Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

The Reaction of Alkyl Hydropersulfides (RSSH, R = CH_3 and ^tBu) with H_2S in the Gas Phase and in Aqueous Solution

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Table S1. Energies of structures in the PES for the $CH_3SSH + H_2S$ reaction (**Mechanism 1**).

ΔE_{water} ($\Delta(E_{water} + ZPE_{water})$) ($\Delta G_{water, T = 298K}$)	**M06-2X**	**ωB97X-D**
$CH_3SSH + H_2S$	0.0 (0.0) (0.0)	0.0 (0.0) (0.0)
INT1-1	-3.2 (-2.0) (6.2)	-2.7 (-1.7) (6.3)
TS1-1	61.8 (63.6) (73.8)	64.5 (66.1) (76.1)
INT1-2	-0.8 (0.9) (8.7)	-0.4 (1.4) (9.1)
$CH_3SH + HSSH$	3.8 (4.6) (3.8)	3.6 (4.5) (3.7)

Table S2. Energies of structures in the PES for the $CH_3SSH + H_2S$ reaction (**Mechanism 2**).

ΔE_{water} ($\Delta(E_{water} + ZPE_{water})$) ($\Delta G_{water, T = 298K}$)	**M06-2X**	**ωB97X-D**
$CH_3SSH + H_2S$	0.0 (0.0) (0.0)	0.0 (0.0) (0.0)
INT2-1	-2.8 (-1.6) (6.9)	-2.4 (-1.6) (5.4)
TS2-1	67.3 (68.1) (77.8)	68.3 (69.1) (78.9)
INT2-2	2.1 (4.0) (11.4)	1.5 (3.2) (10.4)
$CH_3SH + HSSH$	3.8 (4.6) (3.8)	3.6 (4.5) (3.7)

Table S3. Energies of structures in the PES for the $CH_3SSH + H_2S$ reaction (**Mechanism 3**).

ΔE_{water} ($\Delta(E_{water} + ZPE_{water})$) ($\Delta G_{water,\ T = 298K}$)	**M06-2X**	**ωB97X-D**
$CH_3SSH + H_2S$	0.0 (0.0) (0.0)	0.0 (0.0) (0.0)
TS3-1	43.8 (42.2) (42.2)	44.1 (42.5) (42.6)
INT3-1	20.9 (21.5) (21.7)	20.7 (21.4) (21.7)
TS3-2	46.0 (45.5) (54.8)	47.8 (47.3) (56.5)
$CH_3SH + HSSH$	3.8 (4.6) (3.8)	3.6 (4.5) (3.7)

Table S4. Energies of structures in the PES for the $CH_3SS^- + H_2S \rightarrow CH_3SH + HSS^-$ reaction in aqueous solution (**Mechanism 4**).

ΔE_{water} ($\Delta(E_{water} + ZPE_{water})$) ($\Delta G_{water,\ T = 298K}$)	**M06-2X**	**ωB97X-D**
$CH_3SS^- + H_2S$	0.0 (0.0) (0.0)	0.0 (0.0) (0.0)
INT4-1	-5.4 (-4.1) (4.4)	-4.7 (-3.2) (5.4)
TS4-1	-2.2 (-3.4) (5.6)	-1.7 (-2.7) (6.2)
INT4-2	-4.4 (-3.7) (4.4)	-4.5 (-3.3) (5.0)
TS4-2	9.6 (11.3) (20.6)	11.5 (12.9) (21.9)
INT4-3	9.1 (10.8) (18.9)	10.0 (11.7) (19.6)
TS4-3	9.5 (10.7) (19.0)	10.1 (11.5) (19.7)
INT4-4	-2.6 (-0.6) (7.7)	-2.1 (-0.3) (7.1)
$CH_3SH + HSS^-$	2.5 (3.2) (2.2)	2.0 (2.9) (2.0)

Table S5. Energies of structures in the PES for the CH_3SS^- + H_2S → CH_3SH + HSS^- reaction in aqueous solution (**Mechanism 5**).

ΔE_{water} ($\Delta(E_{water} + ZPE_{water})$) ($\Delta G_{water, T = 298K}$)	**M06-2X**	**ωB97X-D**
CH_3SS^- + H_2S	0.0 (0.0) (0.0)	0.0 (0.0) (0.0)
INT4-1	-5.4 (-4.1) (4.4)	-4.7 (-3.2) (5.4)
TS4-1	-2.2 (-3.4) (5.6)	-1.7 (-2.7) (6.2)
INT4-2	-4.4 (-3.7) (4.4)	-4.5 (-3.3) (5.0)
TS5-2	29.8 (30.6) (39.4)	31.9 (32.2) (40.0)
CH_3SH + HSS^-	2.5 (3.2) (2.2)	2.0 (2.9) (2.0)

Table S6. Energies of structures in the PESs for the reaction of CH_3SS^- and H_2S in aqueous solvent when the intermediate CH_3SSH is attacked by the additional nucleophile CH_3SS^- (**Mechanism 6** and **7**).

ΔE_{water} ($\Delta(E_{water} + ZPE_{water})$) ($\Delta G_{water, T = 298K}$)	**M06-2X**	**ωB97X-D**
CH_3SS^- + H_2S	0.0 (0.0) (0.0)	0.0 (0.0) (0.0)
INT4-1	-5.4 (-4.1) (4.4)	-4.7 (-3.2) (5.4)
TS4-1	-2.2 (-3.4) (5.6)	-1.7 (-2.7) (6.2)
INT4-2	-4.4 (-3.7) (4.4)	-4.5 (-3.3) (5.0)
INT6-1	-5.6 (-4.6) (6.1)	-5.9 (-4.8) (6.4)
TS6-1	4.5 (4.4) (15.8)	6.8 (7.3) (19.3)
INT6-2	-5.9 (-6.2) (3.6)	-7.3 (-7.2) (2.2)
TS7-1	5.3 (5.8) (17.4)	6.6 (7.5) (19.2)
INT7-1	-9.7 (-8.7) (2.3)	-9.5 (-8.3) (2.5)

Table S7. Energies of structures in the PESs for the reaction of ^{t}BuSS^{-} and H_2S in aqueous solvent.

ΔE_{water} ($\Delta(E_{water} + ZPE_{water})$) ($\Delta G_{water, T = 298K}$)	**M06-2X**	**ωB97X-D**
tBuSS^{-} + H_2S	0.0 (0.0) (0.0)	0.0 (0.0) (0.0)
INT8-1	-5.7 (-4.7) (3.6)	-5.4 (-4.1) (4.4)
TS8-1	-3.6 (-4.7) (4.5)	-3.2 (-4.3) (4.7)
INT8-2	-5.5 (-4.4) (4.2)	-6.1 (-5.4) (2.3)
INT8-3	-7.6 (-6.6) (5.0)	-8.2 (-7.3) (4.5)
TS8-2	9.8 (10.4) (23.6)	12.8 (13.1) (25.4)
INT8-4	-8.4 (-8.2) (3.1)	-10.0 (-10.1) (0.3)
TS9-1	4.1 (4.8) (17.8)	4.6 (5.1) (17.5)
INT9-1	-10.4 (-9.4) (0.6)	-11.1 (-10.2) (-0.3)

Table S8. Theoretical activation energies (kcal/mol) and Gibbs free energies (in parentheses) of the reactions shown in Scheme 1, at wB97X-D/6-31+G(d) level.

