Electronic Supplementary Information

Theoretical insight of decatungstate photocatalyzed alkylation of N-tosylimine via hydrogen atom transfer and proton-coupled electron transfer

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COMPUTATIONAL DETAILS

1. Correction of translational entropy in solution

We evaluated the electronic energy (E_{sol}) with zero-point energy correction in solution. For each species, the E_{sol} is defined through equation (S1):

$$E_{sol} = E_{sol}^{pot} + E_{gas}^{v_0} \quad \text{(S1)}$$

the E_{sol}^{pot} is the potential energy including non-electrostatic energy in solution and $E_{gas}^{v_0}$ denotes the zero-point vibrational energy in the gas phase. In a bimolecular process, such as the coordination of $*[W_{10}O_{32}]^{4-}$ to methyl tert-butyl ether, the entropy change which can decreases considerably must be taken into consideration. In such case, Gibbs energy (G_{sol}^{o}) need be computed as follows:

$$\begin{aligned} G_{sol}^{o} &= H_0 - T(S_r^o + S_v^o + S_t^o) \\ &= E^T + P\Delta V - T(S_r^o + S_v^o + S_t^o) \\ &= E_{sol} + E_{therm} - T(S_r^o + S_v^o + S_t^o) \end{aligned} \quad \text{(S2)}$$

where ΔV is 0 in solution, E_{therm} is the thermal correction by translational, vibrational, and rotational movements, and S_r^o, S_v^o, and S_t^o are rotational, vibrational, and translational entropies, respectively. In general, the Sackur-Tetrode equation is used to evaluate translational entropy S_t^o. In solution, however, the usual Sackur-Tetrode equation cannot be directly applied to the evaluation of S_t^o, because the translation movement is suppressed very much in solution.[S1-S3] In this context, the translational entropy was corrected with the method developed by Whitesides et al., where the rotational entropy was evaluated in a normal manner. Thermal correction and entropy contributions of vibration movements to the Gibbs energy were evaluated with the frequencies calculated at 299.15 K and 1 atm.

Table S1 Comparison of Gibbs free energy change ($\Delta G°$) without and with translational entropy correction of key intermediates and transition states.

Energies	without translational entropy correction $\Delta G°$ (kcal/mol)	with translational entropy correction $\Delta G°$ (kcal/mol)
1	0.0	0.0
2	7.4	1.5
TS1	9.3	3.4
3	–15.5	–15.5
4	–6.7	–12.6
TS2	–2.3	–8.2
5	–9.6	–15.6
6	–25.6	–31.5
7	–32.6	–44.4
TS3	–35.3	–47.1
8	–47.5	–53.4
9	–6.0	–12.0
TS4	0.5	–5.5
10	–19.4	–25.3
11	4.5	–1.4

2. Absorption spectra for $[W_{10}O_{32}]^{4-}$

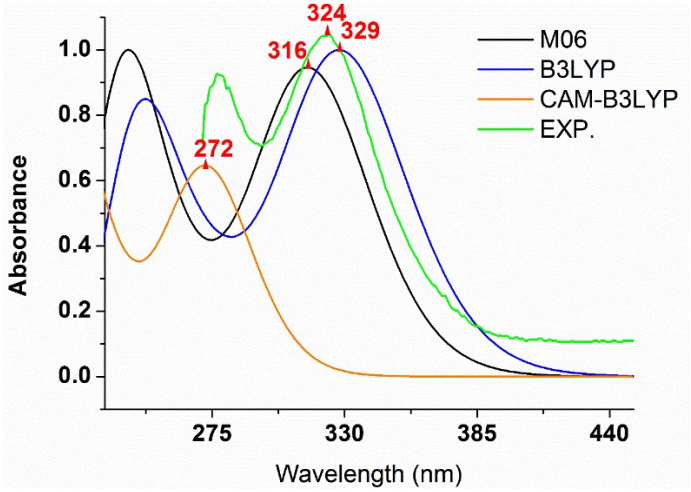

Fig. S1 Comparisons of experimental and calculated absorption spectra of $[W_{10}O_{32}]^{4-}$.

3. Stepwise PCET process for C−H activation

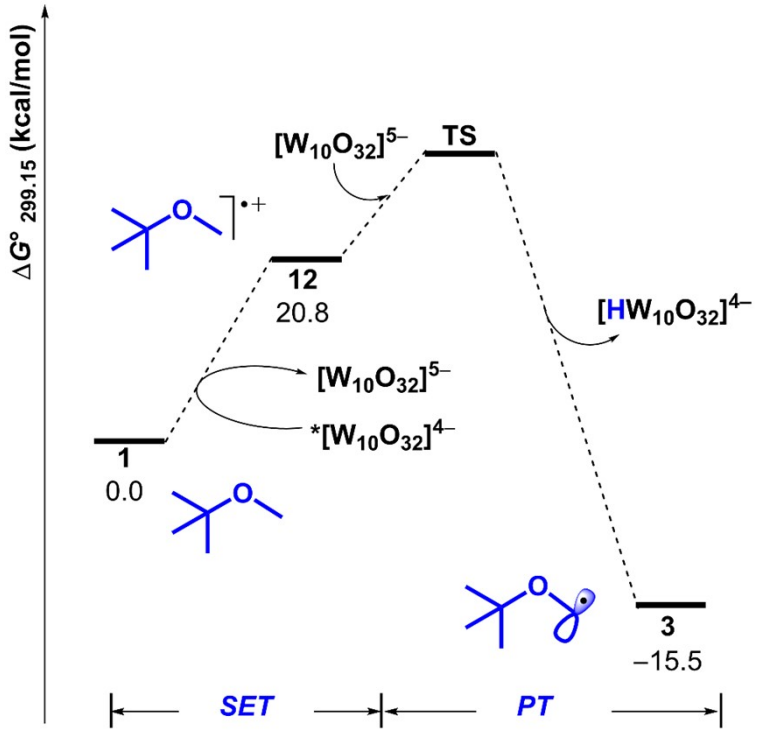

Fig. S2 Gibbs energy profile ($\Delta G°_{299.15}$) of the stepwise PCET process for C(sp^3)–H bond activation.

4. Redox potential

We calculated the standard redox potential ($E^{red}_{1/2}$) according to the equation (S3):[S4]

$$E^{red}_{1/2} = -\frac{\Delta G_r}{nF} - E_{Ag/Ag^+} \quad \text{(S3)}$$

where F is the Faraday constant and n is the number of electrons transferred, $E_{Ag/Ag^+} = 4.47$ V, and ΔG_r is the free energy change of the reaction.

Table S2 The experimental and calculated redox potentials of $[W_{10}O_{32}]^{4-}$.

Redox Potential	$E_{1/2}^{red}$ ($^*[W_{10}O_{32}]^{4-}/[W_{10}O_{32}]^{5-}$)
Cal.	–0.7 V

Exp.	–0.96 V
$\lvert\Delta\rvert$	0.26 V

Table S3 The calculated redox potentials of **5** and **10**.

Redox Potential	$E_{1/2}^{red}$ ($[HW_{10}O_{32}]^{3-}/[HW_{10}O_{32}]^{4-}$)	$E_{1/2}^{red}$ (**5**/**6**)	$E_{1/2}^{red}$ (**10**/**11**)
Cal.	–0.20 V	0.50 V	–1.20 V

5. The fragment charge distribution of HAT process

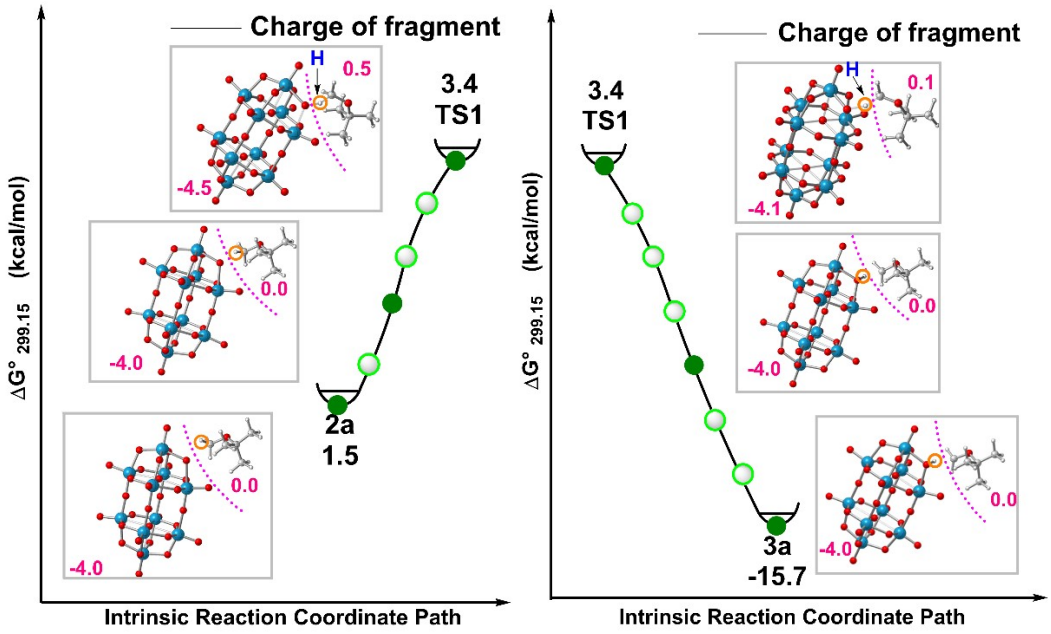

Fig. S3 Fragment charge analysis along the intrinsic reaction coordinate pathway in the hydrogen atom transfer process.

