

Electronic Supplementary Information

Mechanistic Insight into Photocrosslinking Reaction between Triplet State 4-Thiopyrimidine and Thymine

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Figure S1. Optimized geometries of the reactants, intermediates, transition states, and products in S_0 and T_1 states of the (6-4) photocrosslinking reaction between 4-TT and T at M06-2X/6-311++G(d,p) level. Bond lengths are in angstroms. Carbon, oxygen, nitrogen, sulfur, and hydrogen atoms are denoted by gray, red, blue, orange, and white balls, respectively.

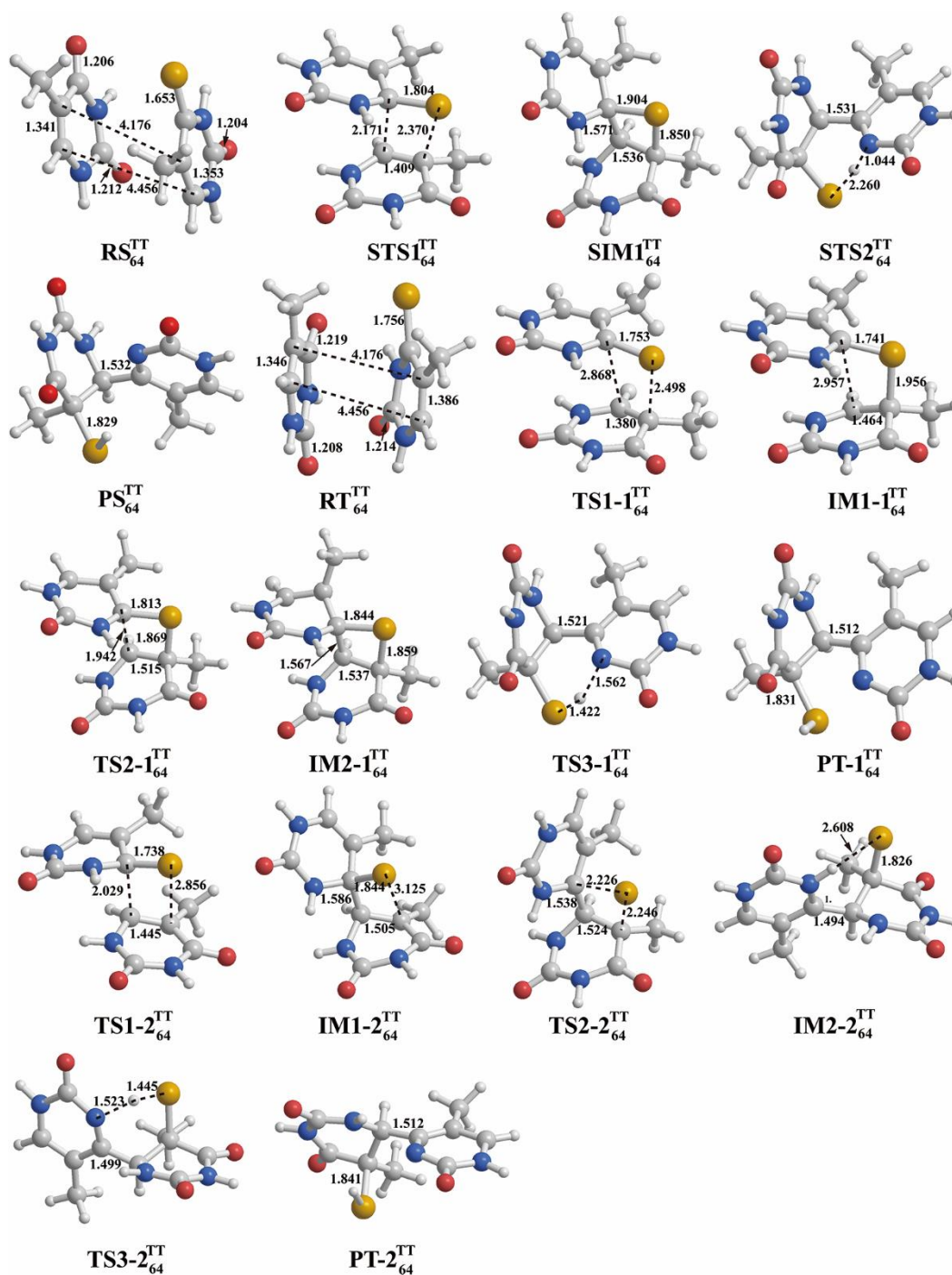


Figure S2. Potential energy profiles of (6-4) photocrosslinking reaction between 4-TT and T. (A)

Energy profiles on the S_0 surface. The concerted pathway towards thietane intermediate $SIM1_{64}^{TT}$ and the subsequent (6-4) photocrosslinking product PS_{64}^{TT} formation pathway are denoted by black solid line. (B) Energy profiles on the T_1 surface. S-attack pathway and C-attack pathway are denoted by green and blue solid lines.

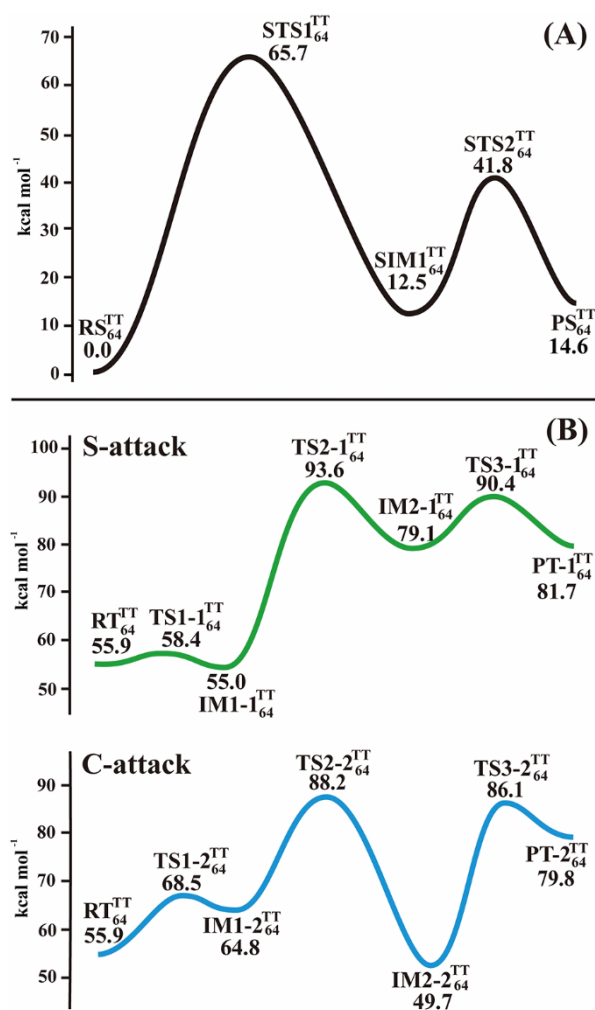


Figure S3. Optimized geometries of reactants, intermediates, transition states, and products in T_1 and S_0 states for the (5-4) photocrosslinking reaction between 4-TT and T at M06-2X/6-311++G(d,p) level. Bond lengths are in angstroms. Carbon, oxygen, nitrogen, sulfur, and hydrogen atoms are denoted by gray, red, blue, orange, and white balls, respectively.

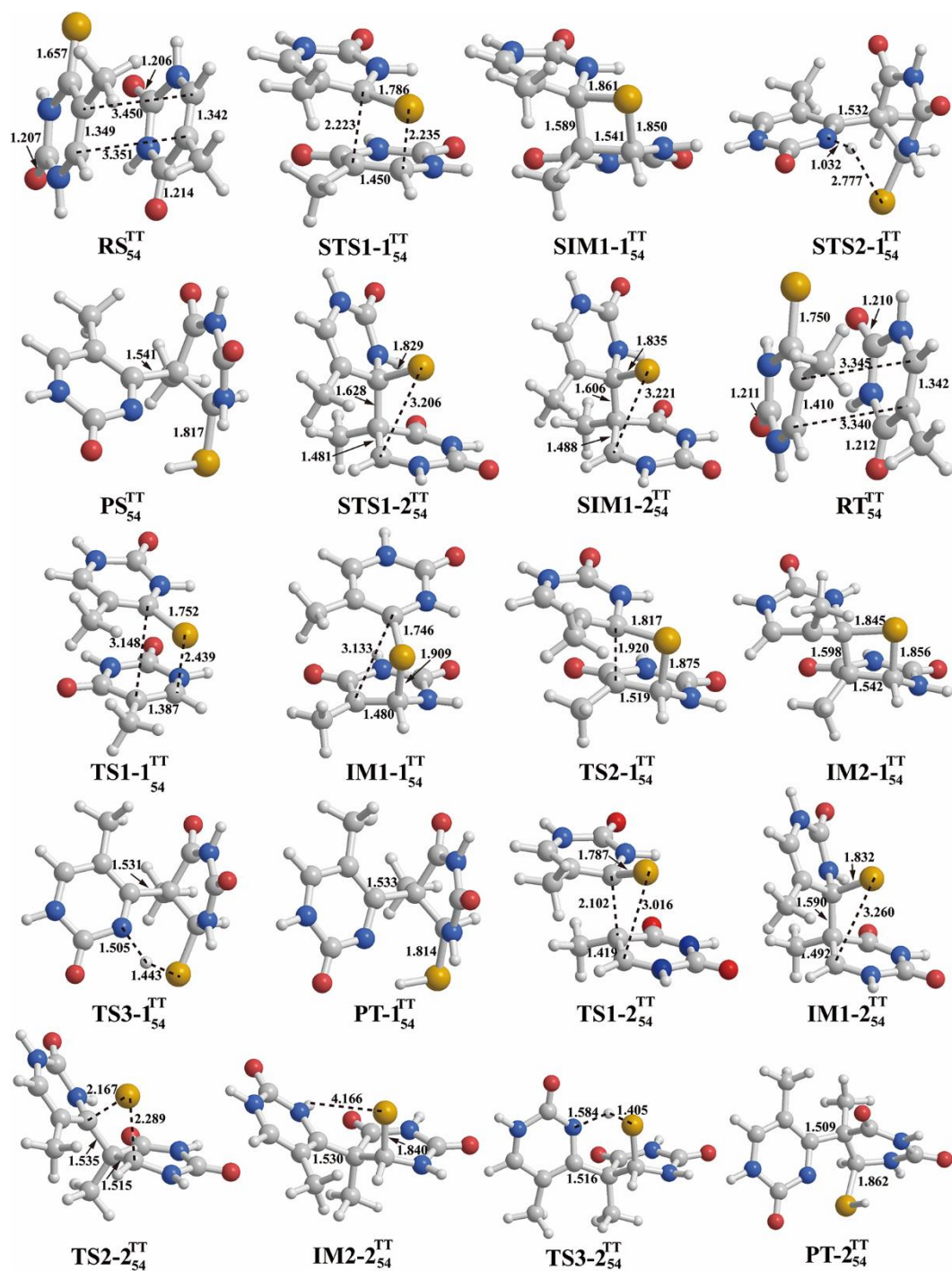


Figure S4. Potential energy profiles of (5-4) photocrosslinking reaction between 4-TT and T. (A) Energy profiles on the S_0 surface. The concerted and consecutive pathways towards the thietane intermediate $SIM1-1_{54}^{TT}$ are denoted by black and orange solid lines. The energy profile of the (5-4) photocrosslinking product PS_{54}^{TT} formation from $SIM1-1_{54}^{TT}$ is denoted by black solid line. (B) Energy profiles on the T_1 surface. S-attack pathway and C-attack pathway are denoted by green line and blue solid line, respectively.

