303123000	-0.059507000
C	-3.592626000	-1.341249000	-0.045214000
C	-2.207474000	-1.449461000	-0.018289000
N	-0.010946000	-0.535400000	-0.027249000
H	-4.223527000	-2.223816000	-0.036182000
H	-1.720265000	-2.417619000	0.029017000
N	0.680194000	0.503632000	-0.021893000
C	2.083913000	0.276481000	0.001321000
C	2.680744000	-0.988583000	-0.021068000
C	2.871447000	1.425049000	0.046464000
H	2.052884000	-1.871185000	-0.055619000
C	4.061180000	-1.091543000	0.003808000
C	4.256780000	1.319906000	0.072168000

H	2.380919000	2.392490000	0.063554000
H	4.534058000	-2.067677000	-0.008805000
C	4.848976000	0.061465000	0.051027000
H	4.872164000	2.211529000	0.112025000
H	-3.858848000	2.047964000	-0.265328000
S	-5.950672000	0.078148000	-0.097805000
O	-6.496812000	-1.193080000	-0.530379000
O	-6.279838000	1.340348000	-0.729865000
N	-6.385378000	0.242114000	1.499449000
H	-6.196710000	-0.582963000	2.057462000
H	-6.057949000	1.103507000	1.921930000
C	6.348951000	-0.069982000	0.020953000
F	6.957914000	1.006306000	0.542667000
F	6.801300000	-0.211464000	-1.237056000
F	6.764618000	-1.145349000	0.710521000

Table S19. During the isomerization of CN-substituted azobenzenesulfonamide atomic cartesian coordinates of intermediates and transition states at ωB97XD/6-31G(d) level.

A1

	Coordinates (Angstroms)		
	X	Y	Z
C	3.826344000	1.132654000	0.126471000
C	4.147279000	0.246424000	-0.908162000
C	3.537864000	-0.997331000	-0.961426000
C	2.573316000	-1.339468000	-0.013522000
C	2.265418000	-0.467266000	1.032784000
C	2.894727000	0.765947000	1.104088000
H	4.882854000	0.530838000	-1.652496000
H	3.796788000	-1.712749000	-1.734906000
N	2.048741000	-2.672135000	-0.089166000
H	1.541443000	-0.752511000	1.787813000
H	2.662571000	1.452429000	1.910942000
C	-1.137285000	-1.973700000	0.980901000
C	-0.164858000	-1.889311000	-0.015791000
C	-0.260414000	-0.929548000	-1.025192000
C	-1.320032000	-0.032385000	-1.018727000
C	-2.267946000	-0.098926000	-0.001114000
C	-2.179427000	-1.057675000	1.005691000
H	-1.057356000	-2.748072000	1.737003000
N	0.834091000	-2.918430000	-0.030992000
H	0.491702000	-0.883453000	-1.805455000
H	-1.399443000	0.734632000	-1.782050000
H	-2.918232000	-1.077775000	1.800081000
S	-3.650447000	1.036195000	-0.012395000
N	-4.867009000	0.288547000	-0.862794000
H	-4.656865000	0.157100000	-1.845669000
O	-3.255276000	2.181763000	-0.808135000
O	-4.126351000	1.140945000	1.352748000
H	-5.235068000	-0.538989000	-0.407646000
C	4.469638000	2.415157000	0.194077000
N	4.990468000	3.449209000	0.244857000

TSA1^{N1}

	Coordinates (Angstroms)		
	X	Y	Z

C	4.653646000	-0.133738000	-1.194285000
C	3.462610000	0.562133000	-1.191993000
C	2.823170000	0.845426000	0.041126000
C	3.417390000	0.412105000	1.253033000
C	4.609125000	-0.281554000	1.214746000
C	5.246597000	-0.568522000	-0.000432000
H	5.139429000	-0.346246000	-2.141094000
H	3.011063000	0.898574000	-2.117805000
H	2.931433000	0.633658000	2.195971000
H	5.060190000	-0.610253000	2.145414000
N	1.677798000	1.512047000	0.061183000
N	0.632606000	2.136823000	0.082118000
C	-2.985661000	1.442051000	-0.022375000
C	-3.005260000	0.053209000	-0.105559000
C	-1.827593000	-0.694901000	-0.145855000
C	-0.606390000	-0.041484000	-0.083598000
C	-0.584127000	1.350109000	0.013926000
C	-1.759402000	2.093649000	0.039762000
H	-3.916867000	1.998542000	-0.029880000
H	-1.877922000	-1.773757000	-0.250136000
H	0.324156000	-0.599738000	-0.119601000
H	-1.693670000	3.175058000	0.100932000
S	-4.582745000	-0.800254000	-0.141393000
N	-4.973400000	-1.116045000	1.439222000
H	-4.364878000	-1.786754000	1.893610000
O	-4.352945000	-2.089213000	-0.762110000
O	-5.567266000	0.150861000	-0.616194000
H	-5.176623000	-0.291591000	1.991969000
C	6.479314000	-1.293584000	-0.020617000
N	7.478537000	-1.883682000	-0.035088000

