Supporting Information

Dithiothreitol-Assisted Polysulfide Reduction in the Interlayer of Lithium-Sulfur Batteries: A First-Principles Study

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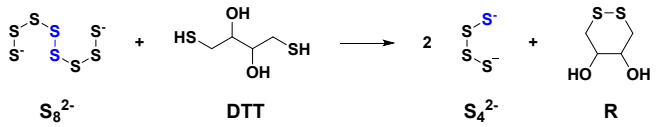
Details of Model Reaction

Ref 64



(1)

Note: Referring to the previous work, the polysulfide in the discharge process exists in the form of ions. Lithium atoms of lithium polysulfide chelate with the DOL and DME molecules, and generate polysulfide dianion (Figure S1). For the existence form of DTT in the system, DTT may react with the alkali anion NO_3^- and $TFSI^-$ in the electrolyte to obtain the thiol anion of DTT. But the energy requirements are high (Figure S2). Therefore DTT participates in the reaction in the form of a neutral molecule.

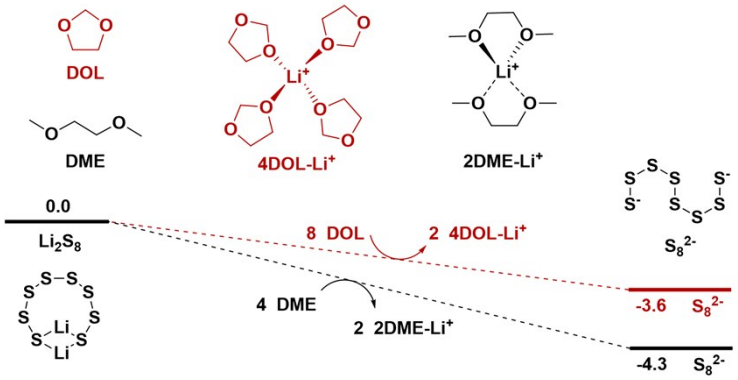


Figure S1

Note: As shown in the red line, the substrate Li_2S_8 reacts with the two molecules of DOL to form 4DOL-Li^+ and S_8^{2-} dianion. The energy barrier of this process is -3.6 kcal/mol. As shown in the black line, the DME molecule captures the lithium atoms of Li_2S_8 to obtain 2DME-Li^+ and S_8^{2-} with free energy of -4.3 kcal/mol.

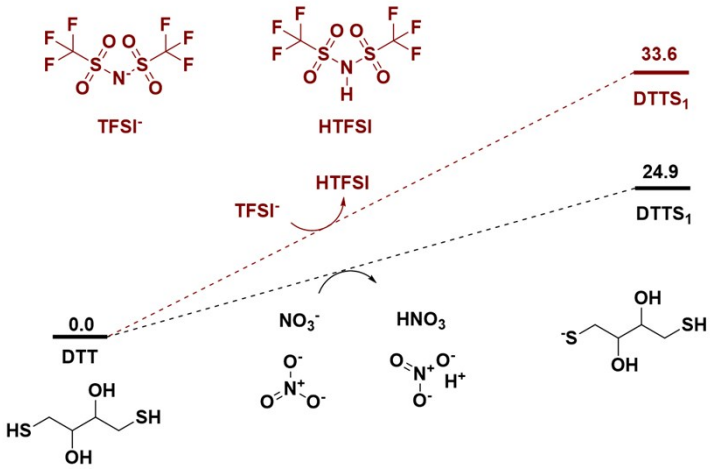


Figure S2

Note: As shown in the red line, the substrate DTT reacts with the $TFSI^-$ anion to form HTFSI and deprotonated **$DTTS_1$**. The energy barrier of this process is 33.6 kcal/mol. As shown in the black line, the NO_3^- anion captures the proton of DTT to obtain HNO_3 and **$DTTS_1$** with free energy of 24.9 kcal/mol.

The rate-determining step of the reaction between DTT and substrate Li_2S_8

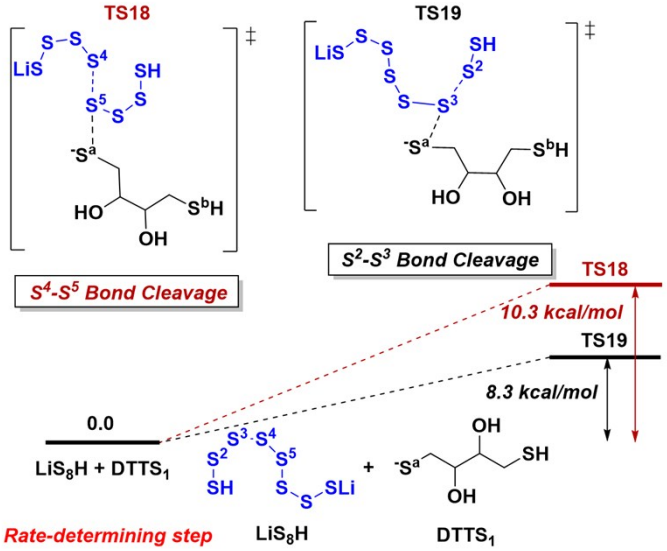


Figure S3

Note: The red line indicates the energy demand of the S^4-S^5 bond cleavage transition state of the rate-determining step. The terminal -$^aS^-$ in **$DTTS_1$** nucleophilically attacks the S^5 atom in LiS_8H, resulting in the cleavage of S^4-S^5 bond. The corresponding transition state is **TS18** in which the formation of S^a-S^5 and cleavage of S^4-S^5 occur simultaneously. The free energy barrier of the S^4-S^5 bond cleavage step is 10.3 kcal/mol (**$DTTS_1$**+LiS_8H→**TS18**, the fixed optimization result is used to estimate the energy).

As shown in the black line, the -$^aS^-$ of **$DDTS_1$** nucleophilically attacks the S^3 atom of the LiS_8H chain, causing the breakage of S^2-S^3 bond. The corresponding transition state is **TS19** in which -$^aS^-$ in the DTT is bonded to the S^3 atomic portion and the S^2-S^3 atom is partially broken. The energy barrier of S^2-S^3 bond cleavage is lower than that of S^4-S^5 bond cleavage (8.3 vs 10.3 kcal/mol, the fixed optimization result is used to estimate the energy).

Therefore, S_2&S_6 fragments are favorably obtained in the presence of Li^+. The Li^+ does not affect the favorable mechanism.

Indeed, our calculation results of generating S_2^{2-}&S_6^{2-} are different from that of generating $2S_4^{2-}$ in ref 66. The difference between them is understandable, because they are different reactions. The research object reaction of our study is DTT involved polysulfide reduction, whereas DTT is not involved in ref 66. When we chose the model reaction to start our investigation, we did not know the favorable mechanism for DTT involved polysulfide reduction, the previous works become our basis to choose the model reaction. Additionally, the method of obtaining favorable mechanism by investigating the the model reaction is common in theoretical calculation works. (For example, the work of *ACS Catal.* **2015**, *5*, 1414-1423, *ACS Catal.* **2016**, *6*, 798-808, *J. Am. Chem. Soc.* **2018**, *140*, 10995-11005, *Org. Lett.* **2018**, *20*, 1730-1734, and so on.)

The Scanning Processes of Proton Transfer

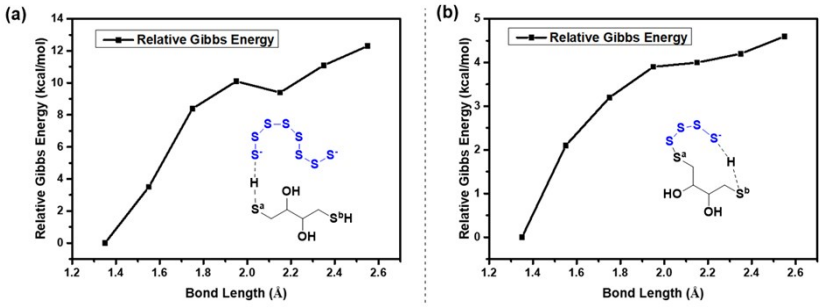


Figure S4

Note: We investigate the reaction processes of DTT deprotonation and intramolecular proton transfer. Firstly, for the DTT deprotonation process, the proton in DTT bonds to the terminal -S^- of the substrate S_8^{2-}, and S^a-H bond in DTT breaks. However, all attempts to locate the transition state fail because the proton always transfers automatically during the relaxed optimization. To estimate the energy demand, we fixed the S^a-H bond in DTT and gradually lengthen it to examine the change in energy during the process. The fixed S^a-H bonds are 1.35, 1.55, 1.75, 1.95, 2.15, 2.35, and 2.55 Å, respectively. The corresponding energies increase as the S^a-H bond elongate (Figure S4a). During the scanning process, corresponding energy increases 12.3 kcal/mol relatively, so we speculate that the DTT deprotonation process is a process of no energy barrier.