ΔE_{water} (ΔG_{water})	**R^2 = H**		**R^2 = S-Me**		**R^2 = S-^{t}Bu**		**R^2 = S-Ad**	
	TS1	TS2	TS1	TS2	TS1	TS2	TS1	TS2
R^1 = Me	17.2 (17.5)	16.2 (16.3)	12.9 (13.7)	12.1 (12.0)	13.3 (14.9)	13.3 (14.6)	14.0 (12.7)	14.2 (13.0)
R^1 = ^{t}Bu	18.2 (18.4)	24.0 (24.6)	15.1 (16.2)	21.2 (22.7)	13.4 (14.4)	20.4 (20.9)	14.2 (15.2)	21.8 (21.6)
R^1 = Ad	18.1 (19.0)	23.8 (24.9)	15.4 (15.8)	21.8 (20.8)	14.0 (14.3)	21.7 (21.2)	11.3 (13.0)	19.4 (20.2)

The IRC plot and structures

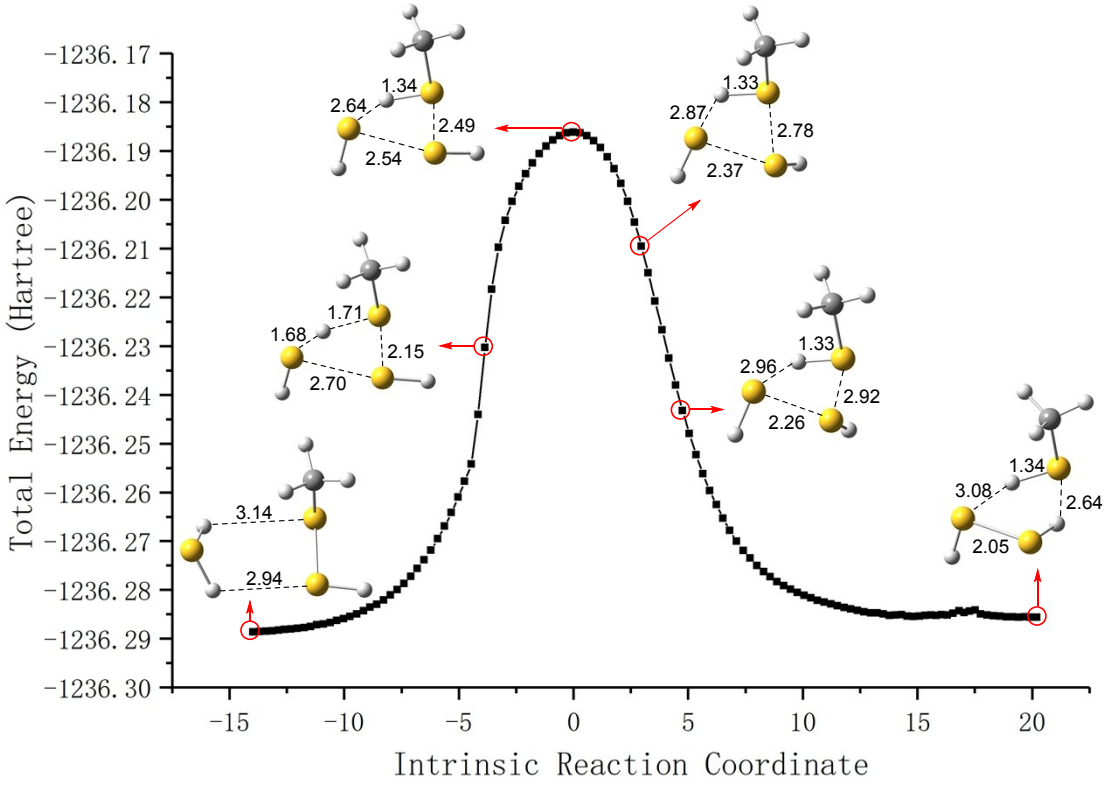

Figure S1. The IRC plot of **TS1-1** and representative structures along the reaction coordinate.

Cartesian Coordinates for Structures under Study

M06-2X, H_2S, gas

S	0.00000000	0.10279800	0.00000000
H	0.96406800	-0.82258000	0.00000000
H	-0.96406800	-0.82218000	0.00000000

M06-2X, H_2S, water

S	0.00000000	0.00000000	0.10260300
H	0.00000000	0.96994200	-0.82082200
H	0.00000000	-0.96994200	-0.82082200

M06-2X, HS^-

S	0.00000000	0.00000000	0.07879000
H	0.00000000	0.00000000	-1.26063400

M06-2X, HSSH, gas

S	1.02432700	-0.05479800	-0.06705200
S	-1.02433500	-0.05503600	0.06685300
H	-1.27578300	0.88025100	-0.85846500
H	1.27591600	0.87709500	0.86164600

M06-2X, HSS^-

S	0.03986900	1.08485700	0.00000000
S	0.03986900	-1.00564100	0.00000000
H	-1.27580600	-1.26745700	0.00000000

M06-2X, CH_3SSH, gas

C	-1.94501400	0.18369400	0.07681200
H	-1.49413300	0.62291800	0.96251000
H	-1.63426900	0.74294200	-0.80493800
H	-3.02836500	0.20009700	0.15483100
S	-1.35806600	-1.50894800	-0.16719600
S	-2.12681900	-2.47072200	1.46489000
H	-1.12301400	-2.24678100	2.32650500

M06-2X, CH_3SSH, water

C	1.63272100	0.68326500	-0.01088900
H	1.49841600	1.30757800	0.86850100
H	2.63025500	0.24452700	0.00567900
H	1.50736300	1.26524200	-0.91995600
S	0.47339700	-0.70211400	0.01843700
S	-1.34321500	0.23835900	-0.08762500
H	-1.51527800	0.50314400	1.21810900

M06-2X, CH_3SS^-

C	-1.61740700	0.66890500	0.00000000
H	-1.48548700	1.28445500	-0.88892500
H	-2.62363700	0.24763700	-0.00062900
H	-1.48630000	1.28370900	0.88955800
S	-0.43779200	-0.69866300	0.00000000
S	1.39403400	0.27183600	0.00000000

M06-2X, CH_3SH, gas

C	-1.15014000	0.01968700	0.00000100
H	-1.51322100	-1.00475600	0.00002200
H	-1.51398200	0.52066600	-0.89195900
H	-1.51398600	0.52071400	0.89193100
S	0.65897500	-0.08641700	0.00000000
H	0.89843800	1.22792700	-0.00000400

M06-2X, CH_3SH, water

C	-1.15071500	0.01946000	0.00000400
H	-1.51866900	-1.00372600	-0.00000500
H	-1.50928500	0.52513300	-0.89154100
H	-1.50927900	0.52511600	0.89156100
S	0.65853200	-0.08695600	-0.00000300
H	0.90500700	1.22801400	0.00001600

M06-2X, $^{t}BuSS^{-}$

C	-0.95472700	0.10987500	0.00000100
S	0.53764200	-0.97856700	0.00005200
S	2.18725500	0.27336200	-0.00001500
C	-0.97993700	0.97996200	1.24788400
H	-0.08985800	1.60850900	1.29182200
H	-1.86036300	1.62791000	1.23552500
H	-1.01570500	0.36746800	2.15001600
C	-0.97981500	0.97997800	-1.24785900
H	-1.01533700	0.36747000	-2.14999300
H	-1.86033100	1.62780900	-1.23563800
H	-0.08980800	1.60863200	-1.29162700
C	-2.14019800	-0.84887300	-0.00008800
H	-2.13371800	-1.48600200	0.88574800
H	-3.07174200	-0.27795000	-0.00032100
H	-2.13343000	-1.48623500	-0.88575400

M06-2X, **INT1-1**

C	0.82667400	1.62695500	0.71339400
H	1.54215900	1.52461800	1.52458100
H	0.88171000	2.63506400	0.30387900
H	-0.18436800	1.42923700	1.06111000
S	1.24878000	0.51155700	-0.64581600
S	0.99168300	-1.32997300	0.20833200
H	2.20863900	-1.47205700	0.75382000
S	-2.60935200	-0.00357300	-0.04982200
H	-1.53884200	0.17057300	-0.83671700
H	-1.96710000	-0.89733300	0.70984900

M06-2X, **TS1-1**

C	-1.63654000	-0.99648200	0.78852000
H	-2.13730100	-0.41927700	1.56052200
H	-2.26126200	-1.82914100	0.47672400
H	-0.66694700	-1.34692300	1.13538000
S	-1.37241200	0.11415700	-0.59464200
S	0.59010800	1.35085800	0.29788000
H	-0.42530000	2.22874700	0.10207000
S	1.64322600	-0.93286000	-0.04687900
H	-0.64481300	-0.72915300	-1.34017900
H	2.18011300	-0.43984700	-1.16738800

M06-2X, **INT1-2**

C	-1.92009500	-0.22112600	1.14216800
H	-2.58334300	0.46998800	1.65585600
H	-2.22237500	-1.23845600	1.37054000
H	-0.89942800	-0.04590000	1.47344400
S	-2.09798900	0.12343200	-0.62756400
S	1.54066500	1.05259500	0.09874100
H	0.28256800	1.23290300	-0.34766600
S	1.56846400	-0.99801100	-0.01378100
H	-1.24839100	-0.81927500	-1.05135500
H	2.01328700	-1.12076900	-1.27215900