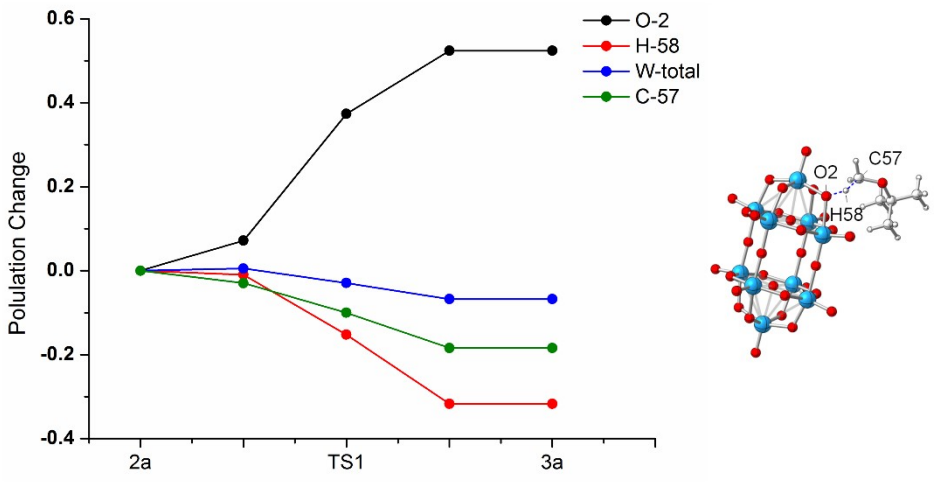

Fig. S4 Changes in electron population (in e) along the intrinsic reaction coordinates of the HAT process.

6. Analysis of regioselectivity for radical addition process

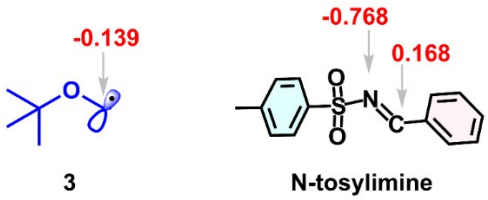

Fig. S5 NPA charge analysis for C-center radical of **1** and **N-tosylimine.**

REFERENCES

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CARTESIAN COORDINATES OF OPTIMIZED STRUCTURES

*$[W_{10}O_{32}]^{4-}$

(U)M06/BSII SCF energy in solution: -3080.2099382 a.u.

(U)M06/BSI SCF energy: -3085.8145166 a.u.

(U)M06/BSI SCF Gibbs free energy: -3085.77942 a.u.

O	-6.08782300	0.00449500	0.01405400
O	-3.89209800	1.97494600	0.00700100
O	-3.88563600	0.16386200	1.81762600
O	-3.93341900	-1.84392100	0.00660200
O	-3.89269400	0.16089900	-1.80552000
O	-2.07601400	4.07802400	-0.00108100
O	-1.90004000	1.94114700	1.82906600
O	0.09794700	2.39655000	-0.00375800
O	-1.90667900	1.93968600	-1.82870200
O	-2.22190600	0.06949500	3.98853200
O	-1.98923500	-1.79509600	1.85377300
O	-0.03665000	0.04477300	2.28379000
O	-1.99449300	0.06491900	0.00291100
O	-2.24403000	-3.99623000	0.00210800
O	-1.99481300	-1.79757700	-1.84844800
O	-2.24255000	0.06490500	-3.98832300
W	-4.36177000	-0.05024500	0.01205900
W	-1.71322500	2.40343000	-0.00075700
W	-1.91550700	0.05921300	2.30471500
W	-1.94683200	-2.31255600	0.00150800
W	-1.94293000	0.05775100	-2.30371200
W	2.10348000	2.33816800	-0.00234400
W	1.89898600	-0.01459400	2.31083100
O	-0.07646000	-2.30653400	0.00128900
O	-0.04859700	0.04227900	-2.28644100
O	3.90540100	1.80104300	0.00107500
O	1.94346500	1.85485300	-1.84238200
O	1.94674700	-0.02899800	-0.00720900
O	2.34416000	4.03336300	-0.00234900
O	1.94087300	1.85561100	1.83911800
O	3.80118400	-0.05992500	1.84164000
O	1.82956800	-1.87304400	1.85524300
O	2.13359500	-0.01538000	4.00576900
W	1.83417500	-2.37502300	0.00071900
W	1.86591100	-0.01689400	-2.30934900
W	4.27505000	-0.15212200	-0.01662300
O	3.78280900	-1.96848300	0.00446200
O	2.04096900	-4.07315600	0.00192500
O	1.82961900	-1.87794300	-1.85243700
O	3.80563900	-0.06340200	-1.84836900

O	2.12043400	-0.02191700	-4.00156100
O	6.00036900	-0.18769500	-0.01208800

$[W_{10}O_{32}]^{4-}$

(U)M06/BSII SCF energy in solution: -3080.2950517 a.u.

(U)M06/BSI SCF energy: -3085.9012962 a.u.

(U)M06/BSI SCF Gibbs free energy: -3085.861015 a.u.

O	-6.01098300	0.14901300	-0.01445700
O	-3.81886400	1.19874800	-1.47548200
O	-3.81923400	1.47407900	1.20185600
O	-3.84187400	-1.16386800	1.42413200
O	-3.84215200	-1.42869200	-1.15787200
O	-2.10698800	2.53354800	-3.11519900
O	-1.88619800	2.62611600	-0.26924500
O	0.03186800	1.45042200	-1.78773700
O	-1.89383900	-0.27887800	-2.61372900
O	-2.10684800	3.11308200	2.53633400
O	-1.89391800	0.25772600	2.61647500
O	0.03244200	1.78259900	1.45850000
O	-1.97036000	0.04206800	-0.00326900
O	-2.22716300	-2.54945300	3.12024300
O	-1.88842300	-2.60244500	0.26660900
O	-2.22860600	-3.12861200	-2.54027900
W	-4.28396900	0.17058400	-0.01640100
W	-1.79689300	1.47472800	-1.80467300
W	-1.79569100	1.80996100	1.46862700
W	-2.03952600	-1.46638300	1.80793200
W	-2.04093000	-1.80299000	-1.47360000
W	2.03953300	1.46637900	-1.80793600
W	2.04092500	1.80299900	1.47359100
O	-0.03186300	-1.45042300	1.78772500
O	-0.03244400	-1.78261000	-1.45851300
O	3.84187800	1.16386500	-1.42412500
O	1.89392900	-0.25773500	-2.61647500
O	1.97035700	-0.04206600	0.00326000
O	2.22717700	2.54944000	-3.12025300
O	1.88842200	2.60245100	-0.26662200
O	3.84214100	1.42869100	1.15787400
O	1.89383200	0.27888400	2.61372600
O	2.22859500	3.12862700	2.54026300
W	1.79690000	-1.47472100	1.80468400
W	1.79568600	-1.80996600	-1.46862200
W	4.28396700	-0.17059100	0.01640000
O	3.81886100	-1.19874400	1.47549400

O	2.10696400	-2.53353200	3.11522400
O	1.88620200	-2.62610900	0.26924900
O	3.81924500	-1.47408700	-1.20184800
O	2.10684500	-3.11309000	-2.53632500
O	6.01098100	-0.14901200	0.01446300

$[HW_{10}O_{32}]^{4-}$

(U)M06/BSII SCF energy in solution: -3080.8978247a.u.

(U)M06/BSI SCF energy: -3086.4920014 a.u.

(U)M06/BSI SCF Gibbs free energy: -3086.443147 a.u.