Similarly, we investigate the process of intramolecular proton transfer of the intermediate **Int3**. As shown in Figure S4b, we fixed the S^b-H bond and gradually lengthen it, fixing S^b-H to 1.35, 1.55, 1.75, 1.95, 2.15, 2.35, and 2.55 Å, respectively. The corresponding energies increase as the S^b-H bond elongate. During the scanning process, corresponding energy increases 4.6 kcal/mol relatively, so the intramolecular proton transfer process is also a process of no energy barrier, and it is not necessary to investigate the transition state of the process.

Gibbs Free Energy Corrections and Electronic Energies in Solvate of related compounds and Transition States

	Thermal Correction of Gibbs Free Energies (Hartree)	Electronic Energy in solvent (Hartree)
DTT	0.104277	-1105.233633350
$DTTS_1$	0.095740	-1104.759680620
R	0.091834	-1104.039847520
S_8^{2-}	-0.034455	-3185.768016850
S_6^{2-}	-0.030942	-2389.388988440
S_4^{2-}	-0.027430	-1593.000413490
S_2^{2-}	-0.020826	-796.590598066
HS_8^-	-0.025658	-3186.238419200
HS_6^-	-0.020649	-2389.865886200
HS_4^-	-0.019155	-1593.481579020
HS_2^-	-0.015591	-797.096717999
HS^-	-0.011848	-398.912047426
Int1	0.091811	-4291.018367590
Int2	0.085782	-4290.995947180
Int3	0.090599	-2697.534062490
Int4	0.089958	-2697.508403430
Int5	0.088341	-3493.911846470
Int6	0.086493	-3493.884296000
Int7	0.090599	-2697.534062490
Int8	0.092777	-1901.148141620

Int9	0.093971	-1502.952870680
TS1	0.084710	-4290.931492910
TS2	0.086678	-4290.963800590
TS3	0.089787	-4290.979294150
TS4	0.091405	-2697.505302780
TS5	0.088889	-4290.981248200
TS6	0.089220	-4290.982056790
TS7	0.091114	-4290.981831070
TS8	0.088399	-4290.975801330
TS9	0.090228	-4290.962451710
TS10	0.089234	-4290.961031950
TS11	0.088049	-3493.882396450
TS12	0.092387	-3494.596602880
TS13	0.091405	-2697.505302780
TS14	0.092825	-2698.207480430
TS15	0.093407	-1901.125968050
TS16	0.096726	-1901.822691250
TS17	0.095055	-1502.935824210
a	0.150018	-1183.367714310
b	0.176633	-1222.668167310
c	0.204852	-1261.941384340
$TFSI^-$	0.008834	-1827.283210520

HTFSI	0.020548	-1827.706750840
NO_3^-	-0.011350	-280.434622304
HNO_3	0.000526	-280.872253384
Li_2S_8	-0.029570	-3200.722601460
LiS_8H	-0.022424	-3193.703025120
DOL	0.066314	-268.315768837
DME	0.109930	-308.814927871
4DOL-Li^+	0.322240	-1080.797761070
2DME-Li^+	0.243360	-625.131662365
TS18	0.091000	-4298.463924320
TS19	0.091664	-4298.467879340

Cartesian Coordinates of Intermediates and Transition States

DTT

C	-1.80012900	-0.74121600	0.20788700
H	-1.70342500	-1.40177100	1.07347500
H	-1.73590500	-1.34484000	-0.69975200
C	-0.69635400	0.32468400	0.20649300
H	-0.77612400	0.90924200	1.13815700
C	0.69635100	-0.32495000	0.20669600
H	0.77602300	-0.90903100	1.13867100
C	1.79991700	0.74119200	0.20784600
H	1.73551100	1.34454600	-0.69995400
H	1.70303400	1.40193400	1.07326600
S	-3.49844000	-0.02236500	0.18306300
S	3.49835400	0.02275400	0.18302000
O	-0.79154200	1.18103600	-0.92391600
H	-1.70931400	1.50645600	-0.94978700
O	0.79188300	-1.18174000	-0.92327800
H	1.70985200	-1.50655300	-0.94944900
H	-3.46888900	0.53928500	1.41087400
H	3.46918400	-0.53812000	1.41119600

$DTTS_1$

C	1.86080700	-0.75919200	-0.29481300
H	1.76255200	-1.34443000	-1.21778800
H	1.73507800	-1.44700000	0.54792700
C	0.73479100	0.28604400	-0.25344800
H	0.78135900	0.86704700	-1.19225800
C	-0.66498000	-0.34375200	-0.20497300
H	-0.77564200	-0.94220100	-1.12566700
C	-1.75218000	0.73865600	-0.20021400
H	-1.66898900	1.34417700	0.70485500
H	-1.65378600	1.39474100	-1.06894300
S	3.53277400	0.04308700	-0.20851200
S	-3.46875800	0.05526500	-0.15774500
O	0.89187000	1.15639100	0.86245500
H	1.86981500	1.27196900	0.91154300
O	-0.76727800	-1.18422400	0.94011600
H	-1.69058800	-1.49201800	0.97349100
H	-3.45141700	-0.53380100	-1.37294300

R

C	-0.14115200	-1.55516900	-0.30977500
H	-0.17846000	-1.52266300	-1.40233400
H	-0.05614700	-2.59965300	0.00804300
C	1.05642000	-0.76339300	0.22133000
H	1.04450900	-0.79154400	1.32239700
C	1.07903000	0.71104600	-0.21322400
H	1.09088200	0.74563100	-1.31090200
C	-0.09296100	1.54919500	0.31339200
H	0.02039100	2.59131700	-0.00561500
H	-0.13555400	1.51906200	1.40583600
S	-1.73279500	-0.95570900	0.37952500
S	-1.70422800	1.00000000	-0.38223700
O	2.22331900	-1.41308700	-0.27684200
H	2.95222400	-0.79002600	-0.10234300
O	2.31277600	1.22333900	0.31005400
H	2.55774400	2.00713900	-0.20772500

S_8^{2-}

S	-2.00495900	-1.05658000	0.87035000
S	-0.40947600	-0.96766800	-0.54672800
S	0.40946300	0.96813800	-0.54649700
S	2.00513900	1.05665300	0.87041300
S	4.39325200	-1.24255600	-0.22627900
S	3.86018700	0.76238900	-0.09754800
S	-3.86016900	-0.76263200	-0.09738300
S	-4.39343900	1.24225600	-0.22632800

S_6^{2-}

S	-3.72743600	0.53623600	-0.06387000
S	-2.14831200	-0.66977800	-0.70837200
S	-0.65440800	-0.85473300	0.77194700
S	0.65429700	0.85408900	0.77241900
S	2.14832300	0.67024300	-0.70795900
S	3.72753700	-0.53605800	-0.06416500

S_4^{2-}

S	-2.29119900	0.71930900	0.21316600
S	-0.92722200	-0.71929900	-0.52673900
S	0.92721300	-0.71932300	0.52672900
S	2.29120800	0.71931300	-0.21315700

S_2^{2-}

S	0.00000000	0.00000000	1.10722000
S	0.00000000	0.00000000	-1.10722000

HS_8^-

S	1.26929000	0.63528100	0.75037700
S	0.56438700	-1.37182200	1.00379300
S	-0.78855500	-1.85803800	-0.52206700
S	-2.72068200	-1.22398400	0.04258700
S	-2.46493700	2.13902800	0.52889900
S	-3.04976500	0.65703700	-0.83180800
S	2.69716000	0.77662500	-0.79156000
S	4.56412700	0.11117300	-0.19607700
H	-1.13637800	2.15517800	0.25369600