M06-2X, **INT2-1**

C	0.97331100	1.60790800	0.69676600
H	-0.05814100	1.51217900	1.02725800
H	1.65824300	1.44386700	1.52408100
H	1.13594700	2.60148700	0.28043500
S	1.30937700	0.44041300	-0.64286700
S	0.82074700	-1.35169600	0.21599000
S	-2.48955000	-0.00081700	0.03113000
H	-3.34183800	0.76075000	-0.66222500
H	-1.48218300	0.25141800	-0.81580000
H	1.99893600	-1.62354300	0.79760000

M06-2X, **TS2-1**

C	-1.18039100	1.56451100	-0.24251900
H	-0.15344500	1.65649000	0.12115700
H	-1.19811000	1.63594400	-1.32649000
H	-1.85904700	2.28681600	0.20185700
S	-1.79961800	-0.08927200	0.14491800
S	0.09066300	-1.11228400	-0.15415800
S	2.34619600	0.39859000	0.01509100
H	2.51560700	0.10461000	1.31037500
H	-1.78779600	0.03401500	1.48166800
H	-0.63071700	-2.25749200	-0.42706600

M06-2X, **INT2-2**

C	-1.53761800	1.14301500	0.00582900
H	-0.89607800	1.08912800	0.88178700
H	-0.91354000	1.09394300	-0.88330400
H	-2.08936800	2.07835500	-0.00218100
S	-2.65639200	-0.27896800	-0.07968500
S	1.08881400	-0.99594800	0.04417300
S	2.30079900	0.65782200	-0.09103200
H	2.70548700	0.70821100	1.18545800
H	-3.32303000	-0.02878600	1.05077900
H	2.01069700	-1.92542500	-0.24281300

M06-2X, **TS3-1**

C	1.62558100	0.70263500	0.00953600
H	2.63147500	0.31566600	0.15890500
H	1.55163800	1.22909500	-0.93882200
H	1.33366000	1.36425600	0.81973500
S	0.48168900	-0.69125200	-0.05083000
S	-1.41755700	0.27407300	-0.02543700
H	-0.29636700	-0.44997000	1.12324200

M06-2X, **INT3-1**

C	1.64856300	0.65068600	0.02399000

H	1.41877100	1.29024800	0.87100200
H	2.62131400	0.17231600	0.12309300
H	1.59341400	1.21977200	-0.89956800
S	0.37118500	-0.62356800	-0.10470300
S	-1.38031600	0.28306500	0.01976800
H	0.62122300	-1.13840000	1.12049700

M06-2X, **TS3-2**

C	2.40863400	1.18803000	-0.00872200
H	1.75119900	1.65239200	-0.73733500
H	2.18800600	1.58860500	0.97700500
H	3.45434600	1.35674400	-0.24800100
S	2.05314400	-0.57976700	0.08633300
S	-0.46316700	-0.34307800	-0.01117800
S	-2.81078600	0.20246300	-0.08853100
H	-3.07588400	-0.18444900	1.16391800
H	2.24719900	-0.85960900	-1.20705400
H	-1.48373300	0.84424800	0.31780900

M06-2X, **INT4-1**

C	-1.03236300	1.58109600	0.69783800
H	-0.04876000	1.49121500	1.15835100
H	-1.14809300	2.58566300	0.28837000
H	-1.80133700	1.40875500	1.44974300
S	-1.19704700	0.40640000	-0.66354300
S	-0.88956000	-1.41662400	0.26680200
H	1.33975600	-0.68821600	0.18660400
S	2.46740800	0.05368500	-0.01914700
H	1.75979100	1.02063700	-0.61588400

M06-2X, **TS4-1**

C	1.46030100	-1.40654900	0.65673700
H	0.45640500	-1.70484600	0.95322200
H	1.98608400	-2.26777400	0.24359800
H	2.00590700	-1.02873300	1.51908800
S	1.38057500	-0.15214000	-0.64018600
S	0.37516200	1.37810600	0.29867000
H	-1.06484000	0.63772300	0.16720500
S	-2.41306300	-0.34599600	-0.04722700
H	-1.62815000	-1.27660100	-0.60366200

M06-2X, **INT4-2**

C	1.38687300	-1.48186700	0.66233100
H	0.36554100	-1.70864100	0.96021100
H	1.85054200	-2.37651700	0.24653100
H	1.96517000	-1.13629100	1.51550700
S	1.39228300	-0.24216000	-0.65043300
S	0.58577000	1.39106400	0.29103800
H	-0.72845100	0.98932800	0.21082400
S	-2.61327000	-0.26141100	-0.04708700
H	-1.61057000	-1.07655900	-0.40334200

M06-2X, **TS4-2**

C	-2.39010700	1.14481000	0.00215100
H	-1.80880200	1.60220600	-0.80111200
H	-3.43564700	1.41212400	-0.15164300
H	-2.06470800	1.59451600	0.94144300
S	-2.16385300	-0.66160400	0.01884000
S	0.57573400	-0.11436200	-0.04919100
H	0.62090400	-1.42148500	0.20048500
S	2.72154600	0.12257900	-0.05976600
H	2.89406900	0.39796600	1.23978400

M06-2X, **INT4-3**

C	2.24214300	1.23624600	-0.02963500
H	1.70859600	1.62309900	0.84194700
H	3.20184400	1.75296200	-0.07511200
H	1.67313000	1.52578000	-0.91526600
S	2.45964500	-0.57599400	0.06119300
S	-0.78379700	-0.47236100	-0.14729100
H	-0.17453900	0.44514200	0.60813400
S	-2.72194300	0.27618200	0.00094200
H	-3.12436400	-0.40967900	1.08059800

M06-2X, **TS4-3**

C	-2.38051100	1.20162000	0.09004300
H	-3.09593500	1.73635500	-0.53619000
H	-1.38889300	1.60386800	-0.13018900
H	-2.60691900	1.44632200	1.12887600
S	-2.44928000	-0.60090600	-0.20446500
S	0.87171900	-0.38732200	0.44596700
H	0.12331200	-0.18491200	-0.64678800
S	2.70621900	0.30302300	-0.21950000
H	3.19298100	-0.84807000	-0.70800100

M06-2X, **INT4-4**

C	2.02103900	0.40118000	-1.06959600
H	1.16058100	1.04233100	-1.24775400
H	2.93111200	0.98109200	-1.20306800
H	2.01843800	-0.42514500	-1.77493900
S	2.01493600	-0.20660300	0.63821700
S	-1.52352100	-1.06052000	-0.20857200
H	0.79151300	-0.77795300	0.56487800
S	-1.65556400	0.98794100	0.16412200
H	-0.40149300	1.23951700	0.57818400

M06-2X, **TS5-2**

C	-0.85511400	0.39132700	0.04107300
H	-1.15606700	1.41360900	-0.08840100
H	-0.66052100	-0.23305400	-0.80935400
H	-0.72973800	-0.00478300	1.03089200
S	1.42212700	1.01687700	0.01747100
S	2.24491300	-0.87157700	-0.10229300
H	2.24028500	-1.22544000	1.19263100
S	-3.11876400	-0.29487600	0.06156800
H	-3.33569300	0.09493800	-1.20015000

M06-2X, **INT6-1**

C	-2.58909700	1.28674500	0.45864600
H	-1.64699700	1.82345100	0.37737400
H	-3.39237400	1.90344000	0.05534500
H	-2.80429300	1.04400300	1.49619800
S	-2.54543900	-0.21417600	-0.54647700
S	-1.09527400	-1.32667800	0.38764900
H	-0.01591300	-0.73561800	-0.17769300
C	1.24455700	1.73600000	0.63906500
H	2.12673500	2.07062800	1.18308400
H	0.71935100	2.60235600	0.23462800
H	0.58415500	1.19266200	1.31595900
S	1.72931100	0.67694500	-0.74007200
S	2.69243800	-0.88842800	0.20695300