O	-6.06326200	-0.00980300	0.00113600
O	-3.93901200	2.01278800	0.00435600
O	-3.87507900	0.08252500	1.82454700
O	-3.90799200	-1.86094200	-0.03954300
O	-3.87438700	0.14027600	-1.81925600
O	-2.11351100	4.04629200	0.06943200
O	-1.89389300	1.88808900	1.89050400
O	0.07963700	2.38778000	0.04916500
O	-1.90312600	1.95955500	-1.80313300
O	-2.21514000	-0.03399200	4.00469000
O	-1.96546600	-1.84517000	1.80263900
O	-0.02733500	-0.01796200	2.28925800
O	-2.01241500	0.10197800	0.01366600
O	-2.20331700	-4.01542100	-0.07976500
O	-1.96076800	-1.76779300	-1.87148500
O	-2.23117800	0.14173800	-4.00276300
W	-4.33586200	-0.07051900	0.02379200
W	-1.73370400	2.37186500	0.06289500
W	-1.91477800	0.00456600	2.32061700
W	-1.91208300	-2.33186800	-0.04499600
W	-1.95379900	0.10153300	-2.31405000
W	2.08142900	2.34626000	0.04365900
W	1.89516900	-0.05566500	2.30641700
O	-0.04739000	-2.30901200	-0.04099600
O	-0.04603300	0.07562900	-2.27779700
O	3.89348700	1.82527500	0.02797500
O	1.92553400	1.89640200	-1.80625300
O	1.94683600	-0.02129000	-0.00328400
O	2.31059800	4.04303100	0.07722200
O	1.93578900	1.82455100	1.87550200
O	3.81059100	-0.08069900	1.82965900
O	1.85773000	-1.91280200	1.81186100
O	2.14596200	-0.09044000	3.99910500
W	1.87331100	-2.37101400	-0.04691000

W	1.85766200	0.03472700	-2.30982500
W	4.27834500	-0.11711800	-0.02170700
O	3.80082500	-1.94968800	-0.04686300
O	2.07859100	-4.06964000	-0.08158700
O	1.84457200	-1.83805600	-1.88936400
O	3.79744000	-0.00804200	-1.85127600
O	2.11167300	0.06640600	-4.00241300
O	6.00428800	-0.14248900	-0.02700900
H	-4.15509700	2.30261000	-0.89557100

$[HW_{10}O_{32}]^{3-}$

(U)M06/BSII SCF energy in solution: -3080.744329 a.u.

(U)M06/BSI SCF energy: -3086.6517063 a.u.

(U)M06/BSI SCF Gibbs free energy: -3086.599651 a.u.

O	-6.05169900	-0.03454600	0.11232100
O	-3.93336500	1.96953600	0.13712400
O	-3.86493100	-0.04178900	1.89724500
O	-3.87234500	-1.83751800	-0.13491200
O	-3.91078600	0.22786200	-1.80769700
O	-2.11876300	3.99732500	0.27801200
O	-1.91060400	1.77332000	1.99408400
O	0.07843800	2.35256800	0.16890800
O	-1.93414300	2.03581300	-1.69993300
O	-2.11772000	-0.25210800	4.00484400
O	-1.96557900	-1.93803400	1.71185400
O	0.00349500	-0.13436700	2.26093500
O	-2.02328400	0.10214300	0.04083600
O	-2.17016300	-3.97533900	-0.29517200
O	-1.97176600	-1.64685700	-1.97490400
O	-2.28559200	0.35824600	-3.99914000
W	-4.33521100	-0.07278400	0.13928600
W	-1.71990700	2.33735100	0.19034200
W	-1.81669800	-0.12488800	2.33208900
W	-1.89993600	-2.30064600	-0.16482500
W	-2.11168500	0.22587800	-2.30905700
W	2.10478500	2.32547100	0.16593500
W	2.02112800	-0.18500500	2.29500200
O	-0.05648100	-2.23612500	-0.16510200
O	-0.09000900	0.21238100	-2.24957000
O	3.90966200	1.80977900	0.12995900
O	1.92188800	2.00184500	-1.69990200
O	1.96823200	-0.00286500	-0.04193600
O	2.31315200	4.01104300	0.30269600
O	1.92683100	1.70843800	1.96736700

O	3.82062700	-0.19657500	1.80350200
O	1.82868700	-1.99803100	1.69555500
O	2.19237600	-0.31116100	3.98470400
W	1.89617100	-2.35416600	-0.18598500
W	1.72804400	0.17052000	-2.29715100
W	4.28266900	-0.10113400	-0.15154100
O	3.77547800	-1.95099000	-0.15226300
O	2.03965400	-4.04647900	-0.30589200
O	1.81554900	-1.73552000	-1.98555300
O	3.79563600	0.08004600	-1.89992500
O	2.03745200	0.29103900	-3.96960100
O	5.99632800	-0.15298600	-0.15069500
H	-4.22265900	2.35503600	-0.70492400

1

(U)M06/BSII SCF energy in solution: -272.862755 a.u.

(U)M06/BSI SCF energy: -272.7749083 a.u.

(U)M06/BSI SCF Gibbs free energy: -272.644233 a.u.

C	0.14045700	0.36673500	0.00000000
C	-0.63020100	0.76106300	1.25513400
H	-1.64991000	0.35403100	1.26334900
H	-0.10513000	0.40147800	2.14991600
H	-0.71510600	1.85371600	1.32054200
C	-0.63020100	0.76106300	-1.25513400
H	-0.71510600	1.85371600	-1.32054200
H	-0.10513000	0.40147800	-2.14991600
H	-1.64991000	0.35403100	-1.26334900
C	1.50742300	1.03081800	0.00000000
H	2.07485900	0.72593600	0.88821900
H	2.07485900	0.72593600	-0.88821900
H	1.41377300	2.12434200	0.00000000
O	0.44694500	-1.02832900	0.00000000
C	-0.63020100	-1.91936100	0.00000000
H	-0.20362600	-2.92823200	0.00000000
H	-1.26939600	-1.82085400	0.89348700
H	-1.26939600	-1.82085400	-0.89348700

2

(U)M06/BSII SCF energy in solution: -3353.0810356 a.u.

(U)M06/BSI SCF energy: -3358.6165472 a.u.

(U)M06/BSI SCF Gibbs free energy: -3358.430697 a.u.

O	-5.60096700	-1.82502700	0.03029400
O	-3.86897100	0.12290500	1.39194300
O	-3.17403500	-2.30611100	1.46771200

O	-3.16088000	-2.56743300	-1.22284600
O	-3.85161000	0.05209500	-1.19802000
O	-2.54897100	2.13461100	2.74602000
O	-1.59610600	-0.52832300	2.67965200
O	-0.10913200	1.53323500	1.62660200
O	-2.29917100	1.85247000	-0.02085300
O	-1.15861800	-3.35737500	3.00523500
O	-0.96591500	-3.22157500	0.16787100
O	0.63700800	-1.67676600	1.71399700
O	-1.66854200	-0.67674300	0.06365700
O	-1.11395100	-3.66195100	-2.68188100
O	-1.63768700	-0.81758000	-2.55997600
O	-2.62972800	1.83231400	-2.86369700
W	-3.92838700	-1.40341100	-0.01513800
W	-1.84373600	1.03359900	1.63584400
W	-1.18563900	-2.18791000	1.75847600
W	-1.15976200	-2.38467000	-1.54877800
W	-2.00488100	0.81052000	-1.63875400
W	1.84817100	2.02264000	1.57819600
W	2.49612900	-1.21835500	1.68610400
O	0.64109400	-1.87376300	-1.54813400
O	-0.20060500	1.30241100	-1.63723000
O	3.68139600	2.12432700	1.20228800
O	1.43758200	2.83058500	-0.10329300
O	2.14879000	0.29006300	-0.01802200
O	1.74602200	3.28979700	2.72379000
O	2.11432200	0.43856200	2.60631200
O	4.28830600	-0.42919600	1.30867700
O	2.74260800	-2.25382400	0.09450900
O	3.05304800	-2.25209300	2.92993300
W	2.49014300	-1.40437400	-1.60829800
W	1.67921200	1.79765900	-1.71485500
W	4.42033000	0.81575400	-0.10881300
O	4.29338200	-0.58707600	-1.34902500
O	3.02011600	-2.55274000	-2.75887900
O	2.04600900	0.16007200	-2.63366100
O	3.59966600	1.97011700	-1.41148900
O	1.58124300	2.95815500	-2.96718100
O	6.08678900	1.25767100	-0.14521300
C	-5.32223500	4.51758300	-0.29424900
C	-6.10070800	5.82704400	-0.35805100
H	-7.04325500	5.67765500	-0.90519700
H	-6.34351100	6.17138400	0.65767700
H	-5.51627300	6.60717900	-0.86654500

C	-4.98487500	4.04594000	-1.70470300
H	-4.36559200	4.79284100	-2.22228200
H	-4.41219100	3.10961800	-1.70969400
H	-5.90989900	3.89387600	-2.28093900
C	-4.04861400	4.70557800	0.52233800
H	-4.29608900	4.93078600	1.57006200
H	-3.40759800	3.81404300	0.49891800
H	-3.46081700	5.54024000	0.11339900
O	-6.23511400	3.62412600	0.33588400
C	-5.70106800	2.35917800	0.69567200
H	-4.98789200	2.42922100	1.53005900
H	-6.54828600	1.73947300	1.01329900
H	-5.19959000	1.84684700	-0.13936900

TS1

(U)M06/BSII SCF energy in solution: -3353.0786527 a.u.