HS_6^-

S	-1.68009500	1.74003400	0.41596500
S	-2.10170900	-0.06566900	-0.56250700
S	-1.06494100	-1.58453600	0.43753500
S	0.90469000	-1.65323600	-0.41594700
S	2.10589800	-0.20353400	0.51899100
S	1.85774600	1.64880500	-0.39496100
H	-0.34540300	1.89020100	0.01476200

HS_4^-

S	-2.21898700	0.65824700	0.25201100
S	-0.85429600	-0.79310800	-0.53367500
S	0.96755300	-0.73424600	0.51736800
S	2.22083600	0.76163000	-0.20464700
H	-1.84170000	1.71963400	-0.49691200

HS_2^-

S	0.04023600	-1.03011200	0.00000000
H	-1.28756200	-1.30877500	0.00000000
S	0.04023600	1.11191000	0.00000000

HS^-

S	0.00000000	0.00000000	0.07972600
H	0.00000000	0.00000000	-1.27561800

Int1

S	0.30056000	-1.29699500	-0.18349500
S	1.98861700	-2.40997200	-0.84054100
S	3.65260000	-1.89285900	0.33572200
S	4.68360800	-0.24824600	-0.56035900
S	2.62179400	2.55791100	-0.60400600
S	4.18391800	1.58434800	0.35991500
S	-0.69745100	-2.30433700	1.38047200
S	-2.04100100	-3.71380900	0.64179200
C	-1.85009900	2.67901900	1.08679500
H	-1.37804600	1.96935100	1.77108400
H	-2.73634100	3.09561800	1.57074900
C	-2.24704800	1.98425300	-0.22276800
H	-1.33919900	1.56200000	-0.68010700
C	-3.19862400	0.81010000	0.04281300
H	-2.66160900	0.10994100	0.70044100
C	-3.55491100	0.07385500	-1.25530200
H	-4.08111400	0.74865100	-1.93421700
H	-2.65251100	-0.29114500	-1.75259100
S	-0.71344900	4.11004300	0.83199700
S	-4.69790700	-1.34945400	-0.97712700
O	-2.87826900	2.88894600	-1.12571300
H	-2.25354100	3.62665500	-1.24557500
O	-4.36433000	1.30497500	0.69886500
H	-4.95285200	0.53607600	0.80769100
H	0.39816500	3.40504400	0.48483800
H	-3.79870100	-2.18299200	-0.36669100

Int2

S	2.00710600	-0.72222300	-0.58918100
S	3.80136400	-1.81836900	-0.18998900
S	4.99585100	-0.76061100	1.17102600
S	6.19220000	0.61535000	0.10937800
S	4.00332600	2.63282600	-1.54473900
S	5.21913100	2.47608800	0.15334100
S	0.62768700	-0.88603700	0.99313900
S	-0.39298300	-2.68665500	0.95359700
C	-5.92654400	1.52685200	1.20167500
H	-5.14325300	1.55466100	1.96918800
H	-6.68233200	0.80405600	1.52534900
C	-5.30659500	1.03685600	-0.11762200
H	-4.43111100	1.67358300	-0.33757500
C	-4.78593800	-0.40637600	-0.03596100
H	-3.99130900	-0.42085400	0.72775100
C	-4.18224500	-0.84469800	-1.37733600
H	-4.94766000	-0.79620200	-2.15536000
H	-3.35381100	-0.19067000	-1.66218100
S	-6.70813400	3.20373900	1.01249100
S	-3.59529500	-2.59642200	-1.39055300
O	-6.24977800	1.12941300	-1.18262200
H	-6.73712000	1.95899500	-0.96834900
O	-5.85224900	-1.27045600	0.35281900
H	-5.49207900	-2.17468200	0.30550600

H	2.91332200	1.97546100	-1.07551900
H	-2.51455700	-2.45478300	-0.57108000

Int3

S	2.05563600	1.54513300	-0.88897500
S	3.39048900	-0.02180400	-0.26316100
S	2.51152500	-1.90870000	-0.58524500
S	1.38454800	-2.54300900	1.04201900
C	-0.39980700	1.20679300	0.98752500
H	-0.03979500	0.17443300	0.97738300
H	-0.76177600	1.43520000	1.99665000
C	-1.51787000	1.44578800	-0.02055500
H	-1.12022600	1.36089600	-1.04435200
C	-2.67017700	0.42738200	0.12781000
H	-2.96780300	0.38682900	1.18682600
C	-2.30245800	-0.97505900	-0.36165700
H	-2.03973100	-0.93859300	-1.42294100
H	-1.45746300	-1.39997900	0.18491200
S	1.06094100	2.31161600	0.77715300
S	-3.71999700	-2.15575300	-0.26492600
O	-2.02468300	2.75912000	0.20392400
H	-2.87496600	2.78906100	-0.27011600
O	-3.73751800	0.97180200	-0.65524400
H	-4.50392900	0.38239400	-0.54295700
H	-3.72511400	-2.30676900	1.07656700

Int4

S	1.19867000	-2.03320800	0.67155200
S	3.05329400	-1.06498500	0.34655200
S	2.92469900	0.95984500	0.89460100
S	2.50257100	2.10092000	-0.81461200
C	-1.05448000	-0.61346100	-0.94951200
H	-0.48603600	0.27988700	-0.68813300
H	-1.43123300	-0.48918400	-1.97077200
C	-2.20790900	-0.85194500	0.01295400
H	-1.80203300	-1.07380300	1.01442900
C	-3.16086400	0.35044600	0.17134500
H	-3.57291200	0.61008400	-0.81292000
C	-2.56813500	1.60253700	0.83550300
H	-3.40559300	2.12006300	1.32046400
H	-1.89410600	1.28883300	1.64434100
S	0.09659500	-2.05800600	-1.09307700
S	-1.71573700	2.78590800	-0.30800300
O	-2.95632100	-1.97059600	-0.46683700
H	-3.79297000	-1.92420800	0.03241600
O	-4.21994900	-0.20211300	0.99851500
H	-4.98828500	0.38399100	0.91074100
H	3.77017600	2.21295800	-1.27794500

Int5

C	-0.76680100	-0.90863000	0.77233700
H	-1.07726900	-0.30116100	1.62677000
H	-0.28226800	-0.24894600	0.04945200
C	-1.96446800	-1.62881700	0.16356700
H	-2.46522300	-2.22876700	0.94093600
C	-3.00043200	-0.64562700	-0.42035700
H	-2.49359500	-0.02244700	-1.17079500
C	-3.65778700	0.25387100	0.62855000
H	-4.14643300	-0.35348900	1.39640400
H	-2.92790300	0.90915700	1.10715600
S	0.50692000	-2.04381900	1.47915300
S	-4.99776700	1.31180100	-0.07566400
O	-1.50221000	-2.47499600	-0.88325000
H	-2.30192400	-2.72477600	-1.38035400
O	-3.96616700	-1.49076100	-1.05569700
H	-4.57179200	-0.91228900	-1.55076500
H	-4.19559200	2.17448000	-0.73444100
S	1.71998700	-2.54407800	-0.14282500
S	3.45802100	-1.35124000	-0.13108000
S	3.10869400	0.39392100	-1.27008700
S	3.05463100	2.08918000	0.02418900
S	-0.25541700	3.10754100	-0.32090800
S	1.18905200	2.34979000	0.95988700

Int6

C	1.39968300	-0.76996400	-0.56340700
H	1.77662600	-0.29201400	-1.47297800
H	0.67470800	-0.09445600	-0.10455100
C	2.54646400	-1.08031300	0.38670300
H	3.21963800	-1.81468700	-0.08670400
C	3.39943300	0.15420800	0.75053100
H	2.74229100	0.94119100	1.14375500
C	4.28100300	0.71933400	-0.37355900
H	5.08816300	1.27389100	0.12188500
H	4.76201000	-0.12105600	-0.89242500
S	0.51163300	-2.27877000	-1.15183000
S	3.44341200	1.84466200	-1.58531000
O	1.99242600	-1.63456600	1.58033800