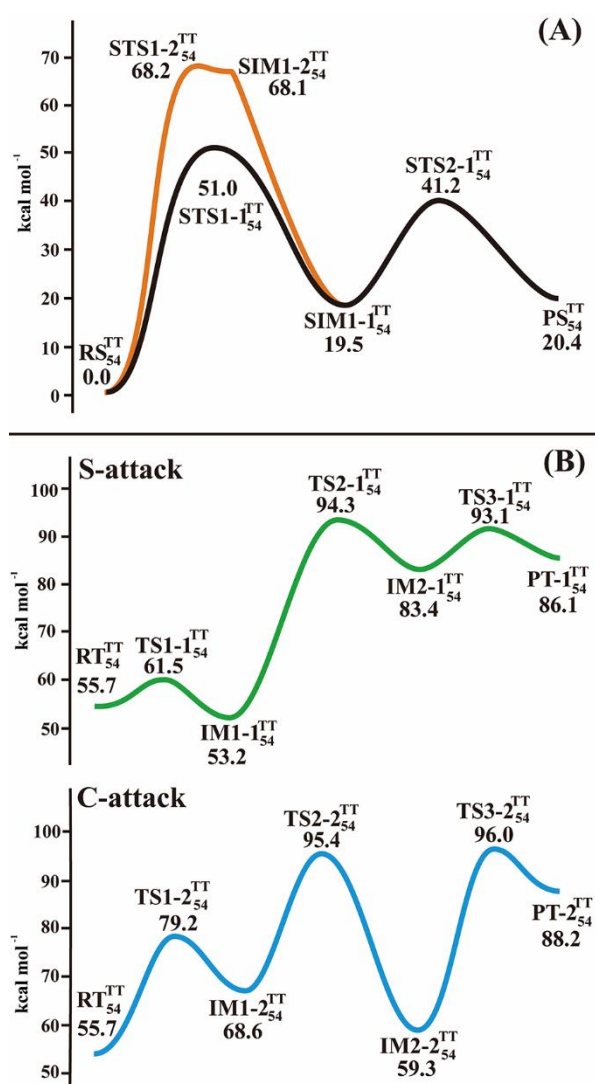


Table S1. Mulliken spin densities (M06-2X/6-311++G(d,p) Level) of the selected atoms in reactants, diradical intermediates and products of (6-4) and (5-4) photocrosslinking reactions between 4-TU and T.

	S	C4	C5'	C6'		S	C4	C5'	C6'
RS ₆₄	0.00	0.00	0.00	0.00	RS ₅₄	0.00	0.00	0.00	0.00
SIM1-1 ₆₄	1.00	-0.27	-1.16	0.68	SIM1-1 ₅₄	0.74	-0.04	0.17	-0.79
PS ₆₄	0.00	0.00	0.00	0.00	PS ₅₄	0.00	0.00	0.00	0.00
RT ₆₄	1.07	0.62	-0.05	0.00	RT ₅₄	1.19	0.50	-0.03	0.00
IM1-1 ₆₄	0.18	0.38	0.03	0.75	IM1-1 ₅₄	0.05	0.50	0.79	0.10
IM2-1 ₆₄	0.03	0.04	-0.02	-0.06	IM2-1 ₅₄	0.03	0.11	0.07	-0.12
PT-1 ₆₄	0.41	0.55	-0.05	0.01	PT-1 ₅₄	0.04	0.39	0.04	0.02
IM1-2 ₆₄	0.90	-0.20	0.68	0.27	IM1-2 ₅₄	0.70	0.13	-0.05	0.96
IM2-2 ₆₄	0.94	0.49	-0.07	0.09	IM2-2 ₅₄	1.034	0.58	0.00	-0.23
PT-2 ₆₄	0.21	0.49	0.01	0.00	PT-2 ₅₄	0.18	0.51	0.01	-0.1

Table S2. Relative free energies (kcal mol⁻¹) of the stationary structures along S₀ and T₁ states of the (6-4) photocrosslinking reaction pathways for 4-TU and T at M06-2X/6-311++G(d,p) level.

	G/kcal mol ⁻¹		G/kcal mol ⁻¹		G/kcal mol ⁻¹
RS ₆₄	0.0	STS2-2 ₆₄	59.1	PT-1 ₆₄	76.3
STS1-1 ₆₄	62.3	RT ₆₄	50.7	TS1-2 ₆₄	64.6
SIM1-1 ₆₄	14.1	TS1-1 ₆₄	54.4	IM1-2 ₆₄	58.0
STS2-1 ₆₄	41.9	IM1-1 ₆₄	50.5	TS2-2 ₆₄	83.4
PS ₆₄	12.4	TS2-1 ₆₄	91.7	IM2-2 ₆₄	46.3
STS1-2 ₆₄	60.2	IM2-1 ₆₄	79.3	TS3-2 ₆₄	80.7
SIM1-2 ₆₄	58.8	TS3-1 ₆₄	83.6	PT-2 ₆₄	74.6

Table S3. Relative free energies (kcal mol⁻¹) of the stationary structures along S₀ and T₁ states of the (5-4) photocrosslinking reaction pathways for 4-TU and T at M06-2X/6-311++G(d,p) level.

	G/kcal mol ⁻¹		G/kcal mol ⁻¹		G/kcal mol ⁻¹
RS ₆₄	0.0	STS2-2 ₆₄	63.4	PT-1 ₆₄	79.7
STS1-1 ₆₄	48.7	RT ₆₄	55.1	TS1-2 ₆₄	74.2
SIM1-1 ₆₄	16.9	TS1-1 ₆₄	56.9	IM1-2 ₆₄	62.3
STS2-1 ₆₄	38.6	IM1-1 ₆₄	49.5	TS2-2 ₆₄	88.1
PS ₆₄	13.1	TS2-1 ₆₄	93.0	IM2-2 ₆₄	51.6
STS1-2 ₆₄	62.5	IM2-1 ₆₄	82.6	TS3-2 ₆₄	85.6
SIM1-2 ₆₄	62.8	TS3-1 ₆₄	84.0	PT-2 ₆₄	81.0

Table S4. Relative energies (without ZPE correction, kcal mol⁻¹) of the stationary structures along S₀ and T₁ states of the (6-4) photocrosslinking reaction pathways for 4-TT and T.

	M06-2X/6- 311++G(d,p)			M06-2X/6- 311++G(d,p)	
	vacuum	E = 4.3		vacuum	E = 4.3
RS ₆₄ ^{TT}	0.0	0.0	IM2-1 ₆₄ ^{TT}	79.1	81.6
STS1 ₆₄ ^{TT}	65.7	65.0	TS3-1 ₆₄ ^{TT}	90.4	92.7
SIM ₆₄ ^{TT}	12.5	14.3	PT-1 ₆₄ ^{TT}	81.7	84.2
STS2 ₆₄ ^{TT}	41.8	34.3	TS1-2 ₆₄ ^{TT}	68.5	70.8
PS ₆₄ ^{TT}	14.6	14.3	IM1-2 ₆₄ ^{TT}	64.8	66.3
RT ₆₄ ^{TT}	55.9	59.1	TS2-2 ₆₄ ^{TT}	88.2	87.6
TS1-1 ₆₄ ^{TT}	58.4	59.8	IM2-2 ₆₄ ^{TT}	49.7	52.4
IM1-1 ₆₄ ^{TT}	55.0	56.8	TS3-2 ₆₄ ^{TT}	86.1	87.8
TS2-1 ₆₄ ^{TT}	93.6	96.0	PT-2 ₆₄ ^{TT}	79.8	81.3

Table S5. Relative energies (without ZPE correction, kcal mol⁻¹) of the stationary structures along S₀ and T₁ states of the (5-4) photocrosslinking reaction pathways for 4-TT and T.

	M06-2X/6- 311++G(d,p)			M06-2X/6- 311++G(d,p)	
	vacuum	E = 4.3		vacuum	E = 4.3
RS ₅₄ ^{TT}	0	0	TS2-1 ₅₄ ^{TT}	94.3	93.9
STS1-1 ₅₄ ^{TT}	51.0	49.9	IM2-1 ₅₄ ^{TT}	83.4	83.5
SIM1-1 ₅₄ ^{TT}	19.5	19.2	TS3-1 ₅₄ ^{TT}	93.1	94.2
STS2-1 ₅₄ ^{TT}	41.2	33.1	PT-1 ₅₄ ^{TT}	86.1	86.9
PS ₅₄ ^{TT}	20.4	19.7	TS1-2 ₅₄ ^{TT}	79.2	78.4
STS1-2 ₅₄ ^{TT}	68.2	69.2	IM1-2 ₅₄ ^{TT}	68.6	67.7
SIM1-2 ₅₄ ^{TT}	68.1	67.8	TS2-2 ₅₄ ^{TT}	95.4	94.3
RT ₅₄ ^{TT}	55.7	56.9	IM2-2 ₅₄ ^{TT}	59.3	59.6
TS1-1 ₅₄ ^{TT}	61.5	60.7	TS3-2 ₅₄ ^{TT}	96.0	95.6
IM1-1 ₅₄ ^{TT}	53.2	52.6	PT-2 ₅₄ ^{TT}	88.2	86.9

Table S6. Mulliken spin densities (M06-2X/6-311++G(d,p) Level) of selected atoms in the reactants, intermediates and products of (6-4) and (5-4) photocrosslinking reactions between 4-TT and T.

	S	C4	C5'	C6'		S	C4	C5'	C6'
RS ₆₄ ^{TT}	0.00	0.00	0.00	0.00	SIM1-1 ₅₄ ^{TT}	-0.73	0.08	0.00	0.79
PS ₆₄ ^{TT}	0.00	0.00	0.00	0.00	PS ₅₄ ^{TT}	0.00	0.00	0.00	0.00
RT ₆₄ ^{TT}	1.15	0.41	0.01	0.00	RT ₅₄ ^{TT}	0.70	0.67	0.10	-0.03
IM1-1 ₆₄ ^{TT}	0.18	0.36	0.01	0.80	IM1-1 ₅₄ ^{TT}	0.02	0.54	0.83	0.00
IM2-1 ₆₄ ^{TT}	0.01	0.06	-0.03	0.01	IM2-1 ₅₄ ^{TT}	0.02	0.34	0.00	-0.08
PT-1 ₆₄ ^{TT}	0.23	0.40	0.04	-0.05	PT-1 ₅₄ ^{TT}	0.01	0.05	0.13	0.01
IM1-2 ₆₄ ^{TT}	0.72	0.02	0.93	-0.08	IM1-2 ₅₄ ^{TT}	0.62	-0.01	-0.16	0.97
IM2-2 ₆₄ ^{TT}	0.94	0.50	-0.09	0.07	IM2-2 ₅₄ ^{TT}	0.95	0.56	-0.08	-0.11
PT-2 ₆₄ ^{TT}	0.06	0.21	-0.05	0.05	PT-2 ₅₄ ^{TT}	0.36	0.60	0.03	-0.11
RS ₅₄ ^{TT}	0.00	0.00	0.00	0.00					

Table S7. Relative energies (kcal mol⁻¹) of the stationary structures optimized in implicit solvent (using the IEF-PCM model with $\epsilon = 4.3$) for the (6-4) photocrosslinking reaction pathways between 4-TT and T at M06-2X/6-311++G(d,p) level.

	E/kcal mol ⁻¹		E/kcal mol ⁻¹		E/kcal mol ⁻¹
RS ₆₄ ^{TT}	0.0	TS1-1 ₆₄ ^{TT}	59.7	TS1-2 ₆₄ ^{TT}	70.7
STS1 ₆₄ ^{TT}	65.3	IM1-1 ₆₄ ^{TT}	56.8	IM1-2 ₆₄ ^{TT}	66.1
SIM ₆₄ ^{TT}	14.3	TS2-1 ₆₄ ^{TT}	96.0	TS2-2 ₆₄ ^{TT}	87.6
STS2 ₆₄ ^{TT}	33.7	IM2-1 ₆₄ ^{TT}	81.6	IM2-2 ₆₄ ^{TT}	52.4
PS ₆₄ ^{TT}	14.0	TS3-1 ₆₄ ^{TT}	92.4	TS3-2 ₆₄ ^{TT}	87.7
RT ₆₄ ^{TT}	59.0	PT-1 ₆₄ ^{TT}	84.1	PT-2 ₆₄ ^{TT}	81.3

Table S8. Relative energies (kcal mol⁻¹) of the stationary structures optimized in implicit solvent (using the IEF-PCM model with $\epsilon = 4.3$) for the (5-4) photocrosslinking reaction pathways between 4-TT and T at M06-2X/6-311++G(d,p) level.