M06-2X, **TS6-1**

C	-0.97721700	-0.91209200	1.26811100
H	-1.69723000	-0.44516700	1.93218300
H	-1.20226500	-1.97178900	1.16703600
H	0.02472400	-0.78352100	1.67017800
S	-1.06649400	-0.08430100	-0.35010500
S	-3.31625900	0.62951800	-0.03586300
H	-3.88489300	-0.53896300	-0.35670100
C	2.61066600	1.64711000	-0.02724200
H	1.63076800	2.11968600	-0.02114600
H	3.26614600	2.16703000	0.67160800
H	3.03826800	1.69173900	-1.02678600
S	2.48049500	-0.06736600	0.52671900
S	1.21624400	-0.89342100	-0.85835100

M06-2X, **INT6-2**

C	-1.01779300	-1.22401500	0.92557200
H	-2.05023800	-0.92044000	1.09615600
H	-0.96971400	-2.28942900	0.71615700
H	-0.41086300	-0.97318300	1.79279400
S	-0.46905300	-0.27064200	-0.50550200
S	-4.25443500	0.69444900	-0.01849000
H	-4.33584600	-0.34829000	0.81745100
C	2.74831700	1.76244200	-0.11307200
H	1.77201600	2.21666600	-0.26623500
H	3.33112500	2.38274800	0.56712000
H	3.27782100	1.65702000	-1.05607400
S	2.56043800	0.15611000	0.68942000
S	1.47570900	-0.88964500	-0.69932500

M06-2X, **TS7-1**

C	-2.72197900	1.54281100	-0.26787300
H	-2.19451800	1.63722500	-1.21782900
H	-3.63252100	2.13942000	-0.32456400
H	-2.08887900	1.96664300	0.51339900
S	-3.11379300	-0.19577700	0.08441400
S	-0.64843500	-0.89737900	-0.01489500
H	-0.63138000	-0.21665800	1.12781100
C	2.30468500	1.62103600	0.75050000
H	2.83062400	1.25043400	1.62729200
H	2.76210100	2.55290400	0.41849500
H	1.25750700	1.80088100	0.98667800
S	2.44348200	0.44644900	-0.61488800
S	1.58129900	-1.23541400	0.16867900

M06-2X, **INT7-1**

C	2.44113400	-1.41660400	0.29497400
H	1.88939700	-2.01570500	-0.42366400
H	3.40656600	-1.88351000	0.47799300
H	1.89195700	-1.35646800	1.23083700
S	2.77690900	0.24034000	-0.35573900
S	-0.71375300	2.03542300	-0.33548000
H	1.51309200	0.70053100	-0.37264300
S	-0.87531800	0.47816200	0.99830300
S	-1.03970800	-1.26854700	-0.07650900
C	-2.74616000	-1.19189300	-0.66463600
H	-2.88859400	-0.28381200	-1.24782900
H	-2.90941200	-2.05769300	-1.30574100
H	-3.44291700	-1.21840500	0.16981900

M06-2X, **INT8-1**

C	1.49697400	-0.43884300	0.11737300
S	0.36384300	0.51687900	-0.98506300
S	-0.66486300	1.83319400	0.22935400
H	-2.28464900	0.23343900	0.23826200
S	-3.07981000	-0.87075700	0.05100200
H	-2.08703900	-1.53400500	-0.55189200
C	2.24297300	-1.38501800	-0.81663300
H	2.92654500	-2.00732700	-0.23445800
H	1.55162100	-2.04431100	-1.34402100
H	2.82866800	-0.83407100	-1.55406400
C	0.69921800	-1.23154000	1.14157300
H	1.37897800	-1.75854900	1.81638100
H	0.06889400	-0.56741700	1.73464300
H	0.05993800	-1.96706300	0.65176300
C	2.47518900	0.49457500	0.81454800
H	1.94093200	1.21465300	1.43506300
H	3.14743200	-0.08211900	1.45511200
H	3.07584900	1.04267100	0.08736400

M06-2X, **TS8-1**

C	1.54864200	-0.39972600	0.10518500
S	0.52378600	0.72230100	-0.94607300
S	-0.86186500	1.56183700	0.31711800
H	-2.02060600	0.38565900	0.14393500
S	-3.11734100	-0.82077800	-0.06195500
H	-2.21528100	-1.76048700	0.23872100
C	0.68223700	-1.48166500	0.73092800
H	1.30165100	-2.13409900	1.35159500
H	-0.09102100	-1.04053200	1.36115400
H	0.19921900	-2.08749500	-0.03669700
C	2.27077900	0.39414400	1.18285700
H	2.88039000	-0.27926900	1.79038500
H	2.92400600	1.14769600	0.74166700
H	1.55642400	0.89258000	1.83863300
C	2.55214900	-1.01463100	-0.86476700
H	3.17369200	-0.24862500	-1.33075700
H	3.20663000	-1.69762400	-0.31920700
H	2.04878600	-1.58029100	-1.65007600

M06-2X, **INT8-2**

C	1.63149000	-0.44760700	0.11019600
S	0.62878800	0.68605300	-0.95175100
S	-0.71488000	1.57175000	0.31481300
H	-1.73102500	0.64137400	0.23948600
S	-3.46734500	-0.78673900	0.03396600
H	-3.47454900	-0.51375200	-1.27742300
C	2.61905400	-1.07338400	-0.86986100
H	3.26463900	-1.76544400	-0.32616300
H	2.10375300	-1.63161000	-1.65244500
H	3.25010100	-0.31561700	-1.33620600
C	2.36842700	0.33780500	1.18292600
H	1.66795300	0.83821600	1.85184200
H	2.97435100	-0.34778800	1.77961700
H	3.02681400	1.08539500	0.74036100
C	0.74506600	-1.51311400	0.73340800
H	0.23219400	-2.09521000	-0.03270600
H	1.35967400	-2.18912900	1.33220800
H	-0.00312500	-1.06567300	1.38895900

M06-2X, **INT8-3**

C	-3.10704400	0.33861000	-0.39792800
S	-2.07866000	0.19867600	1.13222500
S	-0.99587600	-1.52592900	0.90731500
H	0.05300700	-1.01311500	0.22350800
C	2.55504500	1.04153800	0.19320400
S	1.89334800	-0.17097800	-1.03593300
S	2.53972600	-2.04427500	-0.45765800
C	2.02860300	0.73371300	1.58676500
H	2.46214400	1.42975600	2.30957400
H	0.94210800	0.83089200	1.62238400
H	2.29453900	-0.28218100	1.88205600
C	2.03423100	2.39393000	-0.27979500
H	2.37539100	3.17501000	0.40360000
H	2.40168600	2.63236200	-1.27901500
H	0.94252500	2.41045800	-0.29731100
C	4.07562100	1.02326300	0.18283300
H	4.46168300	1.28837200	-0.80240000
H	4.46296300	1.74150800	0.91007400
H	4.44715100	0.03237900	0.44633900
C	-4.06678700	-0.83574700	-0.50362400
H	-4.67664100	-0.72307700	-1.40267000
H	-3.52453400	-1.77871800	-0.57827800
H	-4.72922000	-0.87926000	0.36100600
C	-3.87288200	1.64227900	-0.19398900
H	-3.19515100	2.49270000	-0.11023000
H	-4.52287800	1.80753400	-1.05509400
H	-4.49733600	1.60122100	0.69955000
C	-2.21798500	0.42521000	-1.62767500
H	-1.62983300	-0.48491900	-1.75147800
H	-2.84252100	0.54993000	-2.51505900
H	-1.53450200	1.27245200	-1.56047400

M06-2X, **TS8-2**

C	-2.45125600	-0.73057200	-0.31914000
S	-1.08403100	0.28022300	0.47385300
S	-2.31765000	2.40864400	0.26661800
H	-1.15421100	3.01256400	-0.00031000
C	2.94667900	0.28333200	-0.39204100
S	2.09286800	-0.19728800	1.17769800
S	0.60483100	-1.48151100	0.65240600
C	4.01988700	1.27192900	0.05021600
H	4.71888600	0.81242300	0.75078600
H	4.58405900	1.60307300	-0.82415000
H	3.57932000	2.15065400	0.52327400
C	3.58431300	-0.93821300	-1.03656000
H	2.82665600	-1.68076900	-1.28852500
H	4.09483200	-0.64312000	-1.95647400
H	4.31402300	-1.39708700	-0.36863800
C	1.97508500	0.94564900	-1.35592900
H	1.53753800	1.84407800	-0.91951300
H	2.50568200	1.22272700	-2.27059300
H	1.16378900	0.26510000	-1.61544200
C	-3.80795100	-0.36482300	0.28170400
H	-4.55797300	-1.05527100	-0.11251400
H	-3.79454100	-0.46077500	1.36782000
H	-4.11851600	0.64401900	0.02169800
C	-2.44917200	-0.48241700	-1.82201000
H	-1.50011300	-0.79333300	-2.26138700
H	-3.25080800	-1.05784000	-2.29331500
H	-2.60725900	0.57358900	-2.03852400
C	-2.23139000	-2.21934400	-0.05033000
H	-3.09640400	-2.76168000	-0.43919000
H	-1.34809900	-2.60430500	-0.55599700
H	-2.15031800	-2.42839600	1.01633500