(U)M06/BSI SCF energy: -3358.5966526 a.u.

(U)M06/BSI SCF Gibbs free energy: -3358.410076 a.u.

O	-5.62173900	-1.61837500	0.03395700
O	-3.90914900	0.36272400	1.29456100
O	-3.22321500	-2.13309800	1.52755900
O	-3.17485200	-2.55699000	-1.11391000
O	-3.78750300	0.03119700	-1.35387500
O	-2.54500500	2.38912900	2.51424000
O	-1.64493800	-0.29936800	2.65970500
O	-0.11648200	1.63772800	1.46949000
O	-2.24005900	1.91951100	-0.24133600
O	-1.26772200	-3.10845600	3.19291600
O	-1.01681000	-3.15376200	0.34426400
O	0.57954100	-1.54867500	1.82096500
O	-1.70196900	-0.59870500	0.07034100
O	-1.12887800	-3.79682600	-2.46890900
O	-1.57674500	-0.94616000	-2.55036200
O	-2.53515900	1.72432700	-3.06534200
W	-3.92520700	-1.28189000	-0.00027800
W	-1.87387400	1.18146900	1.49536700
W	-1.25271000	-2.02283100	1.87184600
W	-1.16649500	-2.44253700	-1.42834500
W	-1.95944700	0.76217800	-1.76633300
W	1.82988900	2.10531500	1.43984800
W	2.44650700	-1.12103300	1.80666000
O	0.64544200	-1.97015200	-1.41902700
O	-0.12869400	1.19824500	-1.77149600
O	3.68548300	2.15468900	1.10733400

O	1.49234400	2.80523200	-0.30609200
O	2.15316800	0.26796500	-0.01701100
O	1.72604800	3.45529800	2.48787300
O	2.06698500	0.59994000	2.59179900
O	4.25103100	-0.39270500	1.40992500
O	2.70310500	-2.27338100	0.29446700
O	2.95497500	-2.07221000	3.13521800
W	2.51026900	-1.54071900	-1.46712900
W	1.74557300	1.65271300	-1.83204200
W	4.43382100	0.76032300	-0.08644900
O	4.31179000	-0.74032400	-1.22135700
O	3.04041900	-2.78173800	-2.51880100
O	2.11893700	-0.05502000	-2.61828500
O	3.67280100	1.81537400	-1.49251000
O	1.71089600	2.72345600	-3.16673600
O	6.11049600	1.16708800	-0.11333300
C	-5.29755400	4.20759800	-0.17696800
C	-6.29337600	5.35439900	-0.04425000
H	-7.21012400	5.13817400	-0.61230300
H	-6.56465200	5.49282700	1.01150100
H	-5.85608100	6.28999900	-0.42038900
C	-4.97386000	3.96145000	-1.64405700
H	-4.61894800	4.90114000	-2.09071100
H	-4.17735100	3.21901000	-1.78807000
H	-5.86947600	3.63513200	-2.19375100
C	-4.03266600	4.50600900	0.60758400
H	-4.25572700	4.60428000	1.67744500
H	-3.29421200	3.70558400	0.48190400
H	-3.58175200	5.44255300	0.24619400
O	-6.00342600	3.10697700	0.42597700
C	-5.62528200	1.81479300	0.14387900
H	-4.67907900	1.31879000	0.81843900
H	-6.43682500	1.13767200	0.43605500
H	-5.26437300	1.62481600	-0.87373000

3

(U)M06/BSII SCF energy in solution: -272.2006046 a.u.

(U)M06/BSI SCF energy: -272.1128788 a.u.

(U)M06/BSI SCF Gibbs free energy: -271.994893 a.u.

C	0.35704500	0.00791300	0.01310700
C	0.39480300	-0.38104100	1.48334700
H	-0.43292900	0.07656400	2.03951800
H	0.31478000	-1.47041800	1.58849700
H	1.33875600	-0.05462600	1.93916300

C	0.43963200	1.51767900	-0.16797300
H	1.41763700	1.88166300	0.17269400
H	0.32284400	1.77925200	-1.22739800
H	-0.32694700	2.05087900	0.40816600
C	1.47730500	-0.67410600	-0.75119400
H	1.39007000	-1.76368600	-0.65945300
H	1.42688300	-0.41404200	-1.81590400
H	2.45553500	-0.36590100	-0.36096000
O	-0.84039100	-0.50686200	-0.59999600
C	-2.03151900	-0.13014500	-0.08194800
H	-2.87488600	-0.57591100	-0.60076000
H	-2.13221000	0.86932100	0.34437700

N-benzylidene-4-methylbenzenesulfonamide

(U)M06/BSII SCF energy in solution: -1144.3345819 a.u.

(U)M06/BSI SCF energy: -1144.0952261 a.u.

(U)M06/BSI SCF Gibbs free energy: -1143.903889 a.u.

S	-0.61713700	-1.64370500	0.27911300
O	-0.45077300	-2.38579400	-0.96885400
O	-0.80702900	-2.34913200	1.53641700
C	-1.93190600	-0.47667100	0.06593000
C	-2.48813000	-0.28906300	-1.19287300
C	-2.38618400	0.23355900	1.17404700
C	-3.52004500	0.62957400	-1.33952300
H	-2.11506400	-0.86508500	-2.03695800
C	-3.41329000	1.14896300	1.00696100
H	-1.93685800	0.05877300	2.14984300
C	-3.99608500	1.35733700	-0.24768600
H	-3.96852500	0.78508300	-2.32069900
H	-3.77878900	1.71403300	1.86455400
N	0.68595400	-0.57656900	0.53788700
C	1.67521900	-0.72152100	-0.26456600
H	1.64182400	-1.45974200	-1.08238600
C	2.88990500	0.07545700	-0.15276500
C	3.91566300	-0.12432500	-1.08104200
C	3.04736400	1.02818400	0.86122200
C	5.08609000	0.61875300	-1.00239800
H	3.78721000	-0.86980400	-1.86615700
C	4.21564600	1.76814300	0.93779500
H	2.24020300	1.16631800	1.57799400
C	5.23485500	1.56443400	0.00698700
H	5.88269500	0.46039000	-1.72642700
H	4.33966900	2.50781700	1.72637800
H	6.15194600	2.14746700	0.07216400

C	-5.12903100	2.32566200	-0.40532700
H	-5.22387000	2.67271500	-1.44094500
H	-6.08570300	1.86134900	-0.12792700
H	-5.00023900	3.20442500	0.23847900

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(U)M06/BSII SCF energy in solution: -1416.5451866 a.u.

(U)M06/BSI SCF energy: -1416.2242444 a.u.

(U)M06/BSI SCF Gibbs free energy: -1415.89089 a.u.