	E/kcal mol ⁻¹		E/kcal mol ⁻¹		E/kcal mol ⁻¹
RS ₅₄ ^{TT}	0.0	RT ₅₄ ^{TT}	58.2	TS1-2 ₅₄ ^{TT}	79.5
STS1-1 ₅₄ ^{TT}	48.7	TS1-1 ₅₄ ^{TT}	61.8	IM1-2 ₅₄ ^{TT}	68.8
SIM1-1 ₅₄ ^{TT}	20.3	IM1-1 ₅₄ ^{TT}	53.7	TS2-2 ₅₄ ^{TT}	95.4
STS2-1 ₅₄ ^{TT}	34.3	TS2-1 ₅₄ ^{TT}	94.9	IM2-2 ₅₄ ^{TT}	60.7
PS ₅₄ ^{TT}	20.7	IM2-1 ₅₄ ^{TT}	84.6	TS3-2 ₅₄ ^{TT}	96.3
STS1-2 ₅₄ ^{TT}	68.6	TS3-1 ₅₄ ^{TT}	96.3	PT-2 ₅₄ ^{TT}	87.9
SIM1-2 ₅₄ ^{TT}	68.5	PT-1 ₅₄ ^{TT}	88.1		

Table S9. Relative free energies (kcal mol⁻¹) of the stationary structures along S₀ and T₁ states of the (6-4) photocrosslinking reaction pathways for 4-TT and T at M06-2X/6-311++G(d,p) level.

	E/kcal mol ⁻¹		E/kcal mol ⁻¹		E/kcal mol ⁻¹
RS ₆₄ ^{TT}	0.0	TS1-1 ₆₄ ^{TT}	55.9	TS1-2 ₆₄ ^{TT}	67.3
STS1 ₆₄ ^{TT}	65.6	IM1-1 ₆₄ ^{TT}	52.3	IM1-2 ₆₄ ^{TT}	64.6
SIM ₆₄ ^{TT}	15.3	TS2-1 ₆₄ ^{TT}	90.9	TS2-2 ₆₄ ^{TT}	87.2
STS2 ₆₄ ^{TT}	43.6	IM2-1 ₆₄ ^{TT}	78.2	IM2-2 ₆₄ ^{TT}	49.1
PS ₆₄ ^{TT}	14.8	TS3-1 ₆₄ ^{TT}	85.9	TS3-2 ₆₄ ^{TT}	80.6
RT ₆₄ ^{TT}	52.1	PT-1 ₆₄ ^{TT}	79.6	PT-2 ₆₄ ^{TT}	76.0

Table S10. Relative free energies (kcal mol⁻¹) of the stationary structures along S₀ and T₁ states of the (5-4) photocrosslinking reaction pathways for 4-TT and T at M06-2X/6-311++G(d,p) level.

	G/kcal mol ⁻¹		G/kcal mol ⁻¹		G/kcal mol ⁻¹
RS ₅₄ ^{TT}	0.0	RT ₅₄ ^{TT}	53.5	TS1-2 ₅₄ ^{TT}	76.5
STS1-1 ₅₄ ^{TT}	50.8	TS1-1 ₅₄ ^{TT}	58.2	IM1-2 ₅₄ ^{TT}	67.6
SIM1-1 ₅₄ ^{TT}	21.7	IM1-1 ₅₄ ^{TT}	50.6	TS2-2 ₅₄ ^{TT}	95.0
STS2-1 ₅₄ ^{TT}	44.8	TS2-1 ₅₄ ^{TT}	91.6	IM2-2 ₅₄ ^{TT}	58.9
PS ₅₄ ^{TT}	20.0	IM2-1 ₅₄ ^{TT}	81.7	TS3-2 ₅₄ ^{TT}	91.0
STS1-2 ₅₄ ^{TT}	68.1	TS3-1 ₅₄ ^{TT}	86.8	PT-2 ₅₄ ^{TT}	85.4
SIM1-2 ₅₄ ^{TT}	67.7	PT-1 ₅₄ ^{TT}	81.2		

Cartesian coordinates of the stationary structures for photocrosslinking reactions of 4-TU and T, and of 4-TT and T.

RS₆₄

N	-0.92109300	-1.92364000	0.70866900
C	-2.08433300	-1.27402800	1.07513800
H	-2.47511300	-1.54395800	2.04843700
C	-2.68450700	-0.36738500	0.29080600
C	-3.93242700	0.35788600	0.68176900
H	-3.74428600	1.43379500	0.71169700
H	-4.72168900	0.18886500	-0.05333600
H	-4.27983200	0.03173300	1.66232300
C	-2.10768100	-0.10155900	-1.03245000
O	-2.59269800	0.62017300	-1.86888500
N	-0.90509800	-0.78196100	-1.28669100
H	-0.44259100	-0.56474800	-2.16131800
C	-0.22053800	-1.62312200	-0.43878600
O	0.88374900	-2.06642800	-0.67345900
N	3.05560000	-0.48113200	0.65489200
C	2.21885000	-0.31510700	1.72246800
H	2.47273400	-0.88362600	2.60814100
C	1.15714600	0.51602300	1.66930200
C	0.90701500	1.27957500	0.46922700
N	1.77966900	1.01476400	-0.56556800
H	1.64358000	1.52831700	-1.42875700
C	2.85518500	0.13650700	-0.56970900
O	3.56025600	-0.04163300	-1.52699700
S	-0.30278700	2.39082200	0.30273900
H	0.51949100	0.71331400	2.51678100
H	-0.43657200	-2.52146100	1.35990800
H	3.78260600	-1.18124000	0.66133100

STS1-1₆₄

N	-0.50292800	1.33972800	-0.94810900
C	-0.34136300	-0.05037800	-1.09782600
H	0.24408300	-0.36776600	-1.95142600
C	-1.33299400	-0.89606700	-0.57057200
C	-1.47965100	-2.30125400	-1.05482600
H	-1.91122300	-2.93133300	-0.28011400
H	-2.17179100	-2.29159100	-1.90453800
H	-0.53003800	-2.70679400	-1.40000300
C	-2.59794900	-0.28866500	-0.03631500

O	-3.56681300	-0.94276600	0.25690000
N	-2.59793800	1.09060500	0.01750600
H	-3.40110300	1.53268800	0.44649100
C	-1.55430600	1.95163100	-0.31697900
O	-1.60804400	3.13810600	-0.09841400
N	3.38513400	-0.20405900	-0.55628000
C	2.85611700	-1.47735600	-0.59758100
H	3.48811700	-2.23649100	-1.03853700
C	1.63554100	-1.72994400	-0.09743100
C	0.87505800	-0.64369300	0.49487800
N	1.61735200	0.48086900	0.76582400
H	1.18481100	1.20056200	1.33611400
C	2.82630000	0.83043300	0.17231800
O	3.33591300	1.91455100	0.29046200
S	-0.41305900	-0.97663000	1.69162800
H	1.22872000	-2.72783400	-0.07843000
H	0.25637600	1.96484200	-1.17939600
H	4.30068500	-0.00758300	-0.93439200

SIM1-1₆₄

N	-0.76996400	1.25479800	-1.02756800
C	-0.41644900	-0.14146300	-0.98811300
H	-0.31311700	-0.51680600	-2.01105600
C	-1.38419400	-1.00360300	-0.14641300
C	-1.75962000	-2.32540500	-0.79870800
H	-2.31271500	-2.93996800	-0.08997800
H	-2.39430200	-2.14477200	-1.67157900
H	-0.86627700	-2.86470400	-1.11413700
C	-2.63337600	-0.32912300	0.39441300
O	-3.51081400	-0.95499700	0.93340100
N	-2.69391400	1.04058600	0.27232800
H	-3.49339500	1.50379800	0.68671700
C	-1.82363300	1.87884900	-0.42338800
O	-2.01623700	3.06862100	-0.48465400
N	3.70343900	-0.19216300	-0.05744300
C	3.12574000	-1.27343200	-0.69803400
H	3.81548500	-1.99444400	-1.11599600
C	1.80212200	-1.41227400	-0.78451000
C	0.88820400	-0.41987100	-0.15801100
N	1.60720300	0.76212800	0.20332700
H	1.07906800	1.50094800	0.65049700
C	2.96543800	0.87493500	0.41877500
O	3.47245400	1.83782500	0.94352800
S	-0.15589000	-1.17591200	1.23028500

H	1.37287000	-2.27606500	-1.27060900
H	-0.17247800	1.88437700	-1.54470600
H	4.70312400	-0.09849000	0.02753400

STS2-1₆₄

N	-0.98233700	1.61692900	-0.85482900
C	-0.58258400	0.24994900	-1.15129400
H	-0.65106900	0.09142400	-2.22751400
C	-1.47330900	-0.79411400	-0.48004000
C	-2.86466200	-0.79519100	-1.13498600
H	-3.47876000	-1.54870800	-0.64243800
H	-3.35814100	0.17996900	-1.06064000
H	-2.75954700	-1.07315100	-2.18478300
C	-1.71117500	-0.41274400	0.98577700
O	-2.01228500	-1.17681000	1.85983500
N	-1.61351300	0.95850500	1.27269900
H	-1.89481900	1.23506000	2.20590300
C	-1.38880200	2.01247900	0.39508800
O	-1.54298900	3.16745800	0.71382400
N	3.46258300	0.28182900	0.11061100
C	3.14300500	0.82992700	-1.07909500
H	3.95174300	1.30361300	-1.62153900
C	1.86480400	0.78171800	-1.54678300
C	0.89385900	0.11214600	-0.77412900
N	1.26122800	-0.40534700	0.40910800
H	0.64290000	-1.17246100	0.75296300
C	2.55239800	-0.40291500	0.92781600
O	2.87318100	-0.92687600	1.95305300
S	-0.60446700	-2.37950500	-0.70682400
H	1.59975600	1.23220600	-2.49097200
H	-0.83451600	2.37036500	-1.50963500
H	4.41373000	0.29264500	0.45688500

PS₆₄

N	-0.99402900	1.20668200	-1.40149300
C	-0.49711600	-0.14700800	-1.19499400
H	-0.55738400	-0.67403200	-2.15032200
C	-1.42200000	-0.87570000	-0.20254300
C	-2.80238200	-1.10162100	-0.84215900
H	-3.47987700	-1.53650200	-0.10736200
H	-3.21615000	-0.16029400	-1.20635900
H	-2.71215300	-1.79264900	-1.68367000
C	-1.63724700	-0.02518000	1.05518400
O	-1.79079100	-0.47300300	2.15817400

N	-1.77322800	1.32789800	0.79485700
H	-1.95879500	1.91980400	1.59526400
C	-1.39899800	2.01092400	-0.36100200
O	-1.48396000	3.21145400	-0.44389200
N	3.47705200	0.05833100	0.06692900
C	3.26079200	-0.38047600	-1.18883100
H	4.13584700	-0.63468100	-1.77441300
C	1.98705900	-0.48632900	-1.65046100
C	0.95891400	-0.11599400	-0.73733500
N	1.16082800	0.30435200	0.47695400
H	-0.03221200	-2.11880600	1.27892000
C	2.44846600	0.41983900	0.97056100
O	2.73821800	0.79134800	2.07828200
S	-0.74591800	-2.52176500	0.21484000
H	1.77123400	-0.84827800	-2.64402300
H	-0.61763800	1.73908500	-2.17362100
H	4.41479000	0.14462700	0.43639000

STS1-2₆₄

N	-0.66875700	1.39599100	-0.75482000
C	-0.25438100	0.02885900	-0.74543400
H	0.46393400	-0.14867200	-1.54898600
C	-1.36665600	-0.90810400	-0.79261800
C	-1.23863800	-2.31278600	-1.25372300
H	-1.27636200	-2.99923600	-0.39929700
H	-2.09522900	-2.57140500	-1.88154000
H	-0.31130100	-2.47616000	-1.80044800
C	-2.64245900	-0.49992300	-0.21579800
O	-3.59006300	-1.24619700	-0.08188600
N	-2.69692200	0.82707300	0.20658600
H	-3.56553900	1.13537700	0.62593600
C	-1.79943400	1.84364900	-0.11688600
O	-2.02332300	3.00304400	0.12599500
N	3.21277800	-0.62156700	-0.79191100
C	2.53511100	-1.73567400	-0.30479400
H	2.98891700	-2.69367800	-0.52197000
C	1.40235500	-1.61632800	0.38764600
C	0.82135000	-0.25525300	0.60466700
N	1.84608100	0.75462800	0.46873700
H	1.72749700	1.62573000	0.96797600
C	2.99779500	0.64991400	-0.27082400
O	3.76538600	1.56540700	-0.45348200
S	-0.12671100	-0.05970900	2.07826300
H	0.88420500	-2.47806300	0.77931200