M06-2X, **INT8-4**

C	1.76513700	1.21665900	0.14121500
S	0.72233100	-0.28875100	0.40911400
S	5.20787100	-1.56577700	0.03935700
H	6.15126000	-2.51635800	-0.01837800
C	-3.38972000	-0.54007400	0.26650800
S	-2.29070700	0.75215600	-0.47370200
S	-0.63844800	-0.26812700	-1.11748300
C	-4.59530300	0.25869500	0.75301200
H	-5.08809500	0.77864300	-0.06950700
H	-5.31449300	-0.43155700	1.19764400
H	-4.30859600	0.98836500	1.51098000
C	-3.80665600	-1.55123600	-0.78978900
H	-2.94276100	-2.08472800	-1.18690300
H	-4.47705900	-2.28495900	-0.33701600
H	-4.33028200	-1.06607700	-1.61340200
C	-2.69796500	-1.22815200	1.43213400
H	-1.82146200	-1.78491300	1.09927300
H	-2.38868000	-0.50904800	2.19046100
H	-3.39366300	-1.93692600	1.88671200
C	0.91171300	2.47373000	0.18473800
H	0.20378400	2.50014000	-0.64436500
H	0.35802100	2.54642300	1.12082100
H	1.56368800	3.34565800	0.09700800
C	2.73987100	1.18066600	1.31481800
H	3.34514500	0.27213000	1.29786900
H	3.41298700	2.03654100	1.23424800
H	2.21710700	1.24668200	2.26975200
C	2.51702700	1.11204200	-1.17629000
H	3.14074000	2.00022400	-1.30134700
H	3.16185600	0.23224900	-1.18749900
H	1.82912600	1.06151400	-2.02100900

M06-2X, **TS9-1**

C	-3.11975100	0.71658100	0.05088200
S	-3.06242700	-1.11577100	-0.14773900
S	-0.53437700	-1.63914700	-0.01129500
H	-0.52577000	-0.93388800	-1.13783300
C	2.77889900	0.99294800	-0.14207600
S	2.53948700	-0.46077200	0.97336600
S	1.70586700	-1.92779600	-0.17659500
C	3.81438600	0.67370700	-1.20901400
H	3.94536100	1.53973100	-1.86212200
H	4.77754500	0.43129300	-0.75930000
H	3.49227000	-0.16907400	-1.82174400
C	3.28678000	2.09121000	0.78665300
H	3.49731100	2.98648900	0.19838200
H	2.54303900	2.34547200	1.54265100
H	4.20822300	1.79217600	1.28872400
C	1.46216100	1.40436600	-0.78228300
H	0.69809300	1.59762200	-0.02819400
H	1.61545300	2.31596000	-1.36523700
H	1.09774200	0.62916600	-1.45699800
C	-2.47131700	1.40255500	-1.15018700
H	-2.51327000	2.49022000	-1.03412300
H	-1.42256500	1.11854300	-1.25029200
H	-2.98677800	1.13670100	-2.07399000
C	-4.58004100	1.15264600	0.14273300
H	-5.07106400	0.69291100	1.00143700
H	-4.64240600	2.23990900	0.25451100
H	-5.12933500	0.87033200	-0.75656500
C	-2.39258300	1.14172300	1.32382300
H	-1.34605400	0.83652100	1.29476400
H	-2.43055500	2.22988300	1.43567000
H	-2.85523700	0.69138100	2.20328000

M06-2X, **INT9-1**

C	-3.76266500	-0.36064800	0.20136400
S	-2.29891700	-0.57791600	-0.89436500
S	0.11459100	2.00487500	0.54052700
H	-1.52693300	0.36038100	-0.30479500
S	1.06608700	1.03304300	-1.00453000
S	1.73606800	-0.79782700	-0.36811500
C	3.46140000	-0.52868800	0.24551100
C	3.47072800	0.48904900	1.37532400
H	3.10036400	1.45477400	1.03128300
H	2.84607800	0.15976200	2.20613100
H	4.49365000	0.61659200	1.73875300
C	4.36142600	-0.07039700	-0.89210700
H	5.37811000	0.07200400	-0.51794100
H	4.38807300	-0.81037100	-1.69244800
H	4.01448000	0.87752700	-1.30443500
C	3.90074600	-1.89883200	0.75139200
H	3.87524000	-2.64403100	-0.04508300
H	4.92701200	-1.83053500	1.11883200
H	3.26813200	-2.24116600	1.57131700
C	-4.81026700	-1.36259600	-0.26844100
H	-4.44220500	-2.38610300	-0.18687400
H	-5.70244500	-1.26944100	0.35397700
H	-5.09692600	-1.17662800	-1.30431000
C	-4.29589100	1.06083400	0.07220500
H	-5.16500600	1.18713800	0.72268200
H	-3.53864100	1.78840200	0.36798600
H	-4.59773300	1.27343000	-0.95333700
C	-3.37056500	-0.64387700	1.64611300
H	-2.59483000	0.04628600	1.98122000
H	-4.24219600	-0.51954200	2.29359700
H	-2.99897500	-1.66232600	1.75899200

ωB97X-D, H_2S, gas

S	0.00000000	0.10262800	0.00000000
H	0.96811300	-0.82100800	0.00000000
H	-0.96811300	-0.82103300	0.00000000

ωB97X-D, H_2S, water

S	0.00000000	0.00000000	0.10242800
H	0.00000000	0.97395600	-0.81942400
H	0.00000000	-0.97395600	-0.81942400

ωB97X-D, HS^-

S	0.00000000	0.00000000	0.07888400
H	0.00000000	0.00000000	-1.26213800

ωB97X-D, HSSH, gas

S	1.02488200	0.05487400	0.06747000
S	-1.02488300	0.05488700	-0.06745800
H	-1.28540900	-0.87817900	0.86055100
H	1.28541500	-0.87799800	-0.86073500

ωB97X-D, HSS^-

S	0.03987900	1.08500700	0.00000000
S	0.03987900	-1.00537100	0.00000000
H	-1.27612300	-1.27418200	0.00000000

ωB97X-D, CH_3SSH, gas

C	1.64397700	0.67530800	-0.00565200
H	1.55257600	1.27941100	0.89366900
H	2.63514200	0.22291100	-0.03661100
H	1.50059400	1.28961900	-0.89078600
S	0.46895400	-0.69895900	0.01540200
S	-1.34396800	0.24314100	-0.08763300
H	-1.55193900	0.44929100	1.22333500

ωB97X-D, CH_3SS^-

C	-1.63109700	0.66077200	-0.00002200
H	-1.51341300	1.27953100	-0.88950800
H	-2.63082900	0.22324300	-0.00057400
H	-1.51409100	1.27878500	0.89006700
S	-0.43565300	-0.69345700	-0.00007500
S	1.40096100	0.27182000	0.00008400

ωB97X-D, CH_3SH, gas

C	-1.15013700	0.02000700	0.00000000
H	-1.51677200	-1.00386200	0.00000700
H	-1.51518100	0.52182800	-0.89200600
H	-1.51518000	0.52184100	0.89199900
S	0.65893900	-0.08675100	0.00000000
H	0.90492600	1.22816600	-0.00000100

ωB97X-D, CH_3SH, water

C	-1.15101900	0.01970800	0.00000300
H	-1.52166700	-1.00299100	-0.00000800
H	-1.51033300	0.52612200	-0.89156100
H	-1.51033000	0.52610300	0.89157900
S	0.65862000	-0.08723100	-0.00000200
H	0.91053100	1.22821800	0.00001100