H	2.71127900	-1.55194200	2.23503700
O	4.24048900	-0.34477800	1.82497900
H	4.57313200	0.42535900	2.31227900
S	-0.85808300	-2.75429100	0.34842400
S	-2.78679500	-2.18196000	-0.28548900
S	-3.37429600	-0.37268500	0.61529600
S	-3.09744400	1.21052800	-0.74685000
S	-1.53679200	3.53990400	1.16675500
S	-1.25170500	2.13944100	-0.36833500
H	-1.96956100	4.57961300	0.41698400

Int7

S	2.05563600	1.54513300	-0.88897500
S	3.39048900	-0.02180400	-0.26316100
S	2.51152500	-1.90870000	-0.58524500
S	1.38454800	-2.54300900	1.04201900
C	-0.39980700	1.20679300	0.98752500
H	-0.03979500	0.17443300	0.97738300
H	-0.76177600	1.43520000	1.99665000
C	-1.51787000	1.44578800	-0.02055500
H	-1.12022600	1.36089600	-1.04435200
C	-2.67017700	0.42738200	0.12781000
H	-2.96780300	0.38682900	1.18682600
C	-2.30245800	-0.97505900	-0.36165700
H	-2.03973100	-0.93859300	-1.42294100
H	-1.45746300	-1.39997900	0.18491200
S	1.06094100	2.31161600	0.77715300
S	-3.71999700	-2.15575300	-0.26492600
O	-2.02468300	2.75912000	0.20392400
H	-2.87496600	2.78906100	-0.27011600
O	-3.73751800	0.97180200	-0.65524400
H	-4.50392900	0.38239400	-0.54295700
H	-3.72511400	-2.30676900	1.07656700

Int8

C	0.37721400	0.49727200	0.42863300
H	0.45193400	-0.57301900	0.21897300
H	0.30318400	0.65124100	1.50935200
C	-0.83190700	1.09677500	-0.27784400
H	-0.73482500	0.94706700	-1.36481400
C	-2.16499900	0.46199500	0.16727900
H	-2.24422700	0.55177600	1.26132800
C	-2.30344400	-1.00824400	-0.23787800
H	-2.22016500	-1.10770400	-1.32413600
H	-1.53576300	-1.63013200	0.22601400
S	1.93958000	1.26877600	-0.19311300
S	-3.95922100	-1.71317400	0.17826300
O	-0.86337200	2.49204100	0.02232400
H	-1.72992500	2.80522300	-0.29258500
O	-3.16931000	1.26322400	-0.46105500
H	-4.03261300	0.93052200	-0.15885700
H	-3.79823500	-1.74437200	1.51841900
S	3.41772500	-0.03536000	0.58815000
S	3.43572200	-1.84271200	-0.48361100

Int9

C	0.97369800	-0.05965800	0.29684900
H	0.80157400	-1.06309800	-0.10105800
H	0.96587800	-0.11137500	1.39123800
C	-0.10999900	0.89433100	-0.19223200
H	-0.09180900	0.93656200	-1.29333400
C	-1.52869500	0.46642300	0.23686500
H	-1.54434600	0.37168900	1.33314800
C	-1.98534100	-0.84998600	-0.39799100
H	-1.96443400	-0.76780300	-1.48882000
H	-1.34745800	-1.68435900	-0.10122300
S	2.65025100	0.46953600	-0.27977100
S	-3.73538000	-1.27933600	0.01032500
O	0.15752300	2.18875100	0.34805300
H	-0.63734400	2.71681800	0.15506900
O	-2.37112600	1.54887000	-0.17015800
H	-3.26908700	1.34914200	0.14719200
H	-3.53729200	-1.58478500	1.31038600
S	3.84982800	-1.23835100	0.11715100

TS1

C	-4.27832400	-1.86529800	-0.58103600
H	-4.13189500	-1.14833900	-1.39265600
H	-4.91961400	-1.40831900	0.17514900
C	-2.93837800	-2.26070200	0.04909200
H	-2.30338300	-2.71149800	-0.73173300
C	-2.19643200	-1.01957800	0.57642800
H	-2.01861300	-0.36783400	-0.28989600
C	-0.84084300	-1.41532500	1.18084700
H	-1.00790300	-2.02679500	2.07121100
H	-0.27848400	-2.01955600	0.46017200
S	-5.23393100	-3.30966500	-1.22270800
S	0.20848000	0.01990900	1.66238700

O	-3.11755900	-3.17836300	1.12453200
H	-3.67462000	-3.89922700	0.78005400
O	-3.02617700	-0.35942700	1.52518500
H	-2.83652700	0.60220300	1.47919100
H	-4.38888600	-3.64696300	-2.22072500
H	0.26461600	1.06679200	0.09351500
S	-1.51680500	2.29349000	-1.59208900
S	0.52653700	1.83205900	-1.14339300
S	2.36379400	-0.21890300	-0.45405200
S	4.10184100	-1.17743900	-0.56201900
S	7.38078700	-1.11878200	0.18636900
S	5.73164700	0.06457400	0.11456200
S	-2.18355500	3.80736900	-0.29317100
S	-2.88072900	3.00909300	1.49323800

TS2

C	-1.72718500	-0.58947200	0.34046700
H	-1.49314000	-0.01781600	-0.56432100
H	-1.57221800	-1.65017700	0.12956300
C	-3.19136500	-0.34736400	0.73538900
H	-3.32872000	0.73526000	0.89526900
C	-4.16218600	-0.74897900	-0.38447900
H	-3.90664200	-0.13259500	-1.26191000
C	-5.61258300	-0.44648300	0.01540700
H	-5.89086700	-1.04512400	0.88567800
H	-5.73694200	0.61045800	0.26473600
S	-0.57128100	-0.07782000	1.68519800
S	-6.83555800	-0.90288100	-1.29009300
O	-3.54778400	-1.06372100	1.91484300
H	-2.81503100	-0.91877300	2.54293700
O	-3.98053000	-2.12847200	-0.67913300
H	-4.64137700	-2.35424200	-1.35752500
H	-0.58046100	1.67581000	1.12815400
H	-6.46255300	0.01637300	-2.20637700
S	2.15584100	-1.95092400	-0.80303800
S	1.83648600	-0.16649300	0.14152300
S	3.56779700	1.76510900	-0.67693500
S	2.19105000	3.19525900	-1.22501400
S	-0.77842200	3.04686800	0.51136700
S	1.14734000	3.88375200	0.50985700
S	3.41687400	-3.25904600	0.35400000
S	5.42077000	-2.94556400	-0.11827700

TS3

C	-2.34488000	-1.35366200	1.21532300
H	-1.87470700	-0.94141600	0.31583400
H	-2.37735000	-2.44483100	1.09588700
C	-3.78667600	-0.85041100	1.29776500
H	-3.78739900	0.22950000	1.51448600
C	-4.58019300	-1.07270600	-0.00870500
H	-4.49594700	-2.13410900	-0.29030300
C	-4.09897100	-0.19692300	-1.16843800
H	-4.20400800	0.86034300	-0.90831800
H	-3.05384000	-0.38529700	-1.41760800
S	-1.28916800	-0.90396300	2.66322400
S	-5.11423700	-0.41078300	-2.69950900
O	-4.45219000	-1.55707100	2.34936000
H	-5.39652000	-1.35150200	2.23617600
O	-5.94239500	-0.76649800	0.31608500
H	-6.46974200	-0.92965200	-0.48565600
H	-4.69104200	-1.65421100	-3.01213900
S	4.64404400	-0.99291500	0.85293600
S	3.52162600	0.70010900	1.33554000
S	1.36615400	0.09912700	1.49281700
S	0.54697500	0.57499400	-0.40214100
S	1.05819500	3.98927900	-0.88329600
S	-0.31852600	2.50594700	-0.38527300
S	5.06037700	-1.03494000	-1.21509900
S	3.51267900	-2.04577600	-2.21873800
H	3.94467400	-3.31500400	-2.03411800

TS4

S	1.13698800	-1.06145100	1.49500300
S	2.95984000	-1.27813000	0.47962500
S	3.86921300	0.60359100	0.19520700
S	3.18291300	1.45930200	-1.60300700
C	-0.78799700	0.56978300	-0.37067300
H	0.14535000	1.07811500	-0.11677800
H	-0.92018400	0.60633900	-1.45230800
C	-1.93927400	1.28973400	0.32399400
H	-2.11089400	2.22136600	-0.24490600
C	-3.27925700	0.54826400	0.37283500
H	-3.17786300	-0.30181700	1.05832700
C	-3.78687000	0.04567700	-0.98047000
H	-4.85696000	-0.17177600	-0.87828400
H	-3.69134900	0.84238200	-1.72963300
S	-0.58056500	-1.22195700	0.06153000
S	-2.91800800	-1.49253200	-1.53489900