H	0.03283200	2.10867400	-0.89945600
H	4.11155400	-0.73121700	-1.23680600

SIM1-2₆₄

N	-0.80352700	1.32520900	-0.87564100
C	-0.35161400	-0.05150700	-0.96694400
H	0.06674100	-0.20208300	-1.96756900
C	-1.49817800	-0.98798800	-0.76170600
C	-1.52819500	-2.36719100	-1.31434700
H	-1.40749500	-3.10607300	-0.51279700
H	-2.50694300	-2.56875400	-1.75697200
H	-0.74961800	-2.52063500	-2.06182200
C	-2.61921000	-0.57168300	0.06910600
O	-3.51312000	-1.32165200	0.40474100
N	-2.60947300	0.76482900	0.46670000
H	-3.40161600	1.07956300	1.01233700
C	-1.84324000	1.77653600	-0.10469400
O	-2.09176900	2.94617400	0.06148100
N	3.64616700	-0.70432700	-0.01627000
C	2.80771100	-1.78725600	-0.15272900
H	3.29345100	-2.75021000	-0.24246700
C	1.47482200	-1.65586400	-0.18145800
C	0.85005900	-0.30780500	0.01358900
N	1.83247900	0.73386000	-0.23237400
H	1.52266000	1.67323500	-0.01436100
C	3.19051300	0.60587500	-0.02301900
O	3.93747600	1.54630500	0.09315700
S	0.30384700	-0.40550200	1.76316100
H	0.84107400	-2.52439000	-0.26422200
H	-0.31213800	2.04697200	-1.38068400
H	4.64565500	-0.81348800	0.05507800

STS2-2₆₄

N	-0.72940700	1.28542000	-0.90687100
C	-0.33935700	-0.10787300	-0.94697100
H	0.09104700	-0.30749300	-1.93472500
C	-1.53151800	-0.99048800	-0.73397600
C	-1.55016400	-2.41559400	-1.15270700
H	-1.30266900	-3.06705600	-0.30470100
H	-2.55700300	-2.69431700	-1.46785900
H	-0.84077000	-2.60663300	-1.95903300
C	-2.69972100	-0.47920500	-0.02802400
O	-3.65641900	-1.16917100	0.26062500
N	-2.65218800	0.86873800	0.32280200

H	-3.46203500	1.24363000	0.79992900
C	-1.76923300	1.81492800	-0.18751500
O	-1.93015600	2.99977800	-0.02206800
N	3.66706000	-0.60799100	-0.20230400
C	2.87865400	-1.72868400	-0.36915100
H	3.40957000	-2.64579600	-0.58811400
C	1.54767800	-1.68833800	-0.26953700
C	0.83151200	-0.41751100	0.07084000
N	1.76171300	0.69504900	0.04826000
H	1.41499600	1.56385500	0.43633000
C	3.13945600	0.63844600	0.08028400
O	3.83300700	1.60298600	0.29884900
S	0.08356200	-0.65582200	1.74645200
H	0.96830800	-2.59198900	-0.37480000
H	-0.10270300	1.97449100	-1.29560000
H	4.67330100	-0.66121000	-0.21114200

RT₆₄

N	-2.35214900	-1.20361100	0.82656100
C	-2.65863400	0.13392500	0.91151700
H	-3.32424800	0.40022100	1.72370400
C	-2.17689000	1.05706300	0.05998400
C	-2.46316100	2.51794300	0.21703500
H	-1.53716100	3.06496800	0.41159100
H	-2.89322100	2.93159500	-0.69748800
H	-3.15592600	2.68777900	1.04135900
C	-1.23548200	0.60545500	-0.96765100
O	-0.63201100	1.33652000	-1.72597500
N	-1.04818600	-0.78189200	-1.02248900
H	-0.40310000	-1.13768500	-1.72508200
C	-1.50010800	-1.72896100	-0.12331500
O	-1.18476500	-2.89526700	-0.15094400
N	1.60118700	-1.78759400	0.73485200
C	1.55008600	-0.97374800	1.86842900
H	1.45715800	-1.46683300	2.82185000
C	1.61538700	0.40729100	1.68337300
C	1.74455700	0.91591100	0.41406400
N	1.93340400	0.03250300	-0.65785000
H	1.93142700	0.40112800	-1.60022400
C	1.74744500	-1.32905800	-0.55809200
O	1.69825300	-2.05542000	-1.52788900
S	1.75022000	2.63040200	0.01795900
H	1.55116500	1.12496400	2.48846800
H	-2.70698000	-1.86499400	1.50028600

H	1.34655200	-2.76502500	0.78706700
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TS1-1₆₄

N	0.21529900	0.75861600	1.53937400
C	1.13405000	-0.24335500	1.48056800
H	1.05058100	-1.00805700	2.24200600
C	2.09211100	-0.31073600	0.48842000
C	3.30120500	-1.19368600	0.61357700
H	3.67493300	-1.46113200	-0.37421100
H	4.10039100	-0.66168400	1.13675500
H	3.05570000	-2.10430800	1.16008100
C	2.22432600	0.87273300	-0.39494500
O	3.13486500	1.04888300	-1.16386400
N	1.19856300	1.81668000	-0.26939300
H	1.24230200	2.61775700	-0.88799700
C	0.16456900	1.82584600	0.64682400
O	-0.68711600	2.67384700	0.70042400
N	-3.13200300	-0.29252100	0.41960700
C	-2.56843200	-1.39038600	1.07041000
H	-3.14154200	-1.82149700	1.87598200
C	-1.37134200	-1.90559000	0.59971400
C	-0.73117200	-1.30552700	-0.46817400
N	-1.33892500	-0.17789400	-1.03812000
H	-0.93935100	0.21264200	-1.88146800
C	-2.59216100	0.31198700	-0.70108200
O	-3.14568700	1.18960200	-1.31453500
S	0.84755700	-1.73471200	-1.09622100
H	-0.92943400	-2.77613700	1.06258500
H	-0.56861100	0.70111500	2.17653400
H	-4.04184700	0.05615400	0.68092800

IM1-1₆₄

N	0.34782900	0.71400800	1.68114600
C	1.30692900	-0.26525700	1.54731200
H	1.34563000	-1.02468600	2.31325700
C	1.98443500	-0.44042400	0.26018300
C	3.34364600	-1.11516900	0.36871900
H	3.74393100	-1.31800400	-0.62471400
H	4.04213000	-0.45758000	0.88975900
H	3.24868800	-2.05253400	0.91802400
C	2.08275300	0.86124300	-0.51580000
O	2.92124100	1.07556900	-1.35182900
N	1.09624300	1.79514900	-0.22780000
H	1.07498700	2.63047600	-0.80047000

C	0.17218800	1.76748300	0.81419900
O	-0.68306300	2.60747400	0.95219400
N	-3.19369100	-0.35420000	0.28944500
C	-2.62801900	-1.42400300	0.97410500
H	-3.23022300	-1.86809800	1.75190200
C	-1.38234600	-1.87321200	0.61976900
C	-0.68798200	-1.24784100	-0.41613800
N	-1.32177700	-0.17471100	-1.05886400
H	-0.88025200	0.24983700	-1.86341000
C	-2.59761600	0.28522200	-0.78441900
O	-3.13630300	1.16011500	-1.41520200
S	0.94588300	-1.62620900	-0.88488400
H	-0.92982500	-2.70727700	1.13564800
H	-0.31025100	0.69156100	2.44755400
H	-4.11810400	-0.01958100	0.51420900

TS2-1₆₄

N	0.55876000	0.98601600	1.51007700
C	0.59385600	-0.36839200	1.16791300
H	0.46741500	-1.01777500	2.02784200
C	1.68314000	-0.80881000	0.20990300
C	2.79546300	-1.64911000	0.82064500
H	3.47294900	-1.99533500	0.03947100
H	3.36928300	-1.05021600	1.53315200
H	2.36840800	-2.50967500	1.33623600
C	2.27455800	0.32702600	-0.61009100
O	3.17797900	0.16353200	-1.38702400
N	1.67794000	1.57024900	-0.44433400
H	2.05952600	2.32285000	-1.00656900
C	0.92727300	2.00025300	0.65637100
O	0.66503300	3.16079700	0.83701800
N	-3.44288300	-0.12034200	0.14278100
C	-2.99747800	-1.08142000	1.03645100
H	-3.75634700	-1.59805400	1.60311000
C	-1.74981800	-1.74625600	0.61059900
C	-0.80020600	-0.96273300	-0.03967100
N	-1.28992500	0.22429700	-0.65232500
H	-0.70460100	0.70041600	-1.32528000
C	-2.61810900	0.59768100	-0.70712000
O	-3.02805800	1.49085900	-1.41251600
S	0.56234200	-1.78677200	-0.91166300
H	-1.51700500	-2.75891600	0.90356600
H	-0.05952300	1.28905000	2.25054900
H	-4.39653800	0.21352000	0.16132300

IM2-1₆₄

N	0.18154400	0.92807300	1.41060700
C	0.39376900	-0.43153800	1.00397100
H	0.33746200	-1.07371600	1.88518200
C	1.72355700	-0.67119400	0.26925000
C	2.84204100	-1.30962100	1.06933600
H	3.69688200	-1.51038100	0.42333400
H	3.16297300	-0.62881300	1.86331200
H	2.49656800	-2.24279600	1.51520800
C	2.23642800	0.54915700	-0.48323000
O	3.23806700	0.52168700	-1.14994800
N	1.45702700	1.68997100	-0.38516100
H	1.79069800	2.50067900	-0.89419200
C	0.51025100	1.99030200	0.60941300
O	0.08200500	3.10687800	0.74563700
N	-3.20835400	-0.20139300	0.32176700
C	-2.64755800	-1.17282300	1.13574900
H	-3.22449100	-1.51912300	1.97920400
C	-1.59590300	-1.94442000	0.45275500
C	-0.55664600	-1.02606900	-0.09595500
N	-1.23558500	-0.04266400	-0.91984300
H	-0.72555100	0.43640100	-1.64987100
C	-2.52494400	0.40602600	-0.73199700
O	-3.03941600	1.26063500	-1.41454300
S	0.88185300	-1.78302500	-0.96021600
H	-1.84281400	-2.83143300	-0.13071600
H	-0.57942300	1.12395300	2.04707900
H	-4.11557800	0.20318600	0.50840600

TS3-1₆₄

N	-1.53481300	1.30401100	-1.01029500
C	-0.55305500	0.23438000	-1.08741100
H	-0.40471300	0.00088100	-2.14667800
C	-1.16584500	-1.02232200	-0.42529900
C	-2.43277500	-1.47902200	-1.16626400
H	-2.86203500	-2.34600300	-0.66339000
H	-3.17133900	-0.67716700	-1.18826800
H	-2.18395500	-1.75252800	-2.19374800
C	-1.56131100	-0.66945400	1.01370300
O	-1.57416000	-1.44471100	1.92964300
N	-1.98534700	0.64408900	1.16803100
H	-2.33850100	0.89688900	2.08300800
C	-2.07009800	1.65455700	0.20234800

O	-2.59970400	2.71196900	0.43821100
N	3.40094800	0.93810000	0.19752400
C	2.63673700	2.06492500	-0.10044400
H	3.14976800	3.01359200	-0.08837000
C	1.31602800	1.90273100	-0.47582000
C	0.76278100	0.63186600	-0.44704900
N	1.46822800	-0.32021700	0.29393200
H	0.85450000	-1.80874600	0.45634100
C	2.86533700	-0.33617300	0.29342800
O	3.52987800	-1.33033300	0.44062000
S	0.01538600	-2.40428600	-0.49050900
H	0.73701000	2.75862400	-0.79878400
H	-1.51408800	2.05317800	-1.68627700
H	4.40915800	0.98363000	0.21903400