ωB97X-D, ^{t}BuSS^{-}

C	-0.96083200	0.10934900	0.00000100
S	0.54446500	-0.96971400	0.00011600
S	2.20250800	0.27378000	-0.00005600
C	-0.99812000	0.97970100	1.24940000
H	-0.11970000	1.62443100	1.29603400
H	-1.88778500	1.61497000	1.23863600
H	-1.02489900	0.36969700	2.15358200
C	-0.99792900	0.97968900	-1.24941200
H	-1.02457700	0.36967900	-2.15359300
H	-1.88759000	1.61496600	-1.23878600
H	-0.11949700	1.62441300	-1.29591900
C	-2.13641500	-0.86446900	-0.00008600
H	-2.12683500	-1.50233800	0.88536300
H	-3.07422100	-0.30413100	-0.00017000
H	-2.12668800	-1.50235500	-0.88552200

ωB97X-D, **INT1-1**

C	0.76587400	1.64679200	0.71155400
H	1.50961600	1.61215600	1.50353000
H	0.73747900	2.65034700	0.28695100
H	-0.21892300	1.39028400	1.09510300
S	1.22538200	0.54835100	-0.64858500
S	1.14668400	-1.30966400	0.20649900
H	2.38831000	-1.36295700	0.71526400
S	-2.70417900	-0.07074500	-0.03970000
H	-1.64383700	0.14253900	-0.83290300
H	-2.05410200	-1.00019600	0.67130600

ωB97X-D, **TS1-1**

C	-1.69689800	-0.97212700	0.77330400
H	-2.16099400	-0.37883100	1.55631200
H	-2.37414000	-1.75785500	0.44813900
H	-0.75420600	-1.39289800	1.11702200
S	-1.36028000	0.13894500	-0.59371800
S	0.62407700	1.33020300	0.29776600
H	-0.38129100	2.22797600	0.11767900
S	1.63318600	-0.94576700	-0.03848700
H	-0.64965900	-0.72516300	-1.33347900
H	2.14994400	-0.51456600	-1.19447700

ωB97X-D, **INT1-2**

C	-2.08619800	-0.15514300	1.14099700
H	-2.73330000	0.61364900	1.55643600
H	-2.46750000	-1.13074000	1.42852100
H	-1.07919400	-0.01486900	1.52649600
S	-2.12928100	0.05391100	-0.65841900
S	1.53199200	1.07151100	0.06654200
H	0.26425900	1.15430500	-0.38768600
S	1.70114600	-0.97650000	0.04160500
H	-1.28668600	-0.94372900	-0.95479200
H	2.15789700	-1.13051000	-1.21059700

ωB97X-D, **INT2-1**

C	0.61458000	1.64572300	0.71098800
H	-0.23945300	1.22793800	1.23878100
H	1.45332300	1.78909000	1.38734000
H	0.33483000	2.60459600	0.27436600
S	1.08402600	0.58783000	-0.67791400
S	1.48676500	-1.20670200	0.22092700
S	-2.76459800	-0.31858800	0.05284900
H	-3.31838300	0.70355400	-0.60935100
H	-1.59943700	-0.19280300	-0.60196700
H	2.78255300	-1.00735600	0.51110000

ωB97X-D, **TS2-1**

C	-1.21237200	1.56563200	-0.24184700
H	-0.17671600	1.66873500	0.09567700
H	-1.26191800	1.65617300	-1.32340200
H	-1.88337600	2.27708300	0.23185500
S	-1.80276700	-0.09679000	0.14556500
S	0.09289300	-1.11248300	-0.15097200
S	2.36067800	0.40273000	0.01194400
H	2.59587100	0.14319200	1.30556100
H	-1.79804400	0.02716800	1.48341000
H	-0.61444200	-2.26145000	-0.44660800

ωB97X-D, **INT2-2**

C	2.06065900	-0.13277900	1.15201500
H	1.12184600	-0.62909400	1.38520300
H	2.88264700	-0.75554000	1.49747000
H	2.11428900	0.82926800	1.65424700
S	2.27187200	0.05098300	-0.63793700
S	-1.55958100	-1.02620100	-0.13946700
S	-1.63317000	1.00763900	0.15038300
H	-2.21519800	1.35442400	-1.00765900
H	1.19608600	0.82023900	-0.84619500
H	-2.72955900	-1.34135200	0.43717500

ωB97X-D, **TS3-1**

C	1.64249600	0.69022600	0.00944800
H	2.63886000	0.28419500	0.17558600
H	1.59654400	1.21058200	-0.94441700
H	1.35912400	1.36745900	0.81036500
S	0.47658400	-0.68483000	-0.05086300
S	-1.42303200	0.27481600	-0.02557800
H	-0.30633400	-0.44337400	1.12483100

ωB97X-D, **INT3-1**

C	1.66079100	0.64028600	0.02454800
H	1.45034400	1.28370600	0.87418800
H	2.62523200	0.14370700	0.12150000
H	1.62080900	1.21444400	-0.89712200
S	0.36646700	-0.61675700	-0.10545600
S	-1.38388000	0.28297300	0.02027100
H	0.61746800	-1.14303000	1.11710900

ωB97X-D, **TS3-2**

C	2.51120200	1.15143600	-0.03107100
H	1.86923200	1.69222700	-0.72011000
H	2.37847900	1.55280000	0.97015300
H	3.55554800	1.22879200	-0.32111500
S	2.00589400	-0.57921100	0.05375200
S	-0.45305100	-0.32294000	0.11568600
S	-2.84727800	0.13746600	-0.07180400
H	-2.82378700	1.23932600	0.68817100
H	2.13979500	-0.86705100	-1.24647100
H	-1.47551500	0.48023500	-0.74634900

ωB97X-D, **INT4-1**

C	-1.23164700	1.55102300	0.67498700
H	-0.22031100	1.62013100	1.07548600
H	-1.51251400	2.51635000	0.25043100
H	-1.92338200	1.30145900	1.47916100
S	-1.31550600	0.32932400	-0.65160800
S	-0.75963200	-1.43887900	0.27501000
H	1.41184600	-0.57779700	0.15519500
S	2.55933500	0.15051000	-0.02648300
H	1.88708900	1.17845300	-0.56090900

ωB97X-D, **TS4-1**

C	1.63156900	-1.38389300	0.59034400
H	0.65861200	-1.80289800	0.84164600
H	2.24960400	-2.16192600	0.14009600
H	2.12048100	-1.01558400	1.49079200
S	1.46182200	-0.06621200	-0.63343100
S	0.29677300	1.32843700	0.33638400
H	-1.14155600	0.53664000	0.11817100
S	-2.49900400	-0.37131300	-0.09508500
H	-1.83000000	-1.50745600	0.14134400

ωB97X-D, **INT4-2**

C	1.55618500	-1.46438800	0.61406500
H	0.54967600	-1.79159800	0.86618900
H	2.10445800	-2.29764000	0.17325600
H	2.07791400	-1.12143900	1.50462100
S	1.50518600	-0.16802300	-0.64031800
S	0.52242100	1.35927900	0.31442700
H	-0.76209600	0.89337700	0.15314400
S	-2.74441100	-0.29240900	-0.07328900
H	-1.83820300	-1.27792800	0.00528600

ωB97X-D, **TS4-2**

C	-2.49016700	1.09337600	0.00308700
H	-2.09312300	1.59680600	-0.88039700
H	-3.57488600	1.20182600	-0.01017900
H	-2.11105000	1.61001100	0.88632500
S	-2.02751000	-0.66283500	0.01981900
S	0.49406000	-0.10642400	-0.05344000
H	0.60591000	-1.39693400	0.24978800
S	2.73435800	0.14181000	-0.05972800
H	2.89962000	0.46722000	1.22952200

ωB97X-D, **INT4-3**

C	2.33977700	1.24946200	-0.02751100
H	1.76711600	1.61388200	0.82918800
H	3.29445400	1.77878000	-0.02353300
H	1.80681400	1.55256400	-0.93182600
S	2.57452900	-0.56284200	0.04077100
S	-0.89452300	-0.55653800	-0.06612400
H	-0.17370300	0.55480000	0.12185900
S	-2.78597800	0.29370700	-0.04363300
H	-3.03779000	0.21396400	1.27314300