O	-1.53766100	1.61506500	1.65578600
H	-2.35438100	1.91901300	2.09117300
O	-4.18107800	1.51940900	0.95380400
H	-4.94900800	1.03146800	1.29169500
H	4.01950700	0.83718800	-2.46547600

TS5

C	3.07436400	-0.34838000	1.01204100
H	3.48940100	-1.25410500	1.46816300
H	2.46337500	-0.66993100	0.15809900
C	4.22439600	0.50119300	0.46530800
H	4.77168700	0.96071400	1.30497100
C	5.24117100	-0.31218400	-0.36741700
H	4.69345800	-0.86062500	-1.14883800
C	6.05945100	-1.29681900	0.47214600
H	6.61671800	-0.75613800	1.24311000
H	5.42491300	-2.03779000	0.96082500
S	2.00235000	0.48595400	2.26590500
S	7.35103100	-2.18985800	-0.50443500
O	3.67896400	1.52071000	-0.37429300
H	4.44171100	1.89044800	-0.85246900
O	6.10053000	0.66312200	-0.97239600
H	6.69262000	0.18735800	-1.57999400
H	6.51442900	-2.97220600	-1.21910800
S	-0.17916400	0.59596600	-0.91651700
S	-1.55501900	-0.97676900	-0.63102000
S	-3.26795700	-0.55649600	-1.77830000
S	-4.79910800	0.28604800	-0.54116000
S	-5.78969000	-2.29128100	1.59681400
S	-6.23284400	-1.19802900	-0.10863200
S	-0.30591400	1.96571200	0.66523100
S	-1.84202000	3.41298700	0.05333800
H	-1.04717500	4.23102400	-0.67326200

TS6

C	-2.90271200	-1.32693000	-0.44154300
H	-3.39976700	-2.17753600	0.03777900
H	-2.29342500	-0.83199600	0.32567200
C	-3.97080500	-0.33726000	-0.90788600
H	-4.57855000	-0.80362100	-1.70094000
C	-4.93027700	0.11166400	0.21569600
H	-4.32812000	0.55232600	1.02509800
C	-5.79169300	-1.02021300	0.78143000
H	-6.39497600	-1.46878600	-0.01357700
H	-5.18215100	-1.80226700	1.23695100
S	-1.80527200	-1.97507100	-1.78138600
S	-7.02044200	-0.43771700	2.03513400
O	-3.32157200	0.82975300	-1.41559200
H	-4.02868800	1.48843100	-1.53026800
O	-5.75331700	1.12237500	-0.38135800
H	-6.31340700	1.49076600	0.32361500
H	-6.13683700	-0.13270600	3.00951100
S	0.16909000	0.37416300	-1.38198700
S	1.93540400	-0.77194700	-1.36915500
S	2.24321600	-1.53538800	0.56564700
S	3.48790600	-0.21097000	1.69066100
S	6.55534800	-0.05632300	0.03360300
S	5.49385600	-0.86665200	1.62525000
S	0.85405100	2.46169900	-1.21469100
S	0.88643900	3.03113000	0.80794300
H	-0.41230200	3.38506500	0.94871000

TS7

C	-1.99829900	-1.47229900	0.23424500
H	-1.83335000	-0.72391000	1.01557000
H	-1.62951200	-1.03877200	-0.70343500
C	-3.50197000	-1.70857900	0.08789800
H	-3.88480400	-2.20743500	0.99414600
C	-4.29686500	-0.39826300	-0.10587400
H	-3.85358500	0.15402400	-0.94691000
C	-4.31974300	0.49050700	1.13826000
H	-4.78211000	-0.04541400	1.97251700
H	-3.31589700	0.80335300	1.43038200
S	-1.01548000	-2.98617200	0.64646000
S	-5.34099800	2.01677900	0.91515700
O	-3.73382400	-2.54026100	-1.05295000
H	-4.68214000	-2.43500000	-1.24728900
O	-5.63073900	-0.80990200	-0.45004200
H	-6.11125100	-0.01041900	-0.72520900
H	-4.42544300	2.72538200	0.22132000
S	4.15006600	-1.63568600	0.23939700
S	1.97449500	-1.67672200	0.13654600
S	1.46453100	-0.73319400	-1.67388300
S	1.54392200	1.39614900	-1.50294800
S	-0.72438200	2.69200700	0.82096800
S	-0.34821500	2.27796300	-1.17927800
S	4.79466900	-0.05386700	1.45568100
S	5.22857400	1.62768700	0.26433600

H	6.50093100	1.31215900	-0.07329100

TS8

C	-1.85463400	-0.67415200	1.65607300
H	-1.16892400	-0.68607900	0.80353400
H	-1.81011900	-1.66583900	2.12566600
C	-3.27673800	-0.45935600	1.14128000
H	-3.36964900	0.56622200	0.75350200
C	-3.67249100	-1.43458100	0.01142700
H	-3.51344700	-2.46432700	0.37066500
C	-2.88377700	-1.22110400	-1.28270700
H	-3.00963900	-0.19602900	-1.64246900
H	-1.81703100	-1.39854900	-1.14111800
S	-1.26363400	0.61259900	2.84663000
S	-3.47416000	-2.29501000	-2.66899100
O	-4.18628300	-0.65572300	2.23031300
H	-5.07111200	-0.64806300	1.82636200
O	-5.07198300	-1.21286900	-0.20515900
H	-5.34042100	-1.79558700	-0.93777900
H	-3.04746500	-3.47378200	-2.16655000
S	4.29203200	-0.89170300	-0.96641500
S	3.10860000	0.72807300	-1.63235400
S	2.87778100	2.11315300	-0.09649300
S	0.79266500	1.85909500	0.85877300
S	-1.16352400	2.71941000	-1.87913300
S	-0.35085200	3.34374500	-0.06331900
S	3.05033100	-2.46297800	-0.31320900
S	2.72739000	-2.27073800	1.75367600
H	3.83716300	-2.91305300	2.18719300

TS9

C	3.87338300	1.02980200	0.63649500
H	4.78106000	1.13852600	1.24069300
H	3.16034700	0.43659600	1.22203200
C	4.22146000	0.24936400	-0.63200300
H	4.92910500	0.83763300	-1.24008600
C	4.87655300	-1.11887500	-0.34099300
H	4.19711900	-1.69347100	0.30617100
C	6.25100000	-1.01314500	0.32441600
H	6.93592800	-0.45017500	-0.31678900
H	6.19464900	-0.51386600	1.29310200
S	3.16684300	2.71233100	0.35891900
S	7.07050500	-2.65343000	0.56592100
O	3.02404900	0.01552400	-1.37128000
H	3.25713100	-0.65833300	-2.03366500
O	4.98538400	-1.76124200	-1.61849700
H	5.25928800	-2.67998100	-1.45556000
H	6.25314800	-3.10954200	1.53887100
S	-5.63431000	-0.56453300	-0.85198300
S	-4.36225300	1.12911800	-0.83759700
S	-2.49086200	0.57966900	-1.65437400
S	-1.13378800	0.05110300	-0.16199300
S	-0.52706000	3.15570500	1.57716900
S	0.42822100	1.82259200	0.30909900
S	-5.70933500	-1.42057400	1.06600800
S	-4.17715400	-2.84395500	1.25881800
H	-4.81468600	-3.90287200	0.70719500