A2

	Coordinates (Angstroms)		
	X	Y	Z
C	5.164196000	-1.282491000	0.029511000
C	3.781427000	-1.395374000	0.004529000
C	2.984919000	-0.250888000	-0.014579000
C	3.569863000	1.020208000	-0.011102000
C	4.948310000	1.138533000	0.013349000
C	5.749299000	-0.012918000	0.034199000
H	5.791749000	-2.166832000	0.044726000
H	3.297699000	-2.366215000	-0.000593000
H	2.933039000	1.896836000	-0.027920000

H	5.417121000	2.116645000	0.016071000
N	1.583033000	-0.489453000	-0.038290000
N	0.885399000	0.545386000	-0.042580000
C	-2.697543000	1.338750000	-0.077671000
C	-3.268095000	0.070624000	-0.113090000
C	-2.480530000	-1.081679000	-0.142376000
C	-1.100275000	-0.963707000	-0.118576000
C	-0.516787000	0.307227000	-0.068956000
C	-1.312784000	1.452085000	-0.055025000
H	-3.331279000	2.219209000	-0.090563000
H	-2.953703000	-2.055950000	-0.208137000
H	-0.461976000	-1.839177000	-0.145822000
H	-0.828568000	2.422627000	-0.033088000
S	-5.051668000	-0.088675000	-0.089991000
N	-5.484967000	-0.204656000	1.510883000
H	-5.159676000	-1.052884000	1.960558000
O	-5.376104000	-1.370684000	-0.683234000
O	-5.600406000	1.167544000	-0.561295000
H	-5.303034000	0.637936000	2.044244000
C	7.180213000	0.115323000	0.060820000
N	8.334266000	0.219805000	0.082901000

TSA1^{N2}

	Coordinates (Angstroms)		
	X	Y	Z
C	-2.364171000	-0.233863000	1.200733000
C	-1.084471000	-0.752384000	1.198762000
C	-3.018663000	0.057829000	0.003270000
H	-0.570030000	-0.973146000	2.126741000
C	-0.430047000	-0.986649000	-0.037004000
C	-2.372990000	-0.162640000	-1.213864000
C	-1.092661000	-0.679221000	-1.251924000
N	0.799430000	-1.482898000	-0.052926000
H	-2.874308000	0.095184000	-2.141593000
H	-0.585442000	-0.844560000	-2.195321000
N	1.922427000	-1.954858000	-0.050419000
C	3.014629000	-1.000794000	-0.030976000
C	2.840360000	0.381998000	-0.089431000
C	4.282436000	-1.567424000	0.046705000
H	1.842323000	0.804158000	-0.154633000
C	3.953658000	1.205532000	-0.067605000
C	5.401315000	-0.746057000	0.073627000
H	4.373339000	-2.647775000	0.087680000

H	3.842796000	2.283299000	-0.115559000
C	5.234839000	0.641099000	0.015712000
H	6.397514000	-1.169252000	0.138299000
H	-2.858646000	-0.032240000	2.145809000
S	-4.678317000	0.677985000	0.028259000
O	-4.902022000	1.375328000	-1.224978000
O	-4.893938000	1.292419000	1.325771000
N	-5.701511000	-0.642532000	-0.011917000
H	-5.623901000	-1.169032000	-0.875429000
H	-5.616828000	-1.226666000	0.812983000
C	6.388720000	1.498113000	0.038668000
N	7.319113000	2.188438000	0.057045000

A3

	Coordinates (Angstroms)		
	X	Y	Z
C	-5.164201000	-1.282488000	0.029440000
C	-3.781433000	-1.395377000	0.004430000
C	-2.984921000	-0.250892000	-0.014617000
C	-3.569858000	1.020206000	-0.011043000
C	-4.948305000	1.138537000	0.013440000
C	-5.749298000	-0.012912000	0.034225000
H	-5.791758000	-2.166827000	0.044606000
H	-3.297710000	-2.366219000	-0.000764000
H	-2.933029000	1.896832000	-0.027813000
H	-5.417110000	2.116650000	0.016240000
N	-1.583035000	-0.489462000	-0.038361000
N	-0.885400000	0.545377000	-0.042666000
C	2.480532000	-1.081692000	-0.142317000
C	3.268096000	0.070614000	-0.113098000
C	2.697541000	1.338742000	-0.077775000
C	1.312783000	1.452077000	-0.055152000
C	0.516787000	0.307216000	-0.069016000
C	1.100277000	-0.963720000	-0.118544000
H	2.953708000	-2.055967000	-0.208003000
H	3.331277000	2.219201000	-0.090718000
H	0.828565000	2.422619000	-0.033286000
H	0.461981000	-1.839193000	-0.145739000
S	5.051670000	-0.088681000	-0.089957000
N	5.484941000	-0.204521000	1.510936000
H	5.302989000	0.638111000	2.044225000
O	5.600413000	1.167499000	-0.561360000
O	5.376120000	-1.370741000	-0.683081000