ωB97X-D, **TS4-3**

C	-2.34413300	1.22719700	0.06955000
H	-3.29664600	1.74952200	-0.03860200
H	-1.66165800	1.64301200	-0.67567800
H	-1.94316000	1.47838000	1.05326800
S	-2.54476000	-0.57943600	-0.13208100
S	0.87847700	-0.45804100	0.29048100
H	0.19510400	0.10942600	-0.71063900
S	2.76306400	0.30747000	-0.10435900
H	3.22266700	-0.66341200	-0.91030500

ωB97X-D, **INT4-4**

C	-2.18228500	0.64344600	0.91979800
H	-1.47800300	1.47207100	0.90301900
H	-3.19433800	1.04136000	0.94980000
H	-2.01721400	0.03671700	1.80640500
S	-2.03915200	-0.36170000	-0.58172200
S	1.56273200	-1.03648600	0.30768700
H	-0.77769500	-0.80298500	-0.34861000
S	1.73183000	0.97119800	-0.23754800
H	0.47440600	1.22396400	-0.64407100

ωB97X-D, **TS5-2**

C	-0.88205500	0.36323200	0.03907300
H	-1.17451700	1.39504600	0.00575500
H	-0.71509500	-0.18321800	-0.86760700
H	-0.73345700	-0.11658800	0.98678000
S	1.41512000	1.00863800	0.02401000
S	2.31404400	-0.84705800	-0.10768900
H	2.36034300	-1.19957200	1.18826100
S	-3.16778400	-0.30638600	0.05793600
H	-3.42702100	0.24183700	-1.13573500

ωB97X-D, **INT6-1**

C	-2.68188600	1.23335000	0.58527800
H	-1.73285300	1.76057800	0.64881400
H	-3.43691300	1.90327600	0.17225800
H	-2.99866900	0.90095500	1.57110300
S	-2.56280800	-0.15884100	-0.55794800
S	-1.16061000	-1.37117200	0.32255900
H	-0.04728700	-0.75217100	-0.15655700
C	1.23756700	1.78115100	0.51461800
H	2.10706400	2.24436400	0.98015400
H	0.63805200	2.55324200	0.02979200
H	0.63756900	1.28817500	1.27991300
S	1.74419900	0.60149500	-0.75324300
S	2.82290400	-0.82057100	0.29332800

ωB97X-D, **TS6-1**

C	-0.99651700	-0.91970300	1.26412200
H	-1.72543500	-0.47642800	1.93541000
H	-1.20684100	-1.98101900	1.14497900
H	0.00037200	-0.78768200	1.67849000
S	-1.08829000	-0.06112800	-0.33644000
S	-3.33794200	0.63136400	-0.02565100
H	-3.92094800	-0.51836000	-0.38965100
C	2.73471300	1.60668500	0.02928100
H	1.79318800	2.14910600	0.09138400
H	3.44324100	2.04077600	0.73585600
H	3.14114100	1.68299700	-0.97772300
S	2.50711700	-0.12279600	0.49928000
S	1.17199600	-0.83689400	-0.88588700

ωB97X-D, **INT6-2**

C	-1.04765000	-0.97208000	0.88035500
H	-2.08622800	-0.63790800	0.87711800
H	-1.01441000	-2.05796200	0.84099700
H	-0.55527300	-0.60338200	1.77727200
S	-0.29762300	-0.25108100	-0.59475400
S	-4.89588800	0.60478700	0.00040200
H	-4.35328800	-0.50742400	0.51564300
C	3.12294000	1.65225800	-0.27070600
H	2.22602700	2.18308700	-0.58159900
H	3.72332500	2.30454000	0.36351100
H	3.70940600	1.34866400	-1.13420700
S	2.68900300	0.22338400	0.74389000
S	1.62317600	-0.95900700	-0.54432800

ωB97X-D, **TS7-1**

C	-2.86138700	1.54355400	-0.28192900
H	-2.40734000	1.67169400	-1.26562300
H	-3.81680900	2.06938500	-0.28020600
H	-2.21425500	2.01949600	0.45644500
S	-3.10666000	-0.21429600	0.10355200
S	-0.66958000	-0.85782000	-0.01799000
H	-0.63671100	-0.23351900	1.15566100
C	2.41494500	1.61509000	0.74581500
H	2.93633900	1.23617100	1.62252400
H	2.90863000	2.52304800	0.39802300
H	1.38130300	1.84710700	0.99517900
S	2.48991200	0.42601900	-0.61140900
S	1.56929600	-1.23423100	0.15926400

ωB97X-D, **INT7-1**

C	2.34011700	-1.60262300	0.10311200
H	1.70967400	-1.92514900	-0.72124700
H	3.18174300	-2.28706000	0.18958300
H	1.77460800	-1.61786200	1.03098900
S	3.02676800	0.04515300	-0.21160300
S	-0.31882000	1.97240900	-0.38798800
H	1.85870700	0.72411600	-0.30188100
S	-0.91670200	0.54751100	0.97252500
S	-1.41365500	-1.18073500	-0.02330300
C	-3.06824400	-0.84203900	-0.66549900
H	-3.04127100	-0.00405100	-1.35974800
H	-3.39144500	-1.73444500	-1.20213800
H	-3.76471200	-0.63699600	0.14466500

ωB97X-D, **INT8-1**

C	1.51706400	-0.48209300	0.10735700
S	0.60394400	0.73960400	-0.94320800
S	-0.67736000	1.78612000	0.29795700
H	-2.30212200	0.17782300	0.11539600
S	-3.24124600	-0.81887600	-0.03596000
H	-2.32306100	-1.79371700	-0.02184000
C	2.45739600	-1.19393700	-0.86141400
H	3.03004800	-1.95281600	-0.32347900
H	1.90546600	-1.69378000	-1.65923800
H	3.16513300	-0.49743000	-1.31386100
C	0.55179300	-1.48018500	0.73381200
H	1.09943300	-2.18095200	1.36951000
H	-0.18877100	-0.96823400	1.34942100
H	0.02782000	-2.05272300	-0.03307300
C	2.31721600	0.22942800	1.18992000
H	1.65868000	0.79982700	1.84592000
H	2.85573600	-0.50212600	1.79790300
H	3.04541100	0.91529900	0.75465900

ωB97X-D, **TS8-1**

C	1.56453800	-0.40149400	0.10184700
S	0.54363300	0.75361900	-0.92562300
S	-0.88121400	1.55031600	0.32502500
H	-2.05412000	0.36090300	0.13042300
S	-3.14698400	-0.81931100	-0.07165700
H	-2.26944300	-1.76835900	0.27496500
C	0.69924100	-1.51144000	0.68303400
H	1.31801600	-2.18536200	1.28081600
H	-0.07765200	-1.10188300	1.32939500
H	0.21933600	-2.09190900	-0.10559800
C	2.27476000	0.35795000	1.21418500
H	2.88062800	-0.33297600	1.80561900
H	2.93190000	1.12808400	0.80854500
H	1.55561500	0.83302400	1.88225300
C	2.58105100	-0.97842400	-0.88073700
H	3.20487100	-0.19674100	-1.31716600
H	3.23548500	-1.67570900	-0.35369300
H	2.09086900	-1.52260400	-1.68946000

ωB97X-D, **INT8-2**

C	1.63646600	-0.46518500	0.10492600
S	0.69335700	0.75882900	-0.91986400
S	-0.70670400	1.58419600	0.32645000
H	-1.71174600	0.65501400	0.18423600
S	-3.47683300	-0.83959700	-0.03563400
H	-4.27106900	0.20420200	-0.31256600
C	2.66202400	-1.03153100	-0.87513100
H	3.27385900	-1.77174000	-0.35659900
H	2.18008200	-1.52640400	-1.71941000
H	3.32579200	-0.25444900	-1.25682400
C	2.33287900	0.22788000	1.26697300
H	1.61136000	0.68812700	1.94246100
H	2.90321800	-0.50822000	1.83780400
H	3.02102200	0.99654300	0.91464100
C	0.71110100	-1.56437600	0.60557200
H	0.22214600	-2.07897500	-0.22186600
H	1.29124400	-2.29623600	1.17197000
H	-0.05784500	-1.16343800	1.26687900