TS10

C	-3.68535200	-1.06249700	0.22370200
H	-3.47808100	0.01061000	0.26793700
H	-3.39670100	-1.41143100	-0.77591700
C	-5.18338600	-1.30158700	0.39846100
H	-5.47887900	-1.04177400	1.42783000
C	-6.05419900	-0.46574400	-0.56428600
H	-5.72104500	-0.66214100	-1.59499000
C	-5.99649800	1.03836000	-0.28520200
H	-6.33556400	1.24324300	0.73448600
H	-4.98644900	1.43424600	-0.39891800
S	-2.63757000	-1.87489100	1.51062200
S	-7.13266500	2.01710500	-1.36732000
O	-5.45011800	-2.68543900	0.15214300
H	-6.41909500	-2.75135600	0.09075000
O	-7.38870700	-0.95919300	-0.38514500
H	-7.95368600	-0.49254000	-1.02537200
H	-6.44553600	1.86316300	-2.51915900
S	4.88974400	-0.56383900	-2.09155200
S	2.97000900	0.26932000	-1.84718900
S	3.13038300	2.00113200	-0.64844300
S	2.77104100	1.52476800	1.41036100
S	-0.69565100	-0.08986300	1.67529300
S	0.75471500	1.75678600	1.92075000
S	5.18592900	-2.08291400	-0.66728900
S	6.04925200	-1.24614300	1.05404300
H	7.34645400	-1.29385100	0.67034000

TS11

C	2.64438700	0.88478800	-0.85937900

H	3.43420100	0.64205200	-1.57403500
H	2.44495100	1.95707200	-0.91432400
C	3.08528500	0.56440100	0.57070800
H	2.20825800	0.58704900	1.23688100
C	3.79669900	-0.78353000	0.75482600
H	4.66641500	-0.80283300	0.08286800
C	2.93731800	-2.02490400	0.51653100
H	3.50687100	-2.90357500	0.84461800
H	2.03640900	-1.96987200	1.13747700
S	1.08913200	0.03531900	-1.3999020
S	2.48112900	-2.27338400	-1.25078300
O	3.99980600	1.60631600	0.93737300
H	4.45759900	1.25800400	1.72486500
O	4.25314500	-0.75075700	2.12740500
H	4.94515800	-1.42459300	2.22194000
S	-0.22485100	2.01627100	-1.65036700
S	-0.96861700	2.62980000	0.19265800
S	-2.88539400	1.80857000	0.51669000
S	-2.70307000	-0.01766500	1.56057200
S	-4.48084900	-2.16974800	-0.38723800
S	-2.54176000	-1.59312800	0.18009000
H	-4.75712700	-3.00884400	0.63783400

TS12

C	1.52777000	-1.47294200	0.43228900
H	1.07819400	-0.48355900	0.30738200
H	1.57257400	-1.68429000	1.50784300
C	2.95458400	-1.44673900	-0.11253300
H	2.92655300	-1.29023000	-1.20279300
C	3.81928100	-0.32638200	0.50501200
H	3.78225100	-0.42377600	1.60111000
C	3.37448900	1.08105600	0.10044500
H	3.41801600	1.18965000	-0.98714800
H	2.35612100	1.29862400	0.42603300
S	0.43229300	-2.70190900	-0.40888400
S	4.49247500	2.40109700	0.75404200
O	3.57390000	-2.70158000	0.18352700
H	4.52004200	-2.56792300	-0.00095500
O	5.15198400	-0.58442900	0.04299200
H	5.72904900	0.08105500	0.45709800
H	4.11487300	2.31904000	2.04747300
S	-4.55340200	0.34473100	1.80360500
S	-4.28965500	-1.11461300	0.31324000
S	-2.02181400	-1.40816000	-0.21545000
S	-1.70655200	0.04188200	-1.74374700
S	-0.68776800	1.75496400	-1.02949800
S	-1.97676700	3.26069500	-0.37506700
H	-4.38246600	-0.41945900	2.90867800

TS13

S	1.13698800	-1.06145100	1.49500300
S	2.95984000	-1.27813000	0.47962500
S	3.86921300	0.60359100	0.19520700
S	3.18291300	1.45930200	-1.60300700
C	-0.78799700	0.56978300	-0.37067300
H	0.14535000	1.07811500	-0.11677800
H	-0.92018400	0.60633900	-1.45230800
C	-1.93927400	1.28973400	0.32399400
H	-2.11089400	2.22136600	-0.24490600
C	-3.27925700	0.54826400	0.37283500
H	-3.17786300	-0.30181700	1.05832700
C	-3.78687000	0.04567700	-0.98047000
H	-4.85696000	-0.17177600	-0.87828400
H	-3.69134900	0.84238200	-1.72963300
S	-0.58056500	-1.22195700	0.06153000
S	-2.91800800	-1.49253200	-1.53489900
O	-1.53766100	1.61506500	1.65578600
H	-2.35438100	1.91901300	2.09117300
O	-4.18107800	1.51940900	0.95380400
H	-4.94900800	1.03146800	1.29169500
H	4.01950700	0.83718800	-2.46547600

TS14

C	1.30465500	1.15018900	-0.52051000
H	0.92002000	0.12146500	-0.50152200
H	1.54749000	1.39769900	-1.56172100
C	2.58714600	1.23299500	0.30373300
H	2.34988200	1.08096600	1.36868200
C	3.63389200	0.17403600	-0.10432600
H	3.80307100	0.25047500	-1.18967600
C	3.21197500	-1.25456200	0.24886600
H	3.04679600	-1.34044600	1.32675200
H	2.29363800	-1.54635600	-0.26243900
S	-0.05511600	2.22465400	0.09216900
S	4.52003900	-2.50533300	-0.13097800
O	3.16298200	2.53006600	0.11448900
H	4.05269800	2.47430300	0.50465300
O	4.83128300	0.53369800	0.59688000

H	5.51653800	-0.10595400	0.33438300
H	4.42194000	-2.45279900	-1.47646400
S	-5.69959300	-0.83368800	0.87913500
S	-4.68432600	0.03050600	-0.76438600
S	-2.21251800	0.53404200	-0.21605500
S	-1.30518900	-1.32965900	-0.14366700
H	-5.34494800	-2.13376700	0.74034200

TS15

C	-0.12512900	0.17820000	1.15051600
H	-0.71997500	-0.23759700	1.96637700
H	0.70391900	0.74699700	1.57771800
C	-0.96261600	1.13501400	0.29956600
H	-0.43392100	1.34074700	-0.64473600
C	-2.37707700	0.64535100	-0.03905200
H	-2.90188700	0.44394100	0.90573400
C	-2.45059000	-0.58884300	-0.93789900
H	-3.49405500	-0.72272100	-1.24998700
H	-1.85957300	-0.41395100	-1.84456800
S	0.63098000	-1.22576200	0.20684800
S	-1.89238300	-2.13501100	-0.10283200
O	-1.07646700	2.34382300	1.06352900
H	-1.80977400	2.82725000	0.63954900
O	-2.98898900	1.78227200	-0.69346900
H	-3.94977700	1.64610900	-0.67855700
S	2.86222500	-0.58242300	0.46734600
S	3.36557900	0.88894500	-0.95816300
H	3.01876000	2.01015700	-0.28198900

TS16

C	0.11484800	-0.84254500	0.49791700
H	-0.15352900	0.19803500	0.29020200
H	0.25285500	-0.93545300	1.58315400
C	1.44379600	-1.16692000	-0.18286800
H	1.31170500	-1.12131200	-1.27611700
C	2.58532600	-0.19883500	0.19469500
H	2.68448200	-0.18967400	1.29119600
C	2.36669900	1.22973600	-0.30905800
H	2.27115900	1.23420700	-1.39876700
H	1.46761600	1.67606600	0.11815800
S	1.29536900	-1.90082400	-0.06156200
S	3.79898100	2.34534300	0.04585500
O	1.84404900	-2.48606500	0.20205600
H	2.76264700	-2.57195000	-0.10726800
O	3.76555600	-0.76462100	-0.39198000
H	4.51412200	-0.20360000	-0.12407600
H	3.63218600	2.41446000	1.38382800
S	-5.20730500	1.51580100	-0.08964300
S	-3.37181600	-0.09932500	-0.06214400
H	-5.47595000	1.60017000	1.23487700