PT-1₆₄

N	-1.78729300	1.05673300	-1.04977500
C	-0.67110500	0.13986400	-1.17699200
H	-0.60743300	-0.15858700	-2.23190900
C	-1.00161900	-1.13219900	-0.35472000
C	-2.22928800	-1.87575300	-0.89437300
H	-2.45874800	-2.73418100	-0.26251400
H	-3.09136600	-1.20745800	-0.92048800
H	-2.03383700	-2.22988700	-1.90848100
C	-1.27505700	-0.70271300	1.09155400
O	-0.96472400	-1.34822000	2.06011900
N	-1.98917300	0.46983600	1.19188300
H	-2.26957400	0.75328900	2.12311800
C	-2.29124700	1.39356200	0.17623500
O	-2.96736500	2.36490100	0.40161000
N	3.09145900	1.26378500	0.31767200
C	2.21599400	2.31595600	0.04247500
H	2.56442600	3.30908800	0.27776100
C	0.96398500	2.03248800	-0.46041900
C	0.63896700	0.70459400	-0.69873600
N	1.59729000	-0.26977500	-0.53529500
H	0.72024900	-2.24967700	0.90467700
C	2.77859400	-0.08398100	0.12045800
O	3.51427600	-0.97423200	0.49383700
S	0.44230300	-2.26484100	-0.41318200
H	0.25236700	2.82833000	-0.63675100
H	-1.91655500	1.76808100	-1.75459300
H	3.94481700	1.42388800	0.83126800

TS1-2₆₄

N	-0.54758000	1.25105900	-0.86421400
C	-0.35696800	-0.12084100	-0.88555000
H	0.36027400	-0.44909700	-1.63548300
C	-1.52098800	-0.94081500	-0.67575400
C	-1.51600700	-2.40402600	-0.95085500
H	-1.47642900	-2.97286500	-0.01601300
H	-2.44280800	-2.68875600	-1.45328200
H	-0.66398400	-2.68625100	-1.57087500
C	-2.74501300	-0.33031000	-0.18596000
O	-3.76727200	-0.94221400	0.04267700
N	-2.68705100	1.05620000	0.01118400
H	-3.51112700	1.49718400	0.39883900
C	-1.63573700	1.89466200	-0.28617400
O	-1.65524500	3.08602100	-0.10407600
N	3.39129000	-0.32619900	-0.68340700
C	2.82744300	-1.58135100	-0.50606700
H	3.39180600	-2.41137400	-0.90888500
C	1.66023300	-1.73053900	0.13482600
C	0.94648600	-0.54944600	0.61909600
N	1.76247500	0.60304700	0.67292400
H	1.42404400	1.40453500	1.19086900
C	2.93387700	0.80603700	-0.02601300
O	3.51350800	1.86475100	-0.06428400
S	-0.28349300	-0.69105200	1.84657800
H	1.21862200	-2.70443100	0.28285500
H	0.22251600	1.86926900	-1.08202600
H	4.29114800	-0.21882400	-1.12649100

IM1-2₆₄

N	-0.92651700	1.27384300	-0.99170300
C	-0.45172500	-0.09732700	-0.96422200
H	-0.05791000	-0.33450100	-1.95823600
C	-1.57730000	-1.02793700	-0.63837900
C	-1.57762500	-2.46267300	-1.02470300
H	-1.35716300	-3.09483500	-0.15533500
H	-2.57469200	-2.75595100	-1.36075400
H	-0.84898100	-2.67047700	-1.80884500
C	-2.69378500	-0.54763600	0.16310300
O	-3.57521400	-1.27158400	0.57902700
N	-2.69368200	0.82025500	0.43916100
H	-3.48399700	1.17457600	0.96274100
C	-1.95311500	1.78317400	-0.23957600
O	-2.21104100	2.96077700	-0.17407900
N	3.59011700	-0.50761300	-0.05889300

C	2.80336300	-1.63476500	-0.12405000
H	3.33377300	-2.57671700	-0.17560100
C	1.46534100	-1.56978900	-0.13306400
C	0.77487800	-0.24729000	0.00584600
N	1.70261400	0.82835100	-0.29385700
H	1.34970500	1.76094300	-0.11612300
C	3.06929500	0.77671600	-0.11173600
O	3.77007000	1.75728400	-0.05294900
S	0.24258100	-0.29576200	1.76610400
H	0.87501700	-2.47158100	-0.16284200
H	-0.44606100	1.95480300	-1.56008200
H	4.59479300	-0.56455900	-0.00085000

TS2-2₆₄

N	0.98782800	1.37215900	1.05744200
C	0.52206500	0.00415000	1.13852600
H	0.47887900	-0.28080700	2.19544800
C	1.38147300	-0.99057100	0.37002000
C	1.72034900	-2.30266100	1.02656300
H	0.84277300	-2.77864800	1.46704900
H	2.13971000	-2.97371100	0.27758400
H	2.46717600	-2.16533700	1.81666800
C	2.45318000	-0.45872900	-0.48242700
O	3.22499400	-1.16545800	-1.09571300
N	2.49602900	0.92899600	-0.64788500
H	3.22009200	1.27860600	-1.26264000
C	1.93141500	1.87091300	0.18992600
O	2.23517200	3.04069100	0.16196300
N	-3.52072500	-0.24919300	-0.16758800
C	-2.94451300	-1.36136800	0.37991700
H	-3.56886300	-2.23832300	0.47107200
C	-1.63761300	-1.32264100	0.79803800
C	-0.87285500	-0.15052700	0.52877200
N	-1.59004700	0.99255900	0.19730900
H	-1.06149400	1.82915700	-0.02319500
C	-2.87937600	0.98687700	-0.29136000
O	-3.43016600	1.94718500	-0.75983800
S	-0.15351200	-1.36309600	-1.18606400
H	-1.20152600	-2.16817400	1.30568300
H	0.71121100	2.02918700	1.77210000
H	-4.46811700	-0.26606700	-0.51683600

IM2-2₆₄

N	-0.81287200	1.45373200	-0.23261100
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C	-0.34006000	0.16091100	-0.72843600
H	-0.60929100	0.03745600	-1.78797600
C	-1.12452600	-0.93968400	0.03059100
C	-0.71794000	-2.34326300	-0.41187600
H	0.31799800	-2.54327700	-0.13507700
H	-1.37700600	-3.08399900	0.03708700
H	-0.80987900	-2.41828000	-1.49895200
C	-2.61681100	-0.71306100	-0.23144100
O	-3.41941400	-1.59879200	-0.35763100
N	-2.98333700	0.62114100	-0.29014200
H	-3.97435700	0.82162400	-0.35031400
C	-2.15199500	1.74893800	-0.22278800
O	-2.60980700	2.86179000	-0.16065900
N	3.87511300	0.00156900	-0.38023100
C	3.30928800	-0.32360100	-1.61055100
H	3.99112200	-0.58868200	-2.40274000
C	1.94201900	-0.28208800	-1.74529300
C	1.14828000	0.07741600	-0.66639100
N	1.78595000	0.42383000	0.53110400
H	1.23331200	0.57896700	1.36486500
C	3.15036500	0.36617800	0.74018400
O	3.66718600	0.61465200	1.80315900
S	-0.91610700	-0.84618300	1.84266600
H	1.48560200	-0.52551400	-2.69467500
H	-0.22197000	2.26210400	-0.37627600
H	4.87277700	-0.03504400	-0.23839400

TS3-2₆₄

N	0.96520200	1.54008600	0.08193600
C	0.39150100	0.43893700	0.83961800
H	0.64949000	0.51903800	1.90464500
C	0.97953500	-0.90057500	0.33882200
C	0.60918200	-2.05096500	1.26644900
H	-0.47479800	-2.15884600	1.31135900
H	1.04971900	-2.97709300	0.90094700
H	0.99904300	-1.86440300	2.27122600
C	2.50613900	-0.80124100	0.23705100
O	3.22383600	-1.76357800	0.33267200
N	3.01187700	0.46316200	0.01832900
H	4.00573900	0.52756900	-0.16535200
C	2.29151100	1.64474900	-0.20670100
O	2.83264500	2.64077800	-0.61937400
N	-3.75178200	0.13284000	0.17632200
C	-3.36907300	0.43706400	1.46913300

H	-4.13821800	0.46207600	2.22377100
C	-1.99352700	0.55681200	1.73835600
C	-1.09977600	0.46827900	0.70952200
N	-1.57263900	0.54725200	-0.61449700
H	-0.38004600	-0.09086100	-1.50048400
C	-2.86189200	0.09160900	-0.89593500
O	-3.21005600	-0.26268900	-1.99405200
S	0.38387600	-1.26951100	-1.37441300
H	-1.65597000	0.70152200	2.75715200
H	0.42507500	2.38306200	-0.04921000
H	-4.68367300	-0.19736600	-0.02993900

PT-2₆₄

N	1.02374500	1.49830700	-0.37176700
C	0.40851100	0.67600100	0.68123100
H	0.70564900	1.04351500	1.67218600
C	0.94001700	-0.76230400	0.53832800
C	0.48935400	-1.65827800	1.68512100
H	-0.59895700	-1.71925000	1.70854900
H	0.91963800	-2.65293900	1.57776900
H	0.84231400	-1.23627400	2.62858400
C	2.46874600	-0.77525300	0.42814400
O	3.13892300	-1.71310100	0.77195300
N	3.03055000	0.37404100	-0.08971100
H	4.03461900	0.36630200	-0.22516600
C	2.37314600	1.51330600	-0.58471600
O	2.97966100	2.37916200	-1.16343500
N	-3.72133900	0.40543700	0.01604500
C	-3.32064300	1.33247600	0.97587900
H	-4.10256300	1.89125300	1.46576300
C	-1.98095100	1.47470500	1.24872900
C	-1.07601400	0.67847300	0.55189000
N	-1.53654600	-0.19912300	-0.40402400
H	0.57604700	-0.48724600	-1.83697900
C	-2.84838100	-0.43039800	-0.69341500
O	-3.26107500	-1.25368700	-1.48098500
S	0.26624100	-1.50731100	-1.01546800
H	-1.64150900	2.18262900	1.99304000
H	0.54614700	2.35087000	-0.63154600
H	-4.69889600	0.23612000	-0.16590400

RS₅₄

C	-1.40754500	1.76674400	0.40623200
C	-1.52851700	-0.28466900	-0.95412000

C	-0.61629500	0.32538600	-1.89283000
C	-0.16740500	1.57430900	-1.67241000
O	-1.64168600	2.33653200	1.44247000
S	-2.09938900	-1.83111700	-1.10695100
C	0.21772200	-1.14700100	1.64521800
O	-0.68807900	-1.37932700	2.40784000
C	1.77605300	0.49401700	0.61244200
C	2.15959300	-0.53297800	-0.36176000
C	1.62001500	-1.75634200	-0.24345100
H	-0.33036900	-0.33417600	-2.69730700
H	0.53664900	2.08092000	-2.31939900
H	1.84377700	-2.56165000	-0.93240100
N	-0.58092200	2.28714600	-0.57508700
H	-0.09494200	3.13289300	-0.30831200
N	0.84243300	0.08755200	1.56346000
H	0.49487100	0.79653900	2.20270400
N	0.73376400	-2.07519200	0.76309300
H	0.20270100	-2.93355700	0.71232900
N	-1.93815800	0.52573000	0.08226800
H	-2.50575800	0.09987600	0.80951200
O	2.17521600	1.64114200	0.58957800
C	3.13445500	-0.06493300	-1.39573400
H	2.70722800	0.75770300	-1.97448900
H	4.03786100	0.31958400	-0.91950700
H	3.40632900	-0.87088300	-2.07866400

STS1-1₅₄

C	-0.36876300	0.32298900	1.50282300
C	-2.15681100	1.22657000	0.03053200
N	-2.44325900	-0.09584800	-0.31125000
C	-1.69470100	-1.19751900	0.03867100
C	-0.63369900	-0.98803300	1.00095100
O	-2.79223800	2.14474400	-0.42715700
H	-3.20085400	-0.18705900	-0.97382000
H	-2.25904300	-2.12133900	0.07972700
C	0.70635200	-0.84208600	-0.78539400
N	0.73286100	0.47012600	-1.17535400
C	1.60461500	1.44839300	-0.69910700
N	2.68089400	0.91207000	-0.01754700
C	2.83024100	-0.42249500	0.23106300
C	1.90694300	-1.32341000	-0.17417100
H	-0.02306700	0.81469900	-1.75770100
O	1.45343400	2.62362600	-0.90121200
H	3.32111800	1.58969900	0.37143700