H	5.159657000	-1.052718000	1.960675000
C	-7.180211000	0.115333000	0.060881000
N	-8.334263000	0.219818000	0.082990000

Table S20. During the isomerization of NO_2-substituted azobenzenesulfonamide atomic cartesian coordinates of intermediates and transition states at ωB97XD/6-31G(d) level.

A1

	Coordinates (Angstroms)		
	X	Y	Z
C	-3.598001000	-0.656358000	0.093529000
C	-3.819596000	0.229064000	-0.953952000
C	-3.105526000	1.416990000	-0.981108000
C	-2.152020000	1.678015000	0.004147000
C	-1.953649000	0.784419000	1.059476000
C	-2.686242000	-0.392331000	1.107583000
H	-4.550955000	-0.011332000	-1.715190000
H	-3.275022000	2.149540000	-1.763208000
N	-1.521268000	2.964707000	-0.040163000
H	-1.232408000	1.009590000	1.837294000
H	-2.556100000	-1.107104000	1.910690000
C	1.615821000	2.010511000	0.990830000
C	0.621297000	2.005671000	0.012823000
C	0.619580000	1.041766000	-0.997370000
C	1.601424000	0.060377000	-1.008095000
C	2.570060000	0.049013000	-0.007704000
C	2.580099000	1.012419000	0.998101000
H	1.613443000	2.790300000	1.745404000
N	-0.291247000	3.112253000	0.021905000
H	-0.145093000	1.057274000	-1.766323000
H	1.602854000	-0.711074000	-1.771032000
H	3.333112000	0.973193000	1.778149000
S	3.850688000	-1.199906000	-0.038878000
N	5.098858000	-0.573600000	-0.939305000
H	4.872884000	-0.445091000	-1.918969000
O	3.335096000	-2.320271000	-0.800115000
O	4.357998000	-1.321134000	1.313461000
H	5.550849000	0.226993000	-0.512586000
N	-4.365700000	-1.907251000	0.139419000
O	-4.172484000	-2.653885000	1.085496000
O	-5.149182000	-2.122698000	-0.771934000

TSA1^{N1}

	Coordinates (Angstroms)		
	X	Y	Z
C	4.235908000	0.086364000	-1.193014000
C	3.027273000	0.748099000	-1.188622000
C	2.377491000	1.006773000	0.047416000
C	2.980591000	0.584831000	1.261999000
C	4.189683000	-0.075047000	1.225080000
C	4.815713000	-0.326036000	0.005510000
H	4.744931000	-0.118864000	-2.127066000
H	2.567351000	1.076508000	-2.113024000
H	2.485392000	0.788998000	2.203863000
H	4.663731000	-0.404370000	2.141889000
N	1.215201000	1.636747000	0.067636000
N	0.152109000	2.229321000	0.091035000
C	-3.442609000	1.422844000	0.001746000
C	-3.418109000	0.035903000	-0.108017000
C	-2.217502000	-0.672702000	-0.174098000
C	-1.017492000	0.018448000	-0.109500000
C	-1.039474000	1.407899000	0.015914000
C	-2.237560000	2.112896000	0.065344000
H	-4.391069000	1.949229000	0.013568000
H	-2.233649000	-1.750376000	-0.299221000
H	-0.070155000	-0.508928000	-0.165595000
H	-2.206710000	3.194491000	0.146839000
S	-4.967849000	-0.867958000	-0.145031000
N	-5.336430000	-1.217651000	1.433068000
H	-4.706301000	-1.876885000	1.874408000
O	-4.700501000	-2.139465000	-0.785727000
O	-5.985102000	0.058035000	-0.599555000
H	-5.564994000	-0.409241000	1.999302000
N	6.083270000	-1.026025000	-0.016340000
O	6.606754000	-1.230627000	-1.104972000
O	6.563167000	-1.376895000	1.055152000

A2

	Coordinates (Angstroms)		
	X	Y	Z
C	4.702553000	-1.301575000	0.015031000
C	3.318907000	-1.410886000	-0.009624000
C	2.524628000	-0.264213000	-0.024141000
C	3.109799000	1.007163000	-0.016473000