TS17

C	0.45635500	-0.60628000	-0.87120900
H	0.09225700	-0.23400100	-1.83133000
H	1.16441500	-1.41646200	-1.05625600
C	-0.69443800	-1.16472900	-0.03217000
H	-0.35466500	-1.30147200	1.00717900
C	-1.96865200	-0.30918100	-0.01138800
H	-2.30962000	-0.18515200	-1.04914100
C	-1.83683700	1.06299100	0.64883800
H	-2.84302800	1.48720800	0.75695400
H	-1.42382100	0.94380400	1.65714800
S	1.41936600	0.74936100	-0.05139300
S	-0.81193600	2.24469400	-0.32574700
O	-1.02055900	-2.43898500	-0.60476000
H	-1.89620200	-2.65277500	-0.23265900
O	-2.92195200	-1.12430000	0.71114200
H	-3.80710200	-0.77390000	0.52263200
S	3.40041000	-0.50900600	0.34122900
H	3.05385100	-1.01856900	1.54457900

a

C	-1.67948000	0.40587300	-0.13302200
C	-0.38621800	-0.47137200	-0.15410800
C	0.97829100	0.23863600	-0.06342100
H	1.01507900	0.99044100	-0.86706800
C	2.10375400	-0.77858200	-0.31825000
H	2.10059700	-1.53692500	0.46774400
H	1.97340900	-1.27522700	-1.28276800
S	-3.11450100	-0.80632500	-0.31797800
S	3.79307800	-0.03216900	-0.25706200
O	-0.42725000	-1.47052200	0.86054600
O	1.14758100	0.86550500	1.20389500
H	2.06876800	1.18250500	1.22718300
H	3.67660500	0.74741100	-1.35381300
C	-1.67038000	1.38381400	-1.31833600
H	-0.88455400	2.14613800	-1.21114200
H	-1.51253500	0.85923100	-2.26827000

H	-2.63115700	1.90542400	-1.38287300
H	-0.38456100	-0.95141500	-1.14875100
H	-1.36496300	-1.77524300	0.81250600
C	-1.84593400	1.18974000	1.18037800
H	-1.77870200	0.52091700	2.04341500
H	-1.07106500	1.95793600	1.28902700
H	-2.82700300	1.67618400	1.20049100

b

C	1.62908900	0.41271200	0.30878300
C	0.36871000	-0.46400200	-0.12506000
C	-1.01152200	0.22181000	0.13466800
H	-1.03107800	0.53831200	1.18983100
C	-2.19370400	-0.74553400	-0.08455300
H	-2.18747700	-1.11297100	-1.11385600
H	-2.16395700	-1.59783200	0.59248700
S	3.17855200	-0.41705500	-0.38780800
S	-3.84435500	0.06910100	0.11620900
O	0.43432000	-0.70993700	-1.53267600
O	-1.17057200	1.34955600	-0.71903800
H	-2.08737100	1.65468900	-0.58980000
H	-3.76830200	0.28463700	1.44738100
C	1.74358800	0.50923300	1.84108800
H	0.84759400	0.96680200	2.28727500
H	1.89880800	-0.46676600	2.30839400
H	2.59878800	1.14081000	2.10479500
C	1.58607800	1.84565900	-0.25777900
H	1.43467800	1.83804800	-1.34046900
H	0.78154700	2.43950000	0.19080400
H	2.54019800	2.34105700	-0.04901500
H	1.40360600	-0.84085800	-1.68115700
C	0.38968000	-1.82050900	0.62096800
H	0.03457100	-1.73990900	1.65527100
H	-0.24130400	-2.54297600	0.09528600
H	1.41104600	-2.20843700	0.63338100

c

C	1.50758000	0.70094200	-0.07531900
C	0.30653500	-0.33005400	0.20631200
C	-1.10265300	0.35599200	0.10406500
H	-1.15588800	1.09234900	0.91809500
C	-2.26395800	-0.63915300	0.29599900
H	-2.23872100	-1.39317900	-0.49257200
H	-2.22608800	-1.14002600	1.26236100
S	3.17482900	0.13963200	0.62557100
S	-3.92669700	0.16016000	0.14279000
O	0.23797600	-1.35927400	-0.80473000
O	-1.25734900	1.01494200	-1.15096000
H	-2.18021800	1.32903500	-1.17614400
H	-3.85678300	0.92071300	1.25678200
C	1.19201800	2.07254400	0.56468100
H	0.31501700	2.54840900	0.10745400
H	1.02323900	1.98915700	1.64444000
H	2.05013200	2.73670000	0.42207100
C	1.69327500	0.90961800	-1.59423000
H	2.00789000	-0.01321400	-2.08864400
H	0.77322400	1.25877000	-2.07139800
H	2.47916700	1.65559900	-1.75731100
C	0.39598600	-0.94639900	1.61568800
H	0.16248100	-0.19654500	2.37959500
H	-0.30617200	-1.77847900	1.72756600
H	1.40755000	-1.30284100	1.80848800
C	1.20418800	-2.40242300	-0.80458300
H	2.21801900	-2.02780700	-0.97517600
H	1.19868500	-2.97490100	0.13246900
H	0.91551700	-3.07216100	-1.62200200

$TFSI^-$

N	0.00001200	0.00000800	0.85323100
S	-1.15611100	-0.84204900	0.09342200
S	1.15611200	0.84204800	0.09336500
C	-2.56228700	0.38584900	-0.04239200
C	2.56228900	-0.38584700	-0.04244300
O	-1.65242400	-1.86008400	1.03075500
O	-0.87725500	-1.24749700	-1.29390500
O	1.65244000	1.86011900	1.03065200
O	0.87721700	1.24744900	-1.29396700
F	-2.16906900	1.47993900	-0.70236400
F	-3.57704700	-0.18091200	-0.70701600
F	-2.98733100	0.74096800	1.17387200
F	2.98738400	-0.74090500	1.17382200
F	3.57702100	0.18088500	-0.70713400
F	2.16905200	-1.47997100	-0.70234500

HTFSI

N	-0.00002500	0.00024400	-0.81181900
S	1.25286100	-0.88172400	-0.08582600
S	-1.25327200	0.88214400	-0.08578300

C	2.61112400	0.41422700	0.08599400
C	-2.61077900	-0.41460700	0.08601100
O	1.70293000	-1.83260700	-1.09352900
O	0.85287300	-1.27751500	1.25435300
O	-1.70361000	1.83254500	-1.09377300
O	-0.85364800	1.27829000	1.25441300
F	2.21660000	1.37556900	0.91094600
F	3.68740800	-0.19417200	0.57251700
F	2.87682500	0.92203900	-1.11360800
F	-2.87651200	-0.92213600	-1.11366900
F	-3.68708900	0.19327300	0.57300700
F	-2.21551000	-1.37604100	0.91055000
H	0.00081500	0.00135800	-1.83293800

NO_3^-

N	0.00001400	-0.00003200	0.00022500
O	1.24000200	-0.23351400	0.00010200
O	-0.41775800	1.19058100	-0.00006000
O	-0.82225600	-0.95704000	-0.00023900

HNO_3

N	0.13637900	0.03406500	-0.00011700
O	-1.13189800	-0.53529300	-0.00020200
O	0.19402900	1.24965900	-0.00003600
O	1.03596200	-0.77353700	0.00013900
H	-1.73940100	0.23491800	0.00161700

Li_2S_8

S	-2.31160200	-0.67134100	0.92484300
S	-1.30418800	-2.08816500	-0.33489600
S	0.66242300	-2.31459900	0.28389500
S	2.01399900	-1.07978900	-0.87273500
S	2.15645900	2.11891100	0.28245200
S	3.02759700	0.20430200	0.43314900
S	-2.94839200	0.89244200	-0.27923400
S	-1.40689500	2.32022400	-0.46134700
Li	0.04430600	2.09355100	1.43796500
Li	0.54555800	1.20252500	-1.31064500

LiS_8H

S	2.43175000	1.10732000	-0.53441600
S	0.46911100	1.81549000	-0.83424600
S	-0.57984000	1.91290800	0.99272100
S	-1.30060900	-0.07330800	1.37051000
S	-2.57474800	-1.18396400	-1.55796700
S	-3.08283600	-0.42404100	0.34110100
S	2.27374600	-1.00007700	-0.76710800
S	2.20753900	-1.90307900	1.12107200
H	3.54118300	-2.05175800	1.28598700
Li	-0.34900000	-0.65607200	-1.13088300

DOL

C	-0.97209300	0.77213400	0.00000000
O	0.40669600	1.15103500	0.00000000
C	1.22425600	-0.00202500	0.00000000
C	-0.97505400	-0.76856800	0.00000000
H	-1.46016800	1.18510200	0.88998400
H	-1.46016800	1.18510100	-0.88998500
H	1.86034200	-0.00344900	-0.89785000
H	1.86034400	-0.00344800	0.89784800
H	-1.46509700	-1.17924500	-0.89001800
H	-1.46509800	-1.17924400	0.89001800
O	0.40170300	-1.15279300	0.00000100