S	1.01513400	-0.89414600	-0.13255800
O	0.58331500	-1.50601100	1.12701500
O	0.76498600	-1.60974200	-1.38306400
C	2.74454800	-0.53752200	-0.01522200
C	3.40289400	-0.72748700	1.19183400
C	3.41711100	-0.07626500	-1.14447100
C	4.76242900	-0.44655300	1.26637000
H	2.84949400	-1.09433900	2.05349600
C	4.77075900	0.20255300	-1.04938700
H	2.87731200	0.05565600	-2.08034700
C	5.46237300	0.01964300	0.15366300
H	5.29227000	-0.59297400	2.20749500
H	5.31081800	0.56667500	-1.92373300
N	0.38628200	0.65283800	-0.33033900
C	-0.69860900	0.88093400	0.33647800
H	-1.08195900	0.16942300	1.08140900
C	-1.41604300	2.14558200	0.22672900
C	-2.63147800	2.29383700	0.90302800
C	-0.91482200	3.20552800	-0.53639700
C	-3.33669700	3.48562900	0.82222400
H	-3.02587800	1.45163000	1.47361900
C	-1.61918600	4.39786500	-0.61090200
H	0.03072900	3.07232000	-1.05862100
C	-2.82852300	4.54009500	0.06743000
H	-4.28468400	3.59434200	1.34548100
H	-1.22630500	5.22406100	-1.20074500
H	-3.37890300	5.47737600	0.00521200
C	6.93216600	0.30357500	0.22836100
H	7.28442400	0.34654500	1.26543700
H	7.51223400	-0.47587500	-0.28484500
H	7.18157900	1.25697700	-0.25464900
C	-3.48966500	-2.35919900	0.04233300
C	-2.81648300	-2.16535300	1.39114700
H	-1.75119700	-1.92103900	1.28376800
H	-3.31928300	-1.36739300	1.95506400

H	-2.88215100	-3.09055400	1.97894700
C	-2.74616600	-3.38140900	-0.80312800
H	-2.86302500	-4.37373000	-0.34900500
H	-3.16191000	-3.41897300	-1.81864400
H	-1.66947000	-3.17840900	-0.86655000
C	-4.94354500	-2.76052200	0.21368800
H	-5.48718500	-1.99021600	0.77494100
H	-5.42774000	-2.88054700	-0.76354100
H	-5.01755300	-3.70890300	0.76029500
O	-3.57851600	-1.07592600	-0.63108500
C	-2.47497800	-0.53265600	-1.16252400
H	-2.67968800	0.38467300	-1.70958800
H	-1.64283900	-1.16647700	-1.47205300

TS2

(U)M06/BSII SCF energy in solution: -1416.5427293 a.u.

(U)M06/BSI SCF energy: -1416.2228506 a.u.

(U)M06/BSI SCF Gibbs free energy: -1415.885035 a.u.

S	1.01852500	-0.94026800	-0.13556400
O	0.61780800	-1.57667000	1.12545000
O	0.83047800	-1.70453300	-1.37415600
C	2.72501400	-0.48787500	-0.01085700
C	3.37785500	-0.61246700	1.20716600
C	3.38720600	-0.01961400	-1.14344800
C	4.71973300	-0.25723500	1.29046700
H	2.83371400	-0.98831500	2.07085000
C	4.72268300	0.33344500	-1.04032700
H	2.85341100	0.05827800	-2.08875900
C	5.40769900	0.21898900	0.17506500
H	5.24469200	-0.35262300	2.24090100
H	5.25424300	0.70280200	-1.91787000
N	0.30626500	0.54605800	-0.34772600
C	-0.87796200	0.67083300	0.22762500
H	-1.18462500	-0.00903900	1.03503000
C	-1.58308600	1.95661200	0.17936600
C	-2.75881300	2.12049700	0.91853600
C	-1.11239400	3.01467700	-0.60490500
C	-3.45054600	3.32346100	0.88118200
H	-3.12936700	1.28872300	1.51871700
C	-1.80531700	4.21646200	-0.63926200
H	-0.19445800	2.87450600	-1.17289900
C	-2.97447600	4.37463000	0.10235100
H	-4.36347300	3.44315900	1.46189900
H	-1.43151400	5.03910700	-1.24672900

H	-3.51483100	5.31930900	0.07327600
C	6.85689700	0.59278800	0.25894400
H	7.22273500	0.56808800	1.29185000
H	7.47920700	-0.09440900	-0.33050600
H	7.03331600	1.60132000	-0.13751700
C	-3.30235300	-2.28290300	0.04974300
C	-2.75401100	-2.20684100	1.46403800
H	-1.67397300	-2.00938000	1.47446000
H	-3.27715800	-1.43085100	2.03913400
H	-2.91583700	-3.16799800	1.96981300
C	-2.51147100	-3.26531800	-0.79521400
H	-2.69444600	-4.27710200	-0.41192200
H	-2.83884400	-3.23738300	-1.84309200
H	-1.42801600	-3.09397600	-0.75344600
C	-4.77850800	-2.63517200	0.05533800
H	-5.34807100	-1.88502000	0.61778300
H	-5.17215400	-2.67246000	-0.96801200
H	-4.93279800	-3.61436100	0.52523700
O	-3.29633100	-0.93545500	-0.53016100
C	-2.21958800	-0.45350700	-1.13803700
H	-2.43932600	0.42430000	-1.74476500
H	-1.44971600	-1.14031100	-1.49603000

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(U)M06/BSII SCF energy in solution: -1416.5550189 a.u.

(U)M06/BSI SCF energy: -1416.2364172 a.u.

(U)M06/BSI SCF Gibbs free energy: -1415.897961 a.u.

S	1.15363100	-1.20830200	-0.22875100
O	0.72836300	-1.84093800	1.01900500
O	1.04779400	-1.94574800	-1.48737400
C	2.80780500	-0.62413400	-0.02660700
C	3.40839400	-0.69265300	1.22363600
C	3.48466800	-0.11323700	-1.13320900
C	4.71418200	-0.23803200	1.36498900
H	2.85493700	-1.10384100	2.06491200
C	4.78303500	0.33824700	-0.97069800
H	2.99161000	-0.08022900	-2.10286500
C	5.41553300	0.28286700	0.27770100
H	5.20002100	-0.28930100	2.33898100
H	5.32719200	0.74051000	-1.82542000
N	0.35113300	0.24694600	-0.50517500
C	-0.98744100	0.28359500	-0.01168000
H	-1.06309700	-0.20070200	0.97711400
C	-1.51381500	1.69356100	0.04326900

C	-2.43280300	2.04541200	1.02948000
C	-1.13792500	2.64067600	-0.90743600
C	-2.96602200	3.32852500	1.07146300
H	-2.73348100	1.30293400	1.76962400
C	-1.66925700	3.92451400	-0.86603700
H	-0.41312400	2.36574500	-1.67302100
C	-2.58415600	4.27176400	0.12338900
H	-3.68111000	3.59252600	1.84890700
H	-1.36553700	4.65919100	-1.61017800
H	-2.99864000	5.27803100	0.15584600
C	6.82246700	0.77591500	0.42716400
H	7.18222600	0.67120700	1.45690000
H	7.50905700	0.22166100	-0.22656700
H	6.90372900	1.83508900	0.14879800
C	-3.72563400	-1.75384200	0.13242100
C	-2.88611100	-2.14478700	1.34117300
H	-1.85612300	-2.41904600	1.07667000
H	-2.85121400	-1.32686700	2.07419700
H	-3.33883900	-3.01476000	1.83524100
C	-3.82198200	-2.90398000	-0.86140600
H	-4.33810700	-3.75776600	-0.40297500
H	-4.38957900	-2.59001700	-1.74649200
H	-2.83490900	-3.25626700	-1.18763200
C	-5.11309300	-1.32257700	0.57404600
H	-5.04401700	-0.45830100	1.24712400
H	-5.71588300	-1.03080200	-0.29473600
H	-5.62435300	-2.13910200	1.09965800
O	-3.21225700	-0.57922800	-0.52670800
C	-1.90054300	-0.58552400	-0.97259400
H	-1.85606500	-0.11039900	-1.96290700
H	-1.47573700	-1.59581900	-1.05870600

6

(U)M06/BSII SCF energy in solution: -1416.7392982 a.u.

(U)M06/BSI SCF energy: -1416.3439248 a.u.

(U)M06/BSI SCF Gibbs free energy: -1416.003312 a.u.