H	3.73499900	-0.70494100	0.75264600
H	2.02533800	-2.37813600	0.01164800
S	-0.44556000	-1.86399100	-1.68713800
N	-1.12549600	1.36492300	0.92305700
H	-0.89337100	2.31166500	1.19635900
O	0.50937600	0.61284300	2.30524100
C	-0.15439800	-2.17205600	1.78650800
H	0.78967400	-1.93296900	2.27757100
H	-0.87111000	-2.45247500	2.56534400
H	-0.01296700	-3.03801600	1.13242300

SIM1-1₅₄

C	-1.13770400	1.24092500	0.37582800
C	-3.26611600	0.11114500	-0.29683800
N	-2.67315200	-1.09057000	-0.02104000
C	-1.25974300	-1.24876900	0.09280600
C	-0.52001900	-0.09804200	0.78975500
O	-4.40818700	0.24281000	-0.65625100
H	-3.23763900	-1.88974400	-0.27066400
H	-1.06506000	-2.20041600	0.58608400
C	0.82697000	-0.35472700	0.03360900
N	1.62950800	0.78101800	-0.25203000
C	2.99122800	0.81007800	-0.43932000
N	3.63732200	-0.36584700	-0.09476700
C	2.98258000	-1.41172000	0.52770100
C	1.65423000	-1.43541900	0.64168200
H	1.17117000	1.66355100	-0.44114200
O	3.58611000	1.78217000	-0.84160100
H	4.64308600	-0.33078100	-0.14719900
H	3.61282500	-2.20973200	0.89679100
H	1.16662500	-2.28736500	1.09199100
S	-0.18868600	-1.11513100	-1.41964700
O	-0.55938500	2.29363300	0.51304800
N	-2.43518400	1.21369100	-0.08221400
H	-2.85440900	2.11207300	-0.29133000
C	-0.46075100	-0.11319700	2.31502700
H	-0.05121300	-1.05627800	2.67770500
H	0.17258200	0.70438900	2.66364600
H	-1.46081600	0.01779900	2.73575500

STS2-1₅₄

C	-1.30391500	1.37183000	-0.75842400
N	-2.19220400	0.48029500	-1.30273200
C	-2.37830900	-0.88051600	-0.96719600

N	-1.66194300	-1.27318100	0.12708600
C	-1.28683600	-0.31261000	1.19287100
C	-0.59154700	0.90517300	0.53939500
H	-2.66145300	0.77205900	-2.15227700
O	-3.06901200	-1.58338500	-1.66005200
H	-1.89391500	-2.19721300	0.47498300
H	-2.20783900	0.07635300	1.64082600
C	0.82510900	0.57703600	0.11505500
N	1.09862400	-0.65979500	-0.30136900
C	2.34260400	-1.13490100	-0.71288000
N	3.31382500	-0.12992500	-0.71890400
C	3.08136100	1.14429400	-0.35453200
C	1.84327500	1.54455100	0.05574800
O	2.56281600	-2.26419000	-1.03300700
H	4.23643200	-0.43595000	-1.00362700
H	3.92700400	1.81876100	-0.40757800
H	1.65662000	2.56506800	0.34214900
S	-0.26021900	-1.11459400	2.44108500
H	0.38469500	-1.38281000	-0.13625400
O	-1.09151100	2.45318500	-1.25035600
C	-0.61196700	2.08177400	1.52363900
H	-0.27205200	3.00328000	1.05441600
H	-1.64090500	2.23899200	1.85035200
H	-0.01018000	1.82852200	2.39635800

PS₅₄

C	-1.44154500	-1.46562800	-0.40448700
N	-2.03095200	-1.28402500	0.82596700
C	-1.98060800	-0.13632300	1.64593500
N	-1.52748600	0.96457000	0.99624500
C	-1.39089700	0.99912300	-0.45036100
C	-0.63374900	-0.25911400	-0.92602700
H	-2.46714700	-2.09414100	1.24911700
O	-2.32262000	-0.18701400	2.80163300
H	-1.51086300	1.82684700	1.52039400
H	-2.38499900	0.93589700	-0.91234500
C	0.78598000	-0.40366600	-0.36716200
N	1.35537100	0.64918100	0.13923600
C	2.65799200	0.59651600	0.60995700
N	3.28144100	-0.66189900	0.53110000
C	2.69273700	-1.75786600	0.00281700
C	1.42670700	-1.67964100	-0.47546000
O	3.25579400	1.54060000	1.06329900
H	4.22669800	-0.69618900	0.88908400

H	3.28102300	-2.66691900	-0.00967100
H	0.92586300	-2.53623400	-0.90050300
S	-0.80661600	2.62079200	-1.02124300
H	0.40667100	2.52210200	-0.45080200
O	-1.52756700	-2.51125400	-1.00081900
C	-0.56577200	-0.32781700	-2.45549300
H	-0.20111800	-1.30330100	-2.77307200
H	-1.56126900	-0.18321000	-2.88104100
H	0.09246600	0.45550100	-2.83032500

STS1-2₅₄

C	-1.29299600	1.30589000	0.00779400
C	-3.14265400	-0.31399400	-0.38783700
N	-2.59198800	-1.10424700	0.60034300
C	-1.48694700	-0.77982700	1.33029100
C	-0.56686100	0.27473600	0.87048300
O	-4.12612700	-0.61866000	-1.01148900
H	-3.09689600	-1.96314300	0.77219700
H	-1.25842100	-1.40256500	2.18162000
C	0.61752400	-0.35716400	-0.07983300
N	1.52144800	0.71764300	-0.43955000
C	2.86944200	0.59572600	-0.66496800
N	3.43079200	-0.56460200	-0.14987300
C	2.70360900	-1.47775300	0.58669200
C	1.37330500	-1.40798800	0.68270300
H	1.11822200	1.53483000	-0.88299200
O	3.53576900	1.43581500	-1.22405500
H	4.43313900	-0.62720100	-0.22863400
H	3.27733100	-2.25349600	1.07678700
H	0.81751700	-2.15899900	1.22271500
S	-0.10617100	-1.22065300	-1.50480700
N	-2.49189600	0.90729400	-0.54792500
H	-2.91746700	1.54126700	-1.21399200
O	-0.83809900	2.39964500	-0.22363700
C	0.09416800	0.97936100	2.06120600
H	0.78345800	1.74442000	1.71190700
H	-0.66900000	1.44811100	2.68384500
H	0.64502400	0.25144400	2.65969500

SIM1-2₅₄

C	-1.25793900	1.30283900	0.08935100
C	-3.14185900	-0.30466100	-0.22496400
N	-2.58571900	-1.08256000	0.75467300
C	-1.43788200	-0.77565100	1.44952300

C	-0.52251000	0.30373400	0.98765700
O	-4.14206400	-0.59277100	-0.83429200
H	-3.08577400	-1.94095700	0.93765000
H	-1.21355900	-1.37701800	2.31620400
C	0.67625300	-0.27405000	0.10996100
N	1.60482600	0.79246400	-0.20026300
C	2.92269000	0.61462800	-0.52780900
N	3.44539300	-0.61536700	-0.13005600
C	2.72675300	-1.52246700	0.61020000
C	1.40469000	-1.38899000	0.79933500
H	1.20998600	1.65924000	-0.54945600
O	3.61037400	1.45021100	-1.06448100
H	4.43633000	-0.72367100	-0.27932500
H	3.29070200	-2.34429600	1.03226700
H	0.84694000	-2.12180000	1.36100500
S	0.06371700	-1.18453400	-1.36499100
N	-2.46446900	0.90019600	-0.43475200
H	-2.89541600	1.52291500	-1.10806100
O	-0.78823100	2.38071900	-0.19439600
C	0.05376700	1.04823500	2.20211500
H	0.69148400	1.87043100	1.88567000
H	-0.75979600	1.44235300	2.81272900
H	0.64474300	0.35587700	2.80577900

STS2-2₅₄

C	-1.23233400	1.29001700	-0.02317500
C	-3.28967800	-0.09527600	-0.25115100
N	-2.71586000	-1.00973700	0.59432400
C	-1.46564900	-0.91018200	1.15230600
C	-0.55354300	0.22850200	0.84829700
O	-4.37068300	-0.24016800	-0.76461900
H	-3.27324000	-1.83919500	0.74317100
H	-1.24146600	-1.60604700	1.94586400
C	0.70479200	-0.31385300	0.04072700
N	1.65726200	0.75032700	-0.18283700
C	2.99325200	0.56500600	-0.43827200
N	3.47929700	-0.67695400	-0.04422900
C	2.71084600	-1.57915100	0.65926800
C	1.38538900	-1.43858800	0.76747000
H	1.28811300	1.62525300	-0.53917700
O	3.71341500	1.41031500	-0.91433400
H	4.47816400	-0.78553700	-0.12203000
H	3.24447900	-2.40498700	1.11143000
H	0.79830400	-2.17899900	1.28677600

S	0.11587200	-1.08554700	-1.52963300
N	-2.52270000	1.05406600	-0.43503300
H	-2.93147200	1.75012900	-1.04773800
O	-0.66767700	2.31160900	-0.34113800
C	-0.08352000	0.90884100	2.14795800
H	0.58891100	1.73454400	1.92064400
H	-0.94226400	1.28710500	2.70510800
H	0.44677800	0.18280900	2.76738000

RT₅₄

C	-1.17653100	1.92141400	0.33516000
C	-1.49028200	-0.13136200	-0.93469700
C	-0.57675000	0.27592800	-1.88604800
C	0.03121200	1.50867800	-1.76074600
O	-1.29399700	2.53206300	1.37345100
S	-2.35631800	-1.65596300	-1.00911700
C	0.01811400	-1.11717400	1.57041800
O	-0.96938300	-1.24976800	2.25736800
C	1.79473300	0.34764300	0.63568800
C	2.14815900	-0.73385500	-0.29169900
C	1.50569700	-1.90583600	-0.18061100
H	-0.37154700	-0.41386800	-2.69275900
H	0.74615800	1.91981100	-2.45431200
H	1.72535300	-2.75273000	-0.81950800
N	-0.32522100	2.31311400	-0.67383600
H	0.27583600	3.08238700	-0.41134400
N	0.76222800	0.04502700	1.52555500
H	0.43222200	0.80337500	2.11767600
N	0.50812300	-2.11299300	0.75043900
H	-0.05835900	-2.94854700	0.72516300
N	-1.89317300	0.75570700	0.07864000
H	-2.29866800	0.36138700	0.92219400
O	2.31646900	1.44135900	0.64477300
C	3.23378000	-0.40436700	-1.26659700
H	2.93235500	0.44266200	-1.88708900
H	4.14125900	-0.10555700	-0.73874400
H	3.45927300	-1.25514400	-1.91093600

TS1-1₅₄

C	-0.50470200	0.16324200	1.44179700
C	-2.07071300	1.42022000	-0.02768200
N	-2.65213900	0.20072300	-0.33940400
C	-2.10674300	-1.01473800	0.02016700
C	-1.14473100	-1.08158300	1.01575300

O	-2.42898500	2.45749200	-0.52577300
H	-3.31310700	0.24645600	-1.10173400
H	-2.69205900	-1.88609300	-0.24263800
C	0.92487900	-0.80911800	-1.05796900
N	1.01546800	0.59035900	-1.15784800
C	1.86459400	1.36689800	-0.39418200
N	2.88590900	0.65350600	0.20069800
C	2.93672400	-0.73385000	0.23723400
C	1.94745100	-1.46281000	-0.38475500
H	0.28462200	1.10061200	-1.63546700
O	1.73403000	2.56475900	-0.27379300
H	3.46339800	1.20147700	0.82098300
H	3.76266400	-1.17199500	0.77486900
H	1.94874000	-2.54192200	-0.33662800
S	-0.48091800	-1.58638100	-1.74650300
O	0.44846800	0.21312700	2.19150000
N	-1.05624500	1.33022100	0.90740600
H	-0.55356300	2.19443900	1.08892700
C	-0.67219500	-2.35651400	1.61789400
H	0.41989300	-2.37133600	1.64058100
H	-1.01124300	-2.43060400	2.65590900
H	-1.04109300	-3.21609600	1.05828000