DME

C	-2.98767700	-0.11641500	-0.00021800
H	-3.74792700	0.66892300	-0.00080000
H	-3.12009400	-0.74558100	0.89303100
H	-3.11991100	-0.74674600	-0.89267600
C	-0.64793200	-0.39926400	0.00062800
H	-0.68871200	-1.04749400	0.89039300
H	-0.68773800	-1.04874800	-0.88826100
C	0.64793200	0.39926400	0.00062800
H	0.68871200	1.04749400	0.89039300
H	0.68773800	1.04874800	-0.88826100
C	2.98767700	0.11641500	-0.00021800
H	3.12009400	0.74558100	0.89303100
H	3.74792700	-0.66892300	-0.00080100
H	3.11991100	0.74674600	-0.89267600
O	-1.72300800	0.52457000	-0.00051800
O	1.72300800	-0.52457000	-0.00051800

4DOL-Li^+

Li	0.04397800	-0.03352400	0.00635600
C	1.23005500	-2.66232900	-0.78984700
O	1.10099600	-1.66637600	0.26265700
C	2.34656000	-1.68586600	0.98471000
C	2.72354400	-3.05067900	-0.74252000

H	0.57205300	-3.50879900	-0.57737600
H	0.93689500	-2.19054100	-1.72916300
H	2.53884400	-0.69571400	1.39854600
H	2.29080600	-2.45149000	1.77214200
H	3.20248800	-3.06606500	-1.72185500
H	2.86802100	-4.01667000	-0.24334800
O	3.32031800	-2.00029300	0.03129200
C	-1.25730700	-0.68610400	2.64228500
O	-1.11410700	0.28282200	1.56892300
C	-2.39593700	0.92219500	1.44722000
C	-2.78604400	-0.76260900	2.86549800
H	-0.82203100	-1.62575700	2.29860800
H	-0.72630100	-0.33298700	3.53032000
H	-2.45726900	1.74478700	2.17498400
H	-2.52566500	1.27734500	0.42498400
H	-3.07881500	-0.25071000	3.79010800
H	-3.17633100	-1.78084200	2.86947900
O	3.33220100	-0.08025600	1.72707700
C	2.63918200	3.18915100	0.59785100
O	3.36795900	2.05225800	0.11619100
C	2.51819400	1.48525000	-0.83757500
C	1.18076800	2.69094100	0.62498300
H	3.02906600	3.45354400	1.58117600
H	2.76004000	4.03595300	-0.08931500
H	2.51029300	2.06870200	-1.77021700
H	2.80020500	0.44723600	-1.01231000
H	0.47612700	3.43074000	0.23688300
H	0.86271500	2.35785900	1.61463100
O	1.20153400	1.52959800	-0.25011000
C	-2.26693300	-1.05813100	-1.61017700
O	-1.05767600	-0.24843400	-1.61173300
C	-1.33672600	0.87355900	-2.46751400
C	-3.31119400	-0.15440000	-2.30350400
H	-2.08813100	-1.98746600	-2.15655500
H	-2.52168500	-1.27322000	-0.57098600
H	-0.73738100	1.72404700	-2.14480900
H	-1.11576100	0.59385500	-3.50804800
H	-4.25681000	-0.08948500	-1.76485500
H	-3.49252200	-0.47315500	-3.33722800
O	-2.69754300	1.14362300	-2.28846300

2DME-Li^+

C	-1.39468400	2.16841800	-1.62986800
H	-0.42527400	2.22411700	-2.12798300
H	-1.48469000	2.97863000	-0.89588900
H	-2.19598600	2.25782300	-2.37206900
C	-2.68142400	0.68615900	-0.25994300
H	-2.75577600	1.42693400	0.54791200
H	-3.54296100	0.80464000	-0.92860400
C	-2.65331500	-0.72160900	0.29620200
H	-2.69942000	-1.46575200	-0.51069800
H	-3.50868000	-0.87352200	0.96608100
C	-1.30891100	-2.14599700	1.67247300
H	-1.37576600	-2.96426400	0.94493100
H	-0.33443100	-2.16378300	2.16345000
H	-2.10109400	-2.25801700	2.42141700
O	-1.45933600	0.89171300	-0.98318100
O	-1.42293000	-0.87726100	1.01745500
Li	-0.00012000	0.01969600	0.00083500
C	1.30653600	-2.14734800	-1.67172100
H	0.33130400	-2.16517500	-2.16119900
H	1.37459400	-2.96565700	-0.94434000
H	2.09755900	-2.25927200	-2.42191200
C	2.65301500	-0.72281700	-0.29769300
H	2.70083600	-1.46708900	0.50898700
H	3.50723300	-0.87435600	-0.96913200
C	2.68181100	0.68486300	0.25863600
H	2.75503300	1.42583800	-0.54912600
H	3.54420500	0.80321600	0.92620700
C	1.39709000	2.16694800	1.63060800
H	1.48612200	2.97723900	0.89659700
H	0.42840100	2.22268900	2.13012100
H	2.19946400	2.25616200	2.37166900
O	1.42145000	-0.87865300	-1.01681500
O	1.46068800	0.89030300	0.98365500

TS18

C	2.67249500	-1.29738400	0.94776100
H	2.05772000	-0.40920100	0.76717500
H	2.89128900	-1.33637300	2.02222100
C	3.99241100	-1.14707000	0.19194400
H	3.79319400	-1.13163800	-0.89175600
C	4.75488200	0.14617800	0.55349900
H	4.89400600	0.17107200	1.64552300
C	4.04141900	1.42302400	0.10159600
H	3.90293500	1.41223900	-0.98359700
H	3.06328300	1.52915400	0.57341600
S	1.69120300	-2.78174500	0.45367800

S	5.02117300	2.95426500	0.43849400
O	4.82669000	-2.25977200	0.51880700
H	5.70453200	-2.03349900	0.16469200
O	6.02648700	0.02227200	-0.09331400
H	6.55340600	0.80079200	0.15861400
H	4.90351500	2.93799200	1.78356100
S	-4.42512100	-0.76276800	1.39614400
S	-3.41786900	-1.68780300	-0.20362500
S	-1.20080100	-1.80749200	0.11616000
S	-0.57854600	0.15678000	-0.40539400
S	-2.09102600	1.01600100	-3.32106900
S	-0.27128300	0.33945000	-2.47893900
S	-4.50117600	1.29886700	0.89199000
S	-3.00391300	2.33079800	1.94361800
H	-3.72591700	2.59015700	3.05710300
Li	-3.06428800	0.57306700	-1.25553100

TS19

C	-3.05001000	-1.26698600	-0.02575500
H	-3.69960100	-2.02352300	0.42738700
H	-2.54165600	-0.74275600	0.79301000
C	-3.91805000	-0.25364900	-0.77211400
H	-4.37912900	-0.74005900	-1.64703600
C	-5.05257100	0.33129000	0.09778500
H	-4.60720500	0.74262300	1.01685500
C	-6.12936100	-0.69281400	0.46615400
H	-6.59011100	-1.09425800	-0.44138500
H	-5.71928700	-1.52377500	1.04249500
S	-1.80522700	-2.15123100	-1.06654000
S	-7.53026000	0.04297900	1.42194300
O	-3.08769900	0.82733300	-1.20007600
H	-3.70244500	1.53071200	-1.47386600
O	-5.61490500	1.39172000	-0.68412800
H	-6.28257700	1.83394800	-0.13142300
H	-6.85312900	0.26650600	2.56846200
S	0.26349600	0.14738100	-0.95125300
S	1.86184400	-1.22347100	-1.05371400
S	2.42524100	-1.86909500	0.87839400
S	3.72187600	-0.36375600	1.66320400
S	5.67453800	-0.63263800	0.94997100
S	1.36088600	2.05796800	-0.97024800
S	1.42948800	2.87136700	0.97334100
H	0.26317700	3.55309800	0.91968400
S	5.85080800	0.46374100	-0.84533000
Li	3.52990800	0.74870100	-0.86442600