S	1.01736100	-0.78148200	-1.85072800
O	0.55011200	-2.15006100	-1.49399800
O	1.78739100	-0.67834800	-3.09673500
C	2.20601900	-0.41686100	-0.52339100
C	2.78519600	-1.43743100	0.21952100
C	2.55500900	0.90724600	-0.26661200
C	3.72179900	-1.13579400	1.20470300
H	2.48274000	-2.46363300	0.01641700

C	3.48915400	1.20071800	0.71688200
H	2.06175600	1.69541500	-0.83668600
C	4.08790900	0.18359100	1.46666200
H	4.17549400	-1.93963800	1.78869900
H	3.75909600	2.23966900	0.91910800
N	-0.06125700	0.35479800	-1.78346200
C	-0.88653500	0.31830400	-0.59237100
H	-0.35651700	-0.08884900	0.29461700
C	-1.33210600	1.71625600	-0.21251400
C	-1.97718200	1.95044400	1.00598500
C	-1.12434100	2.79516800	-1.07199800
C	-2.40322600	3.22680300	1.35488200
H	-2.15255100	1.10967500	1.67728000
C	-1.55117900	4.07391000	-0.72514400
H	-0.60732600	2.59402200	-2.00901800
C	-2.19212700	4.29722200	0.48938200
H	-2.90071600	3.38854400	2.31194100
H	-1.37699000	4.90543900	-1.40939000
H	-2.52202900	5.29988600	0.76340700
C	5.07991200	0.51664500	2.54334300
H	5.58743300	-0.38280200	2.91540100
H	5.85187000	1.21078100	2.18233200
H	4.59739900	1.00081900	3.40521000
C	-2.68598800	-2.13126400	0.94816200
C	-1.25446800	-2.31510400	1.44453000
H	-0.53589200	-2.36029500	0.61373000
H	-0.97104200	-1.48857500	2.11203400
H	-1.17670900	-3.25410300	2.01304900
C	-3.07374500	-3.29179200	0.03357200
H	-3.08966600	-4.23418100	0.59955000
H	-4.07388100	-3.11975100	-0.38735100
H	-2.35948800	-3.41425800	-0.79041600
C	-3.64239100	-2.06766700	2.13048200
H	-3.38490700	-1.21667500	2.77573400
H	-4.67288800	-1.92762500	1.77770500
H	-3.59380600	-2.98863000	2.72787500
O	-2.88453100	-0.88071700	0.29573500
C	-2.09480000	-0.59931000	-0.85094100
H	-2.75021800	-0.10410500	-1.58405000
H	-1.70538600	-1.51449300	-1.31212000

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(U)M06/BSII SCF energy in solution: -4497.5197461 a.u.

(U)M06/BSI SCF energy: -4502.870248 a.u.

(U)M06/BSI SCF Gibbs free energy: -4502.452573 a.u.

O	4.49019000	1.83077200	-1.84087800
O	3.25650600	0.40754900	0.34473200
O	2.29156000	2.82831600	-0.37821700
O	1.80829300	1.84586900	-2.81463600
O	2.73940600	-0.48080400	-2.08299400
O	2.42419600	-0.82241700	2.59525800
O	1.18205300	1.54851200	1.73650900
O	-0.21473700	-0.80661200	1.82795800
O	1.63460100	-1.74869700	0.02686700
O	0.46064800	4.21841500	1.08833600
O	-0.15840400	2.97013100	-1.42586500
O	-1.32446600	2.14283400	0.87796800
O	0.84713400	0.64863600	-0.62990000
O	-0.52055500	2.25362900	-4.18689600
O	0.25024800	-0.29114300	-3.08146900
O	1.50591200	-2.84393900	-2.61153200
W	2.91405700	1.40480300	-1.33288000
W	1.43636900	-0.30842600	1.29727900
W	0.35778800	2.65146600	0.40843000
W	-0.11362200	1.54531500	-2.69169700
W	1.15103500	-1.39224700	-1.78780200
W	-2.10275900	-1.32384700	2.38381600
W	-3.19350100	1.64331700	1.44828000
O	-1.85307900	1.03092800	-2.09816100
O	-0.72065600	-1.87341400	-1.19343600
O	-3.95146800	-1.59524600	2.46775500
O	-1.90865000	-2.72581200	1.11192600
O	-2.86209200	-0.41091000	0.35589100
O	-1.66754600	-2.02070000	3.87857500
O	-2.32449800	0.54017200	2.76284600
O	-4.80210600	0.74482100	1.71964200
O	-3.66813400	1.99779400	-0.37169500
O	-3.54544200	3.09472300	2.27448200
W	-3.62111300	0.54596200	-1.63450600
W	-2.40458600	-2.37789000	-0.72624800
W	-5.02521600	-1.07289600	0.87737500
O	-5.25404100	-0.12358500	-0.72960500
O	-4.45635100	1.14441300	-2.99766200
O	-3.23504900	-1.27223700	-2.07348700
O	-4.35364600	-2.54160700	0.01593000
O	-2.50085800	-3.94234800	-1.40436800
O	-6.62090400	-1.50876400	1.34847000
H	4.22177800	0.17491400	0.67128300

S	6.62057800	0.63028900	2.07682100
O	6.62365400	0.13665000	3.47166000
O	7.97604300	0.92657300	1.55155500
C	5.70174500	2.15969000	2.08234200
C	4.40443900	2.17648300	2.59055900
C	6.26482300	3.30644300	1.54325500
C	3.66173400	3.34553600	2.52398200
H	3.96690400	1.26326600	2.99487900
C	5.51491400	4.47898200	1.50039900
H	7.27550100	3.25259600	1.14216400
C	4.20320600	4.50968300	1.97062300
H	2.62133600	3.33859900	2.85184600
H	5.94291200	5.38261400	1.05826600
C	6.17276900	-2.64676000	1.39043600
C	5.07419200	-2.79097400	2.23803500
C	7.08615700	-3.69808400	1.29359800
C	4.89084000	-3.96447300	2.96221300
H	4.36550200	-1.96684900	2.33138300
C	6.91068500	-4.87090400	2.02256800
H	7.93837200	-3.59069400	0.62012900
C	5.80610800	-5.00945700	2.85967500
H	4.01892000	-4.05682600	3.60966000
H	7.63797900	-5.68168800	1.93417000
H	5.65900500	-5.92885700	3.43015000
C	3.35220300	5.73716400	1.84167900
H	2.95567200	6.06286800	2.81509400
H	3.91416700	6.57476300	1.40374500
H	2.48004900	5.52458200	1.20689000
C	6.32159700	-1.40863700	0.52241700
H	7.40095200	-1.26106900	0.32121800
C	5.64411100	-1.65239100	-0.82792500
H	5.77277700	-0.75560400	-1.45679500
H	4.56182800	-1.77502000	-0.66070600
O	6.22372000	-2.78735000	-1.44334200
C	5.35999800	-3.66550500	-2.15796500
C	4.73668800	-2.94746300	-3.34873200
H	4.10498700	-3.63267200	-3.93153300
H	4.10026300	-2.11142600	-3.02924900
H	5.53208700	-2.55112200	-3.99834100
C	4.29498000	-4.28159400	-1.25393800
H	3.55613100	-3.55249900	-0.89923700
H	3.73320400	-5.04656400	-1.80901700
H	4.77197700	-4.74587900	-0.37854900
C	6.30336200	-4.76294200	-2.63571800

H	6.76748100	-5.25513900	-1.76872500
H	5.76212100	-5.51578600	-3.22673400
H	7.10138000	-4.32983800	-3.25574800
N	5.71755900	-0.20893600	1.06292000

TS3

(U)M06/BSII SCF energy in solution: -4497.5235839 a.u.

(U)M06/BSI SCF energy: -4502.864302 a.u.

(U)M06/BSI SCF Gibbs free energy: -4502.44714 a.u.

O	4.05850400	-3.08953700	-0.95421000
O	3.07167700	-0.39573200	-1.06262500
O	1.74735500	-2.35941300	-2.40407800
O	1.40349900	-3.61156200	-0.07147900
O	2.66654700	-1.70074200	1.18790200
O	2.43180700	2.20487600	-1.36935900
O	0.85532500	0.17378400	-2.60565600
O	-0.20152800	1.82034700	-0.70029200
O	1.71545200	0.82538600	0.97595000
O	-0.27822700	-1.91866800	-4.19561200
O	-0.70110800	-3.04433700	-1.59567600
O	-1.72252500	-0.62263100	-2.26258500
O	0.63204700	-1.09168900	-0.38841500
O	-0.96040100	-4.73622000	0.71123400
O	0.16556100	-2.38118200	1.92722900
O	1.77204200	-0.55271300	3.48248000
W	2.56456500	-2.26693500	-0.77901800
W	1.36333000	0.94404500	-0.92489300
W	-0.13447000	-1.46534900	-2.55686000
W	-0.44822300	-3.16625300	0.28894500
W	1.21401800	-0.77523100	1.88401100
W	-1.98798700	2.74845900	-0.42489000
W	-3.49933900	0.29541700	-2.02620000
O	-2.09872300	-2.22226600	0.51835400
O	-0.57252400	0.15342000	2.10649400
O	-3.77769200	3.15597600	-0.06262000
O	-1.59819000	2.59475700	1.43317700
O	-2.88402700	0.67407200	0.21579900
O	-1.44954100	4.30850100	-0.85947700
O	-2.48176900	1.92636300	-2.08215900
O	-4.96171500	1.21088600	-1.32157200
O	-4.02605100	-1.30185900	-1.11472300
O	-4.05537200	0.08199000	-3.62608700
W	-3.77544400	-1.40166000	0.79246700
W	-2.16079300	0.99627400	2.36841300