IM1-1₅₄

C	1.38758000	-0.12185500	-1.45029300
C	0.30338400	1.94283300	-0.58190500
N	1.15006700	1.87005300	0.50270000
C	1.79949600	0.66475000	0.92502200
C	2.16403200	-0.20054400	-0.22127100
O	-0.47633700	2.84733200	-0.75152400
H	0.94446000	2.56507300	1.20702000
H	2.67545700	0.90508000	1.53198600
C	-0.57969200	-0.78318900	1.07759500
N	-1.65678700	0.11035900	0.97127400
C	-2.72705200	-0.03237600	0.10781300
N	-2.62221200	-1.13261300	-0.72745700
C	-1.59199800	-2.06380500	-0.67012100
C	-0.57893800	-1.89576800	0.23369200
H	-1.71063100	0.91287300	1.58335400
O	-3.66267200	0.72830200	0.07848600
H	-3.39902300	-1.25281800	-1.35924600
H	-1.64682900	-2.88729600	-1.36504300
H	0.23600200	-2.60374400	0.27970500
S	0.73608100	-0.35547200	2.13882400

O	1.51749800	-0.88935900	-2.38439300
N	0.44602400	0.90420300	-1.49366400
H	-0.11440600	0.97895500	-2.33276700
C	3.23184400	-1.22020400	-0.08027900
H	3.21273200	-1.90467700	-0.92690900
H	4.21651500	-0.73924000	-0.04313400
H	3.10894100	-1.77990700	0.85182600

TS2-1₅₄

C	-0.49582800	0.67688700	1.22129800
C	-2.56846500	0.98071200	-0.12401500
N	-2.65531900	-0.38481300	-0.23106900
C	-1.60979700	-1.32245100	0.04536200
C	-0.48095200	-0.76444300	0.89384500
O	-3.40076100	1.73444400	-0.56676500
H	-3.44789800	-0.68895900	-0.77835800
H	-2.04317200	-2.22486800	0.47467700
C	0.75786900	-0.84607800	-0.54126100
N	0.94164400	0.46090300	-1.09127800
C	1.94089200	1.32129500	-0.68927900
N	2.97963700	0.69976700	-0.00876100
C	3.14349200	-0.65867400	0.15302400
C	1.94936600	-1.47738200	-0.15563800
H	0.14752700	0.92431300	-1.51025300
O	1.93801500	2.50658900	-0.92365400
H	3.68164700	1.34442000	0.32696900
H	3.86111300	-0.97182200	0.89795200
H	1.95207700	-2.53282500	0.06933400
S	-0.52001400	-1.82287200	-1.39041800
O	0.34472800	1.18933700	1.92962100
N	-1.45307700	1.44227300	0.56942900
H	-1.40989900	2.44503600	0.70764100
C	-0.03323200	-1.65503500	2.02202800
H	0.13843900	-2.67134000	1.66173200
H	0.88164500	-1.26533600	2.46798000
H	-0.80737500	-1.69152600	2.79495700

IM2-1₅₄

C	-0.59152000	0.94513500	0.93049300
C	-2.82832300	0.79797700	-0.14139600
N	-2.77198500	-0.56216300	0.03104300
C	-1.55298900	-1.30259600	0.12714000
C	-0.38390200	-0.55404900	0.79836400
O	-3.80049800	1.38757700	-0.53770700

H	-3.59454600	-1.03617500	-0.31545200
H	-1.76349900	-2.25115200	0.61664600
C	0.66793400	-0.78485600	-0.38145100
N	1.18957300	0.39398800	-1.04183900
C	2.36726500	1.04483100	-0.72081300
N	3.18432700	0.36858100	0.17335300
C	2.88197500	-0.86613500	0.71924700
C	1.85743100	-1.61710900	-0.01028600
H	0.56460000	0.94153300	-1.61894600
O	2.67361100	2.11500700	-1.19392700
H	3.97534200	0.90975500	0.49283000
H	3.22445500	-1.08689000	1.72030300
H	2.13086300	-2.40975500	-0.70335500
S	-0.59585100	-1.60993000	-1.43551500
O	0.19174400	1.64282800	1.52196100
N	-1.66799000	1.47747800	0.24621800
H	-1.76107200	2.48684400	0.27053200
C	-0.00670000	-1.13918600	2.15417400
H	0.29056800	-2.18437500	2.04461600
H	0.81149100	-0.57406200	2.59875900
H	-0.86793400	-1.08939800	2.82543000

TS3-1₅₄

C	1.67333800	-1.30696100	0.44121400
C	2.41570800	0.32676900	-1.29150800
N	1.60510400	1.25163900	-0.70669800
C	1.12917100	1.12870800	0.65846200
C	0.61106300	-0.30142000	0.92108500
O	3.03188200	0.49286200	-2.31480200
H	1.60244000	2.16237400	-1.14308100
H	1.93824600	1.31832500	1.37439800
C	-0.66130600	-0.60668400	0.14345400
N	-1.33850200	0.43089900	-0.52901100
C	-2.74107100	0.38090800	-0.60914000
N	-3.23654400	-0.89891300	-0.77685000
C	-2.44904900	-2.02727700	-0.59152100
C	-1.16385800	-1.87099700	-0.06504700
H	-0.92199700	1.87086100	-0.02107900
O	-3.43243400	1.36755400	-0.60141400
H	-4.24248700	-0.96906400	-0.83685400
H	-2.91679500	-2.98389800	-0.75996600
H	-0.57702200	-2.74483600	0.19194000
S	-0.10845200	2.41586000	0.99682300
N	2.48277700	-0.88757600	-0.59136000

H	3.10599400	-1.57864100	-0.99109500
O	1.77448400	-2.41515300	0.90873600
C	0.38236200	-0.52479800	2.42144000
H	0.10074800	-1.56245300	2.59230600
H	1.29748000	-0.32298900	2.98461800
H	-0.41081500	0.13263400	2.77627800

PT-1₅₄

C	-1.55214700	-1.27699700	-0.69298700
C	-1.90792400	-0.43025400	1.63373400
N	-1.36898200	0.75351000	1.23024600
C	-1.35272200	1.10638700	-0.18234900
C	-0.67297700	-0.04490600	-0.96339300
O	-2.21515500	-0.71658500	2.76470800
H	-1.35140900	1.49039200	1.92073200
H	-2.38221200	1.15628700	-0.56116200
C	0.72171500	-0.39025400	-0.44344700
N	1.51182600	0.66597600	-0.06007100
C	2.76286300	0.41146300	0.44335600
N	3.25588300	-0.89773000	0.47344000
C	2.55762900	-1.96070900	-0.04334500
C	1.22173200	-1.67191100	-0.48029200
H	0.51250700	2.55966000	-0.14100100
O	3.47204400	1.30442800	0.87302300
H	4.18149400	-1.00361900	0.86399500
H	2.98926300	-2.94564200	-0.00289500
H	0.61791600	-2.48896000	-0.85869500
S	-0.77475800	2.80615400	-0.44206700
N	-2.09162600	-1.34315800	0.57672600
H	-2.56796100	-2.20067300	0.82794300
O	-1.72826300	-2.16104400	-1.49606800
C	-0.63101200	0.24438300	-2.46468800
H	-0.36553700	-0.66312500	-3.00586300
H	-1.60557800	0.58723500	-2.82119400
H	0.10598000	1.02219200	-2.66400000

TS1-2₅₄

C	-1.13289100	1.34473200	0.09911400
C	-3.18370500	-0.07268000	-0.09010800
N	-2.67805700	-0.82261400	0.94315000
C	-1.47070000	-0.57548700	1.56605400
C	-0.57414300	0.37909000	1.07264400
O	-4.23359900	-0.30284700	-0.64021600
H	-3.25749800	-1.60050100	1.22157600

H	-1.23817100	-1.19792800	2.41826900
C	0.70027500	-0.51890000	-0.37101700
N	1.64118000	0.46871200	-0.74221900
C	2.96715100	0.52148200	-0.39183600
N	3.42059700	-0.61055500	0.28056900
C	2.60359100	-1.66271400	0.62112600
C	1.29182000	-1.65570400	0.31969700
H	1.29013100	1.32493700	-1.16023200
O	3.69784100	1.44866500	-0.64570900
H	4.40332100	-0.60720300	0.50575100
H	3.07753200	-2.47911000	1.15024700
H	0.65370700	-2.47976200	0.60484200
S	-0.37213600	-1.11715800	-1.68961900
N	-2.36744200	0.99799300	-0.43971500
H	-2.73384300	1.60657300	-1.16197200
O	-0.55785400	2.34342800	-0.28145500
C	0.48845200	0.90981600	2.00344800
H	1.15586000	1.59054300	1.47709900
H	0.03017900	1.46512900	2.82461900
H	1.06881900	0.08533600	2.42552900

IM1-2₅₄

C	-1.24881400	1.33039100	0.04207500
C	-3.16688900	-0.21534600	-0.36686700
N	-2.65848200	-1.03664600	0.60107900
C	-1.51517400	-0.78812000	1.32967500
C	-0.56407000	0.29038100	0.93455100
O	-4.15798800	-0.45622300	-1.01166500
H	-3.18488000	-1.88685600	0.74306500
H	-1.33167800	-1.41933000	2.18462800
C	0.65036500	-0.26882900	0.08234300
N	1.62599900	0.77989700	-0.12351400
C	2.94647300	0.57607300	-0.41537900
N	3.41145700	-0.70027000	-0.08732900
C	2.63402500	-1.63732600	0.53892200
C	1.30761600	-1.46400000	0.69681700
H	1.27048300	1.67899100	-0.43190800
O	3.68728200	1.41730400	-0.86435400
H	4.40137300	-0.83788000	-0.22008300
H	3.14813200	-2.51857700	0.90048500
H	0.70417000	-2.21359200	1.18408600
S	0.09987100	-1.10693400	-1.46061500
N	-2.44913700	0.97396200	-0.52634600
H	-2.84312800	1.62547500	-1.19505900

O	-0.74162800	2.40208400	-0.19918800
C	-0.02464100	0.98195400	2.19685700
H	0.62105000	1.81802000	1.93811300
H	-0.85642700	1.34688300	2.80111400
H	0.54943300	0.26281700	2.78585700

TS2-2₅₄

C	-1.19574400	1.30622800	0.05991900
C	-3.25059800	-0.03185200	-0.41142200
N	-2.66717400	-1.07188600	0.24741500
C	-1.29653100	-1.14827100	0.54373100
C	-0.58082700	0.14700400	0.85322900
O	-4.36834300	-0.03471100	-0.86730700
H	-3.21455100	-1.92028800	0.23650400
H	-1.09165300	-1.97045700	1.22104800
C	0.81993600	-0.14075800	0.32218200
N	1.65759400	0.91442000	-0.04557700
C	2.97641500	0.78762400	-0.40727300
N	3.51796600	-0.47594600	-0.15245500
C	2.82585800	-1.49263600	0.44381200
C	1.49147400	-1.33719400	0.74277000
H	1.22499700	1.80266600	-0.28164600
O	3.63970600	1.67469200	-0.87974300
H	4.48737900	-0.57882600	-0.41365700
H	3.37378000	-2.39771700	0.66061700
H	0.98677900	-2.09974200	1.31322500
S	0.12277200	-1.49872500	-1.21344800
N	-2.43466000	1.10675000	-0.48555600
H	-2.84493900	1.89657800	-0.96980300
O	-0.64089200	2.37981900	-0.04331700
C	-0.57631500	0.54978900	2.33916000
H	-0.00374800	1.46804400	2.48246500
H	-1.59713800	0.71517700	2.69081400
H	-0.12710200	-0.24720800	2.93509800

IM2-2₅₄

C	0.93075200	-1.25960400	-0.39353200
C	3.22945400	-0.36817500	0.00115400
N	2.65734600	0.67421300	0.69069800
C	1.27614000	1.04786500	0.50302900
C	0.37094400	-0.19394600	0.56002900
O	4.41626400	-0.53775300	-0.10695400
H	3.31723000	1.38754400	0.96834500
H	1.00506700	1.72282400	1.31417500

C	-1.05623400	0.18815100	0.24048000
N	-1.96800800	-0.85325000	0.01382400
C	-3.32362300	-0.68357800	-0.17927000
N	-3.76432500	0.61856400	-0.01447900
C	-2.92303600	1.69681300	0.22807900
C	-1.57062100	1.47188000	0.36944800
H	-1.60553500	-1.74566800	-0.30286400
O	-4.07097100	-1.59026700	-0.46026100
H	-4.75494300	0.74650300	-0.15155200
H	-3.38332700	2.66946900	0.29693400
H	-0.93862000	2.31736700	0.59912300
S	1.16532200	1.94328100	-1.10172900
N	2.30253000	-1.25823900	-0.54274500
H	2.69815000	-2.01642300	-1.08589900
O	0.26400200	-2.12216400	-0.91309500
C	0.43741900	-0.82142800	1.97686700
H	-0.22760600	-1.68477000	2.02327700
H	1.45029000	-1.13905100	2.23058000
H	0.09980100	-0.08570600	2.70923800