C	4.489023000	1.126199000	0.007673000
C	5.261547000	-0.031708000	0.023647000
H	5.345043000	-2.172972000	0.026937000
H	2.834191000	-2.381012000	-0.018017000
H	2.474048000	1.884407000	-0.029679000
H	4.975898000	2.093445000	0.014216000
N	1.121513000	-0.502023000	-0.047088000
N	0.426031000	0.534032000	-0.048868000
C	-3.154515000	1.336493000	-0.081638000
C	-3.728173000	0.069688000	-0.112311000
C	-2.943749000	-1.084825000	-0.139547000
C	-1.563176000	-0.970495000	-0.118278000
C	-0.976728000	0.299249000	-0.073266000
C	-1.769410000	1.446404000	-0.061318000
H	-3.786026000	2.218523000	-0.096149000
H	-3.419606000	-2.058025000	-0.201593000
H	-0.927484000	-1.847879000	-0.143830000
H	-1.282713000	2.415760000	-0.042817000
S	-5.512451000	-0.085241000	-0.085971000
N	-5.943310000	-0.194956000	1.515709000
H	-5.621016000	-1.042874000	1.968035000
O	-5.840153000	-1.368377000	-0.674827000
O	-6.058190000	1.170921000	-0.560781000
H	-5.760144000	0.648971000	2.046455000
N	6.725976000	0.096126000	0.050828000
O	7.382660000	-0.932849000	0.068629000
O	7.194595000	1.223341000	0.054402000

TSA1^{N2}

	Coordinates (Angstroms)		
	X	Y	Z
C	-2.785129000	-0.157952000	1.213849000
C	-1.522418000	-0.715731000	1.262333000
C	-3.423983000	0.058606000	-0.007466000
H	-1.019708000	-0.877669000	2.208725000
C	-0.871885000	-1.069081000	0.053761000
C	-2.781047000	-0.279786000	-1.198752000
C	-1.519295000	-0.840740000	-1.186316000
N	0.342989000	-1.601355000	0.079299000
H	-3.269484000	-0.081445000	-2.147616000
H	-1.012973000	-1.097552000	-2.109451000
N	1.450747000	-2.107410000	0.084323000
C	2.570574000	-1.183283000	0.053692000

C	2.432966000	0.203670000	0.117123000
C	3.821434000	-1.785184000	-0.037503000
H	1.447496000	0.652119000	0.193771000
C	3.567333000	0.999058000	0.086351000
C	4.963532000	-0.995285000	-0.075267000
H	3.882956000	-2.867396000	-0.080607000
H	3.505912000	2.078974000	0.137556000
C	4.810973000	0.382484000	-0.011612000
H	5.954114000	-1.425528000	-0.151241000
H	-3.276314000	0.136848000	2.135964000
S	-5.059600000	0.739915000	-0.045289000
O	-5.256200000	1.325651000	-1.358880000
O	-5.251256000	1.479880000	1.188562000
N	-6.132076000	-0.538420000	0.035470000
H	-6.074247000	-1.149523000	-0.771954000
H	-6.074346000	-1.041163000	0.914492000
N	6.016411000	1.228400000	-0.045516000
O	7.095040000	0.666665000	-0.141316000
O	5.858086000	2.435870000	0.023983000

A3

	Coordinates (Angstroms)		
	X	Y	Z
C	-4.488870000	1.126188000	0.008033000
C	-3.109673000	1.007063000	-0.016380000
C	-2.524579000	-0.264340000	-0.024538000
C	-3.318946000	-1.410949000	-0.010225000
C	-4.702568000	-1.301554000	0.014681000
C	-5.261495000	-0.031659000	0.023779000
H	-4.975669000	2.093468000	0.014958000
H	-2.473860000	1.884270000	-0.029445000
H	-2.834290000	-2.381102000	-0.018993000
H	-5.345112000	-2.172912000	0.026430000
N	-1.121546000	-0.502228000	-0.047840000
N	-0.426073000	0.533824000	-0.049735000
C	2.943753000	-1.084913000	-0.139107000
C	3.728111000	0.069643000	-0.112269000
C	3.154403000	1.336430000	-0.082221000
C	1.769295000	1.446273000	-0.062149000
C	0.976650000	0.299091000	-0.073741000
C	1.563180000	-0.970636000	-0.118099000
H	3.419668000	-2.058112000	-0.200655000
H	3.785880000	2.218473000	-0.097012000

H	1.282533000	2.415608000	-0.044139000
H	0.927533000	-1.848062000	-0.143382000
S	5.512384000	-0.085195000	-0.085690000
N	5.943173000	-0.194221000	1.515993000
H	5.760020000	0.649921000	2.046384000
O	6.058183000	1.170777000	-0.560927000
O	5.840269000	-1.368574000	-0.673918000
H	5.621028000	-1.042017000	1.968634000
N	-6.725873000	0.096263000	0.051240000
O	-7.194457000	1.223479000	0.055262000
O	-7.382646000	-0.932645000	0.068842000