W	-4.92847300	1.68926400	0.63511400
O	-5.29840900	-0.12929400	0.92415100
O	-4.69673600	-2.75957400	1.26512400
O	-3.15069200	-0.66009000	2.43773500
O	-4.06086100	1.86101600	2.23812800
O	-2.04403200	1.44760200	4.01245300
O	-6.44393500	2.47570700	0.85009400
H	4.14232800	-0.06961400	-1.15778200
S	6.24910300	0.99306900	-2.33832900
O	7.61937200	0.50421400	-2.60149700
O	5.33144900	1.07449900	-3.47286900
C	6.51033300	2.68024100	-1.74755100
C	7.79334900	3.18965300	-1.60556700
C	5.40558200	3.41714300	-1.32205300
C	7.97968200	4.43961800	-1.01861800
H	8.63238000	2.57984500	-1.93755900
C	5.60553000	4.65607500	-0.73221100
H	4.39977400	3.00113900	-1.42357200
C	6.89157700	5.17773400	-0.55873100
H	8.98993200	4.83828700	-0.88866500
H	4.74392000	5.22054300	-0.37096700
C	6.04187000	1.20652800	1.10550400
C	4.72295800	1.49274800	1.45904000
C	7.06758400	1.92469300	1.71572100
C	4.43059300	2.47833400	2.39326000
H	3.90326900	0.94666000	0.99504800
C	6.78360300	2.92311300	2.64536500
H	8.10194600	1.70551600	1.44106800
C	5.46330300	3.20207000	2.98860600
H	3.38710900	2.66906600	2.64260600
H	7.60014500	3.48904800	3.10021400
H	5.23794400	3.98311900	3.71683100
C	7.08456300	6.48084600	0.16089400
H	8.11153600	6.85788400	0.05019900
H	6.39697500	7.25680900	-0.20563500
H	6.88758600	6.36640000	1.23769800
C	6.32888200	0.11720300	0.09027200
H	7.40711100	0.14689400	-0.15291400
C	6.05721500	-1.25381700	0.69389100
H	6.23243200	-2.02589800	-0.07095700
H	4.99818600	-1.31633200	0.98409700
O	6.91657400	-1.43834200	1.80883000
C	6.37905600	-2.15156300	2.91551400
C	5.87203200	-3.52562800	2.48780900

H	5.55306700	-4.10729100	3.36533500
H	5.01130100	-3.44428000	1.81159700
H	6.66929100	-4.07787100	1.96826000
C	5.27492400	-1.35964500	3.60962300
H	4.36540600	-1.28462700	3.00026400
H	4.98833400	-1.85135300	4.55121400
H	5.62565000	-0.34188700	3.83334800
C	7.57176500	-2.29872400	3.85182700
H	7.95036500	-1.30362700	4.12389000
H	7.28917900	-2.83473500	4.76944600
H	8.38070900	-2.84993100	3.35119800
N	5.52932300	0.24327500	-1.12775800

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(U)M06/BSII SCF energy in solution: -1417.2234441 a.u.

(U)M06/BSI SCF energy: -1416.8967518 a.u.

(U)M06/BSI SCF Gibbs free energy: -1416.544334 a.u.

S	1.13653600	-1.21960900	-1.60273100
O	0.45101400	-2.39461800	-1.06906300
O	1.74191400	-1.26086900	-2.92512700
C	2.33096100	-0.71496000	-0.39294700
C	2.39112500	-1.36766500	0.83081600
C	3.20468300	0.32539700	-0.70329200
C	3.34287600	-0.96455600	1.76175900
H	1.70281000	-2.18449200	1.03997100
C	4.14669000	0.71094000	0.23470200
H	3.13845700	0.81764000	-1.67177900
C	4.22888600	0.07397300	1.47938600
H	3.40034500	-1.46899700	2.72597800
H	4.83803900	1.52212000	0.00543700
C	-0.85218900	0.29071000	-0.57059800
H	-0.40776900	-0.15111300	0.33512200
C	-1.12868300	1.75246800	-0.30214000
C	-1.76979200	2.11947100	0.88398100
C	-0.79914600	2.74827000	-1.22002500
C	-2.07657300	3.44897800	1.14202200
H	-2.03934900	1.34683500	1.60239600
C	-1.10744700	4.08094800	-0.96332500
H	-0.27107600	2.48830600	-2.13585400
C	-1.74801600	4.43594500	0.21731000
H	-2.57333500	3.71650300	2.07333700
H	-0.83841600	4.84530500	-1.69078600
H	-1.98659600	5.47868300	0.42009900
C	5.25490300	0.51246100	2.47960400

H	5.22179200	-0.09779000	3.38919700
H	6.26931300	0.44341800	2.06501400
H	5.10136600	1.55969200	2.77265300
C	-3.21659800	-1.68643800	0.92088100
C	-1.90403500	-2.12569400	1.55982900
H	-1.15434600	-2.41486300	0.81057300
H	-1.49090900	-1.32158700	2.18622300
H	-2.07779100	-2.99723000	2.20545300
C	-3.80036900	-2.80168600	0.06217600
H	-4.05157200	-3.66952500	0.68620600
H	-4.71592200	-2.45443600	-0.43351200
H	-3.09580600	-3.14662700	-0.70563200
C	-4.21292600	-1.28117000	1.99377000
H	-3.80994700	-0.45873900	2.59933600
H	-5.14819700	-0.93935000	1.53354800
H	-4.43526900	-2.12646800	2.65759400
O	-3.05720100	-0.48776100	0.14560200
C	-2.13047600	-0.49691400	-0.90349200
H	-2.60313400	-0.01941100	-1.78008200
H	-1.83601100	-1.51470600	-1.19721100
N	0.12983700	0.11895600	-1.64699900
H	-0.23919100	0.21098000	-2.59439100

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(U)M06/BSII SCF energy in solution: -1416.545325 a.u.

(U)M06/BSI SCF energy: -1416.2208153 a.u.

(U)M06/BSI SCF Gibbs free energy: -1415.886295 a.u.

S	1.21646400	-0.88357300	0.73884600
O	1.14940000	-0.80906100	2.19821800
O	0.86564400	-2.12126700	0.05575800
C	2.83897500	-0.38683100	0.22975600
C	3.73800600	0.09584200	1.17114000
C	3.18523200	-0.49468200	-1.11494200
C	5.00728700	0.47825700	0.75329600
H	3.43841300	0.16168300	2.21481700
C	4.45319400	-0.10331200	-1.51369300
H	2.46301700	-0.88530500	-1.82948500
C	5.38180100	0.38465000	-0.58743800
H	5.72395100	0.85640000	1.48228700
H	4.73783200	-0.17918700	-2.56342000
N	0.27940400	0.32542800	0.01146700
C	-0.56205100	0.89335800	0.80323700
H	-0.54837900	0.70350800	1.88677500
C	-1.54526100	1.85590000	0.31735900

C	-2.43479200	2.43734300	1.22677600
C	-1.62944400	2.19095800	-1.03962700
C	-3.40320300	3.33080800	0.78912600
H	-2.36309700	2.17439400	2.28310100
C	-2.59528900	3.08567200	-1.47415100
H	-0.92686900	1.73524100	-1.73513200
C	-3.48456200	3.65374100	-0.56255300
H	-4.09513000	3.77641900	1.50106100
H	-2.65999000	3.34365900	-2.52955000
H	-4.24382200	4.35292700	-0.90860600
C	6.75888500	0.77471200	-1.03248800
H	7.26009200	1.40774300	-0.29103200
H	7.38988400	-0.11155100	-1.18739200
H	6.73429000	1.31995700	-1.98439000
C	-3.27441500	-2.01793300	-0.60685600
C	-2.11713400	-1.68115600	-1.53244600
H	-1.64936100	-0.72885300	-1.25142100
H	-1.34126700	-2.45366500	-1.47028200
H	-2.47148700	-1.60495700	-2.56974300
C	-4.33681800	-0.92961200	-0.62407200
H	-4.82728000	-0.92372000	-1.60588400
H	-5.10562900	-1.11820600	0.13768700
H	-3.91446500	0.07221700	-0.46445200
C	-3.88207200	-3.36228400	-0.96453200
H	-3.12476400	-4.15066400	-0.87744900
H	-4.71245600	-3.60487200	-0.28916900
H	-4.25947000	-3.35132000	-1.99493900
O	-2.73647300	-2.23049700	0.72026000
C	-2.44937600	-1.17865100	1.49757400
H	-1.88444100	-1.45579100	2.38532800
H	-3.16118200	-0.35096100	1.55278300

TS4

(U)M06/BSII SCF energy in solution: -1416.5357607 a.u.