ωB97X-D, **INT8-3**

C	-3.07201700	0.35666600	-0.38636000
S	-2.11518800	-0.03210900	1.15285800
S	-1.02330500	-1.71491800	0.73985700
H	0.05187400	-1.12693800	0.14601400
C	2.40644400	1.11951300	0.21915200
S	1.91614800	-0.20527600	-0.97989900
S	2.87603600	-1.95055200	-0.43185600
C	2.01079200	0.73561400	1.63817000
H	2.32681000	1.51476700	2.33652100
H	0.92999100	0.61600900	1.72619100
H	2.48625000	-0.20068900	1.93272700
C	1.62635000	2.35207700	-0.23065600
H	1.86233900	3.19265100	0.42577700
H	1.88548700	2.63923400	-1.25114600
H	0.54959100	2.17983000	-0.18393700
C	3.90437800	1.38022900	0.13680900
H	4.19232400	1.70936600	-0.86268400
H	4.18759000	2.15922300	0.84930200
H	4.46765200	0.47752800	0.37658200
C	-4.00885700	-0.78810300	-0.74307900
H	-4.58150000	-0.52257000	-1.63436300
H	-3.45300500	-1.69992300	-0.96299500
H	-4.70943600	-0.99327200	0.06661200
C	-3.86741800	1.60146300	0.00143000
H	-3.21073000	2.43244900	0.26266600
H	-4.47749900	1.90964700	-0.84936300
H	-4.53568300	1.40561300	0.84117200
C	-2.12478700	0.66366900	-1.53712000
H	-1.51691600	-0.20453800	-1.79323400
H	-2.70575300	0.94020900	-2.41981200
H	-1.45774400	1.49030500	-1.29147500

ωB97X-D, **TS8-2**

C	2.45231100	-0.73347300	0.34190500
S	1.11132700	0.28235200	-0.50641800
S	2.28562400	2.42024500	-0.29373500
H	1.19995900	2.95227400	0.27920400
C	-2.94350000	0.26769000	0.40973500
S	-2.09544300	-0.17083000	-1.18160000
S	-0.59192600	-1.46520200	-0.72755900
C	-4.02940600	1.25640200	-0.00674900
H	-4.73256200	0.80759200	-0.71026200
H	-4.59048100	1.56697700	0.87704300
H	-3.60297300	2.14997500	-0.46510700
C	-3.56789300	-0.97303800	1.03414300
H	-2.80485300	-1.71469500	1.27278800
H	-4.07937200	-0.70168700	1.96083500
H	-4.29597200	-1.42922700	0.36244500
C	-1.97395300	0.92176000	1.38397100
H	-1.54563000	1.83323000	0.96658400
H	-2.50255200	1.17776400	2.30586600
H	-1.15503400	0.24693300	1.63246400
C	3.82420500	-0.39584900	-0.24218500
H	4.57045000	-1.05192600	0.21341100
H	3.84303000	-0.56029500	-1.32011000
H	4.11592000	0.63179200	-0.03988500
C	2.42099100	-0.44971000	1.83963300
H	1.45950000	-0.73599900	2.26801800
H	3.20355400	-1.02351400	2.34370700
H	2.59012200	0.60802500	2.03946000
C	2.22048100	-2.22635600	0.10502400
H	3.06232300	-2.77171100	0.53870700
H	1.31459300	-2.58730200	0.58788600
H	2.17725500	-2.46779600	-0.95693800

ωB97X-D, **INT8-4**

C	1.74798600	1.24842300	0.12659300
S	0.70696300	-0.25400100	0.45037800
S	5.41711700	-1.55645500	0.04229200
H	6.36073600	-2.51054600	0.04619400
C	-3.44656800	-0.54040800	0.27353000
S	-2.32403500	0.68691100	-0.54962400
S	-0.64294000	-0.35077000	-1.08359900
C	-4.67074400	0.29894600	0.63491200
H	-5.13372400	0.73676100	-0.25053900
H	-5.40860300	-0.34650200	1.11439300
H	-4.41793900	1.09971000	1.33086700
C	-3.82642000	-1.65072300	-0.69556100
H	-2.95142400	-2.21956700	-1.01112300
H	-4.51229200	-2.34063900	-0.19944200
H	-4.32173600	-1.25159800	-1.58070300
C	-2.79997000	-1.11162000	1.52706200
H	-1.91425300	-1.70006000	1.28723300
H	-2.51783500	-0.32391100	2.22530100
H	-3.51354700	-1.77260100	2.02366200
C	0.89378400	2.50782500	0.12301200
H	0.19088600	2.51076500	-0.71031900
H	0.33374600	2.61403400	1.05184900
H	1.54506000	3.37730700	0.01110500
C	2.71845900	1.25803200	1.30667500
H	3.32989500	0.35408300	1.33101300
H	3.38907800	2.11245200	1.19964400
H	2.19424500	1.35723500	2.25799300
C	2.50513000	1.10043300	-1.18533000
H	3.13217400	1.98155400	-1.33802100
H	3.14899900	0.22022100	-1.17297600
H	1.82290700	1.02490000	-2.03263100

ωB97X-D, **TS9-1**

C	3.10886300	0.72916500	-0.04899300
S	3.03540200	-1.11018600	0.12802400
S	0.57448800	-1.64609500	0.01253400
H	0.53441900	-0.89654300	1.10830900
C	-2.78620100	0.99406900	0.13693400
S	-2.54231200	-0.48285500	-0.95622400
S	-1.68615200	-1.94644300	0.18716400
C	-3.80305500	0.68615300	1.22740000
H	-3.94159000	1.56626300	1.85982800
H	-4.76921300	0.41547500	0.80050700
H	-3.46154200	-0.13326000	1.86094900
C	-3.32520200	2.06350500	-0.81061300
H	-3.53590900	2.97181900	-0.24279000
H	-2.60028200	2.31062200	-1.58727400
H	-4.25300200	1.74504500	-1.28868600
C	-1.46728200	1.44548000	0.74928700
H	-0.71635300	1.64046400	-0.01654500
H	-1.62842500	2.36518200	1.31692400
H	-1.07476300	0.69486900	1.43521600
C	2.47291700	1.40749900	1.16490100
H	2.53840300	2.49565400	1.06787000
H	1.41758000	1.14967300	1.26171800
H	2.98034800	1.11778000	2.08599100
C	4.57745200	1.14166500	-0.13878300
H	5.06186900	0.68903600	-1.00521900
H	4.65793800	2.22907100	-0.23489200
H	5.12673300	0.84069800	0.75472800
C	2.38266300	1.17829400	-1.31560000
H	1.33120000	0.89109200	-1.28867100
H	2.43497700	2.26693200	-1.41486000
H	2.83387100	0.73440700	-2.20427900

ωB97X-D, **INT9-1**

C	-3.91171400	-0.32990000	0.21549700
S	-2.48281600	-0.59781000	-0.92229000
S	0.08614900	1.89124600	0.51398800
H	-1.64770700	0.30576200	-0.35626500
S	1.11527500	0.97030600	-1.01504500
S	1.89983300	-0.81686900	-0.38422600
C	3.60825900	-0.47736500	0.25738400
C	3.56137100	0.49885000	1.42495700
H	3.15626900	1.46190600	1.11518000
H	2.94501700	0.11453500	2.23792600
H	4.57332800	0.65773700	1.80598700
C	4.49602900	0.06280000	-0.85569400
H	5.50132900	0.24188900	-0.46690900
H	4.56960800	-0.64516400	-1.68179400
H	4.11070100	1.00721200	-1.24141700
C	4.10799900	-1.84403700	0.72068500
H	4.12916500	-2.56289300	-0.09989400
H	5.12548300	-1.74194300	1.10381800
H	3.48591700	-2.24755900	1.52081200
C	-5.00779100	-1.29104400	-0.23514500
H	-4.67802900	-2.32892200	-0.17218400
H	-5.87928800	-1.17274000	0.41170300
H	-5.31848800	-1.08734200	-1.26083700
C	-4.39542100	1.11255500	0.10663800
H	-5.24504000	1.26724100	0.77644100
H	-3.60855500	1.81254200	0.39073400
H	-4.71328600	1.34616300	-0.90955500
C	-3.49426700	-0.63839200	1.64968100
H	-2.68686100	0.01951600	1.97367800
H	-4.34420500	-0.48848000	2.32011600
H	-3.15720000	-1.67022900	1.74960200