(U)M06/BSI SCF energy: -1416.2128311 a.u.

(U)M06/BSI SCF Gibbs free energy: -1415.877545 a.u.

S	0.87365100	-0.96485600	1.27300800
O	1.04342100	-0.57480800	2.67329000
O	0.50316400	-2.33136300	0.93812600
C	2.36938800	-0.56967600	0.39759300
C	3.29769800	0.29203500	0.96747000
C	2.56866300	-1.11284900	-0.86789200
C	4.44780800	0.60803100	0.25441100
H	3.11834700	0.69414300	1.96292600

C	3.72091100	-0.78465400	-1.56594300
H	1.82567700	-1.78962800	-1.28706700
C	4.67615400	0.07588200	-1.01567900
H	5.18690700	1.27919400	0.69216600
H	3.89037400	-1.20359600	-2.55816300
N	-0.23134300	0.04995800	0.49134900
C	-0.30545000	1.27171200	0.98186600
H	0.15217200	1.52238900	1.94919200
C	-1.08280300	2.29298800	0.32586000
C	-1.29253700	3.52518100	0.96823600
C	-1.65579300	2.08885500	-0.94358100
C	-2.05761900	4.51426600	0.37020400
H	-0.84877400	3.69117000	1.95036000
C	-2.42225800	3.07977700	-1.53509500
H	-1.46451600	1.14744400	-1.45733200
C	-2.62995700	4.29497900	-0.88154500
H	-2.21274700	5.46264400	0.88176300
H	-2.85719300	2.91111000	-2.51915800
H	-3.23227200	5.07110500	-1.35018800
C	5.93221000	0.39672400	-1.76825800
H	6.37884200	1.33808300	-1.42692600
H	6.68690900	-0.39049200	-1.63189700
H	5.74587500	0.47952100	-2.84618000
C	-2.98039100	-2.27185200	-0.68246900
C	-1.73409100	-2.22621900	-1.54985400
H	-1.21111200	-1.26830100	-1.43464500
H	-1.03923000	-3.02052000	-1.25147700
H	-2.00919500	-2.36403600	-2.60421500
C	-3.96939200	-1.17691500	-1.04746600
H	-4.39327600	-1.39602100	-2.03562500
H	-4.79563700	-1.13948600	-0.32498900
H	-3.50463400	-0.18383400	-1.10610500
C	-3.64312500	-3.63472700	-0.74651800
H	-2.94706800	-4.40782400	-0.40027000
H	-4.53754800	-3.66369600	-0.11145100
H	-3.93856700	-3.86496800	-1.77777100
O	-2.56337200	-2.16876200	0.70985800
C	-2.18924900	-1.00705900	1.20737600
H	-1.86083900	-1.06793900	2.24349900
H	-2.65821900	-0.08787900	0.85348500

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(U)M06/BSII SCF energy in solution: -1416.5730561 a.u.

(U)M06/BSI SCF energy: -1416.2506432 a.u.

(U)M06/BSI SCF Gibbs free energy: -1415.909621 a.u.

S	0.62325900	-1.56965900	-1.09946600
O	0.40198900	-1.73458700	-2.53301000
O	1.53592500	-2.44765600	-0.38818500
C	-0.94866800	-1.56292000	-0.28360900
C	-2.09469400	-1.24202300	-1.00401300
C	-0.99958400	-1.82678800	1.08075200
C	-3.30350800	-1.14609200	-0.33174200
H	-2.02520200	-1.05898000	-2.07465700
C	-2.22026300	-1.73386900	1.73552600
H	-0.09020900	-2.10101600	1.61327500
C	-3.38038000	-1.37381500	1.04534300
H	-4.20712700	-0.87975600	-0.88005900
H	-2.27665300	-1.93773600	2.80475600
N	1.16274100	0.05998200	-0.80879000
C	0.32822200	0.99891800	-1.46103800
H	0.47243900	1.14560000	-2.53776500
C	-0.71533200	1.68729800	-0.80671900
C	-1.61513100	2.46806200	-1.57624000
C	-0.93665800	1.60629000	0.59074800
C	-2.69032800	3.10236800	-0.98465200
H	-1.45389300	2.54423100	-2.65194100
C	-2.01574100	2.24659100	1.17121100
H	-0.24965500	1.02015000	1.19770400
C	-2.90451700	2.99174900	0.39237000
H	-3.37491900	3.68830400	-1.59580400
H	-2.17302800	2.16419600	2.24605900
H	-3.75360100	3.49107600	0.85563200
C	-4.67975000	-1.19406800	1.76857000
H	-4.86330000	-0.12815200	1.96709600
H	-5.52742500	-1.56127500	1.17706900
H	-4.68511600	-1.71419800	2.73351500
C	3.58703200	0.50720100	1.02152200
C	2.66416200	-0.17897200	2.02044600
H	1.61149200	-0.02373900	1.75751600
H	2.85817200	-1.25906500	2.01969300
H	2.83545300	0.21331000	3.03257200
C	3.27402200	1.99074400	0.90256700
H	3.44580000	2.47344400	1.87325300
H	3.93101300	2.47668100	0.16791800
H	2.22943800	2.18001900	0.62140200
C	5.03591900	0.31205500	1.44023400
H	5.27570400	-0.75786100	1.47025100
H	5.71166600	0.79427200	0.72261200

H	5.21513200	0.73954600	2.43535500
O	3.50720100	-0.17978200	-0.24280300
C	2.59943800	0.21260500	-1.19413500
H	2.82202000	-0.38740000	-2.09029100
H	2.69410800	1.27720900	-1.46303100

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(U)M06/BSII SCF energy in solution: -1416.6910744 a.u.

(U)M06/BSI SCF energy: -1416.2960354 a.u.

(U)M06/BSI SCF Gibbs free energy: -1415.955686 a.u.

S	0.75164600	-1.74978900	-0.89980400
O	0.55525600	-2.24833000	-2.26708700
O	1.66152500	-2.49645600	-0.02523400
C	-0.84373100	-1.66667800	-0.11737700
C	-1.96910600	-1.35227000	-0.87183700
C	-0.92228200	-1.81192900	1.26059700
C	-3.17009900	-1.11857800	-0.22120700
H	-1.88034300	-1.24822700	-1.95021300
C	-2.14225200	-1.60510800	1.89658700
H	-0.02500400	-2.07182900	1.82036900
C	-3.26686000	-1.21926100	1.16920700
H	-4.04385300	-0.80883500	-0.79594900
H	-2.21382200	-1.70477600	2.98077500
N	1.17658600	-0.08827000	-0.89924700
C	0.25305600	0.71475100	-1.64299400
H	0.20731900	0.53060400	-2.72102000
C	-0.76039500	1.46639500	-1.02684000
C	-1.77599800	2.08717400	-1.82122700
C	-0.90358400	1.66364300	0.38069300
C	-2.82095100	2.79972700	-1.26618000
H	-1.71811300	1.96951400	-2.90684500
C	-1.96212100	2.37407300	0.91961800
H	-0.17029600	1.21152000	1.04873000
C	-2.94913600	2.95791400	0.11966200
H	-3.56731700	3.24182000	-1.93206700
H	-2.02163700	2.47241400	2.00740300
H	-3.77497500	3.52093000	0.55396600
C	-4.54524900	-0.84638800	1.85700800
H	-4.66445100	0.24697200	1.85136100
H	-5.42283600	-1.26969000	1.34955200
H	-4.56059700	-1.18042000	2.90241000
C	3.41650800	0.80262100	0.95724100
C	2.51656300	0.15277800	2.00284900
H	1.48206400	0.10447900	1.64749200

H	2.85608100	-0.87439600	2.18974500
H	2.54583100	0.72015700	2.94534400
C	2.93688600	2.20586200	0.60936500
H	2.96056500	2.83138000	1.51264700
H	3.59874900	2.66778900	-0.13772600
H	1.91057900	2.21486800	0.22036500
C	4.84480700	0.86234800	1.48440600
H	5.21109000	-0.15315500	1.68409500
H	5.50802000	1.32543700	0.74138200
H	4.89631000	1.44422200	2.41541500
O	3.51452900	-0.05143500	-0.18571700
C	2.59844000	0.08988500	-1.23012600
H	2.93450600	-0.64024100	-1.98542300
H	2.63224400	1.09196800	-1.68258900