TS3-2₅₄

C	-1.06293300	-0.91571000	1.02590900
C	-3.11873400	0.22501200	0.18406500
N	-2.49743900	0.34971600	-1.03584000
C	-1.05539300	0.40642600	-1.13543800
C	-0.44327800	-0.79935900	-0.37964500
O	-4.26318200	0.53534000	0.39790100
H	-3.03251800	0.91253600	-1.68311000
H	-0.79364100	0.31092700	-2.18866600
C	1.04990500	-0.65732400	-0.23952400
N	1.46916000	0.38817900	0.61460600
C	2.77161100	0.88176500	0.49233500
N	3.70957500	-0.01587500	0.00051100
C	3.36441600	-1.26152600	-0.48375400
C	1.99541000	-1.55528400	-0.64499700
H	0.37098200	1.53992500	0.46719300
O	3.07406300	1.99851800	0.83444600
H	4.65105800	0.34033600	-0.07883000
H	4.16149700	-1.90884800	-0.81087200
H	1.71945400	-2.50125000	-1.09059400
S	-0.39739600	2.05299600	-0.59310600
N	-2.31781400	-0.35172500	1.17172900
H	-2.76810200	-0.47649600	2.07054200
O	-0.53232400	-1.51210000	1.92407200

C	-0.82698200	-2.09232100	-1.11923500
H	-0.49314000	-2.96043700	-0.54947800
H	-1.90811600	-2.15066500	-1.24393500
H	-0.36611500	-2.11016000	-2.10924800

PT-2₅₄

C	-1.10938400	-1.05139300	0.92034000
C	-3.09357000	0.28575100	0.18484600
N	-2.42799400	0.54627400	-0.99233000
C	-0.99787200	0.48911500	-1.07251900
C	-0.45214000	-0.81545200	-0.45407700
O	-4.23350900	0.61044100	0.39747900
H	-2.92454200	1.18441100	-1.59898500
H	-0.69540700	0.52913100	-2.11914600
C	1.03241600	-0.68806500	-0.29012000
N	1.41089000	0.50105500	0.32340300
C	2.70420400	0.94654400	0.37155100
N	3.64531100	-0.06140400	0.14618100
C	3.31306600	-1.35774000	-0.23586200
C	1.99280300	-1.67423600	-0.46938800
H	-0.67300100	1.87571500	0.89676300
O	3.03818900	2.08528300	0.61837500
H	4.60646200	0.24251900	0.17879200
H	4.13142900	-2.04825800	-0.36705800
H	1.72710800	-2.67185800	-0.78910300
S	-0.19320500	2.01277700	-0.35187300
N	-2.33074000	-0.40984900	1.12263500
H	-2.81665200	-0.63466700	1.98349100
O	-0.64551200	-1.77028000	1.76015800
C	-0.85298300	-2.00499300	-1.33872500
H	-0.55540600	-2.93607000	-0.85549600
H	-1.93226400	-2.02697900	-1.49720300
H	-0.35130700	-1.93165300	-2.30568200

RS^{TT}₆₄

N	-0.95584300	-1.28989100	1.57973700
C	-2.12643700	-0.56020200	1.51183400
H	-2.52539800	-0.24089600	2.46702400
C	-2.71918400	-0.24930900	0.34986400
C	-3.96823600	0.56864100	0.26236600
H	-3.77844600	1.47857100	-0.31234300
H	-4.75386700	0.01780500	-0.25846100
H	-4.32251900	0.84401300	1.25609200
C	-2.13396600	-0.76997000	-0.89131400

O	-2.61189300	-0.63847900	-1.99126100
N	-0.93663400	-1.48225700	-0.71225200
H	-0.47091300	-1.79587500	-1.55542500
C	-0.25732800	-1.70298900	0.46478000
O	0.83930700	-2.21557300	0.52642500
N	3.03759900	-0.18268600	0.73014100
C	2.18188600	0.57704600	1.48077400
H	2.40735900	0.61697700	2.53994500
C	1.13344700	1.24635300	0.94919400
C	0.93580700	1.16412600	-0.48844000
N	1.82006100	0.34216000	-1.15386400
H	1.70792300	0.26635000	-2.15827000
C	2.87636500	-0.38672000	-0.62682100
O	3.59203800	-1.09180100	-1.28951100
S	-0.23981000	1.97481400	-1.32189900
H	-0.48256800	-1.43151500	2.45860600
H	3.74473900	-0.75637300	1.16539100
C	0.24027100	2.13754900	1.75693000
H	0.33990700	3.17477200	1.43040000
H	-0.80708500	1.86314600	1.61304800
H	0.49017200	2.07437700	2.81781800

STS1^{TT}₆₄

N	-0.41728000	1.20680300	-1.31831800
C	-0.50697200	-0.19888500	-1.21639100
H	-0.08474900	-0.73813600	-2.05377900
C	-1.56127400	-0.78158600	-0.48642500
C	-2.17144600	-2.08102200	-0.91323300
H	-2.76364800	-2.50604600	-0.10623800
H	-2.83104500	-1.88090400	-1.76639500
H	-1.40790300	-2.79248300	-1.22038000
C	-2.50676000	0.15185700	0.21621700
O	-3.55065200	-0.20284600	0.70073000
N	-2.10635700	1.47911400	0.23560600
H	-2.72382400	2.12391400	0.71413700
C	-1.13950300	2.09009700	-0.57114100
O	-0.99311200	3.28965400	-0.59305500
N	3.12935800	0.49314300	-0.29148300
C	2.91158200	-0.83566200	-0.58947200
H	3.71455500	-1.32993800	-1.12153700
C	1.77267800	-1.47260900	-0.24362400
C	0.76844100	-0.70049400	0.46769000
N	1.16950500	0.52437600	0.91620200
H	0.57144200	0.99237700	1.59071900

C	2.29916500	1.23945400	0.52057300
O	2.53461900	2.36301800	0.87632600
S	-0.49075400	-1.44893100	1.52025800
H	0.30915500	1.62776700	-1.87764700
H	4.00163400	0.94139600	-0.53287900
C	1.52507900	-2.90541100	-0.60364400
H	1.16492600	-3.46047700	0.26279000
H	0.76342600	-2.98339600	-1.38405400
H	2.43873700	-3.36828400	-0.97820400

SIM1^{TT}₆₄

N	0.96847000	0.59486700	1.66953700
C	0.53473000	-0.55938200	0.93121800
H	0.39682400	-1.37984200	1.63403300
C	1.51854600	-1.01314400	-0.15783700
C	2.42951800	-2.17330600	0.20254800
H	3.01889500	-2.46832800	-0.66570400
H	3.11624700	-1.87697700	1.00129200
H	1.83341800	-3.02284200	0.53887900
C	2.33533500	0.12153200	-0.75663000
O	3.10344100	-0.03748700	-1.66775100
N	2.12155200	1.37713500	-0.19782700
H	2.68237100	2.12908500	-0.58326100
C	1.60629800	1.65359100	1.08204800
O	1.75382100	2.73297500	1.59450700
N	-3.34327500	0.63254700	-0.31730400
C	-3.18385300	-0.57031700	0.34871600
H	-4.10265600	-1.04707300	0.66715200
C	-1.98772500	-1.12055700	0.58293500
C	-0.76419700	-0.43637000	0.05544300
N	-1.05009200	0.91862000	-0.31677200
H	-0.29342800	1.45589000	-0.72322900
C	-2.27875100	1.42668900	-0.68614400
O	-2.41336000	2.48754300	-1.24958100
S	0.12828300	-1.42049900	-1.30800600
H	0.49964500	0.83627800	2.53110300
H	-4.25641100	1.00824400	-0.51730900
C	-1.85777700	-2.44015300	1.28940900
H	-1.20410900	-3.11648200	0.73175700
H	-1.44946400	-2.33230500	2.29868500
H	-2.83442200	-2.91560900	1.38362000

STS2^{TT}₆₄

N	0.86823800	1.78473800	-0.00783100
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C	0.52486400	0.65549500	0.84464800
H	0.49257600	0.99594800	1.87824800
C	1.54668200	-0.48029100	0.78350800
C	2.85576000	-0.03856600	1.46014700
H	3.56699000	-0.86261500	1.40881200
H	3.29296200	0.84618400	0.98402900
H	2.65480500	0.17304200	2.51152000
C	1.92114900	-0.76550400	-0.67611500
O	2.34718300	-1.80604500	-1.09292400
N	1.79431200	0.32721000	-1.54985700
H	2.18052100	0.19614900	-2.47728800
C	1.44876100	1.63766100	-1.24274500
O	1.64014200	2.55677000	-2.00313000
N	-3.31358400	-0.33884600	-0.63706700
C	-3.19428300	0.70133800	0.21574100
H	-4.10510800	1.25235700	0.41962200
C	-1.99994300	1.04243200	0.78209600
C	-0.89068100	0.21950400	0.45667500
N	-1.06188100	-0.80833800	-0.38854600
H	-0.35357300	-1.56896700	-0.28951000
C	-2.26311700	-1.19474900	-0.97349400
O	-2.39901500	-2.15048100	-1.68018600
S	0.76796100	-1.88185100	1.64710300
H	0.72694500	2.74026800	0.28169100
H	-4.20997400	-0.59096500	-1.03359900
C	-1.88941900	2.20070200	1.73415200
H	-1.25195300	2.99312300	1.33751300
H	-2.87332800	2.63327200	1.91590000
H	-1.48297300	1.87839200	2.69475000

$\text{PS}_{64}^{\text{TT}}$

N	-1.11589500	-0.53926900	1.70757400
C	-0.46310400	0.53407600	0.97616100
H	-0.37039300	1.38498100	1.65263100
C	-1.38059900	0.97125300	-0.18582100
C	-2.65463500	1.63200000	0.36558100
H	-3.33876700	1.85238300	-0.45403900
H	-3.14664600	0.97540300	1.08405900
H	-2.39895300	2.56906300	0.86609200
C	-1.81085300	-0.25366600	-1.00486900
O	-1.95163000	-0.25348000	-2.19823200
N	-2.14631700	-1.34562500	-0.22886000
H	-2.46425100	-2.16624400	-0.73024000
C	-1.73781000	-1.59529500	1.08379700

O	-1.98072500	-2.64169400	1.63078200
N	3.26104300	-0.73665100	-0.42446900
C	3.24992400	0.38792400	0.32698500
H	4.21015400	0.85952900	0.50312100
C	2.08470000	0.88523300	0.81997900
C	0.92257400	0.11649300	0.47498100
N	0.92603000	-0.96217400	-0.24983900
H	-0.03085400	1.32894200	-2.11867400
C	2.10740600	-1.46671100	-0.76667000
O	2.19808500	-2.44892200	-1.45915700
S	-0.54321100	2.20813600	-1.24211600
H	-0.73007700	-0.80311900	2.60343900
H	4.12672700	-1.10612300	-0.79429500
C	2.03815300	2.15014100	1.63100400
H	1.40871600	2.90029900	1.14613200
H	1.65074300	1.97665500	2.63817600
H	3.04057900	2.56815200	1.73271500

RT₆₄^{TT}

N	-2.45001600	0.26625200	1.30411000
C	-1.92754000	1.53579000	1.24970700
H	-2.07213000	2.12907800	2.14453900
C	-1.28249400	2.02424400	0.17432200
C	-0.67808900	3.39414000	0.16727700
H	0.40539400	3.32862800	0.04219000
H	-1.06266900	3.98504900	-0.66681800
H	-0.89899400	3.91501400	1.09916500
C	-1.08891400	1.12518300	-0.96483000
O	-0.42767600	1.38465800	-1.95091400
N	-1.72253100	-0.11708500	-0.84604700
H	-1.58907200	-0.78206100	-1.60566600
C	-2.35132200	-0.64131800	0.26833700
O	-2.76984800	-1.77154100	0.34283800
N	0.38593200	-2.38195600	0.55091200
C	1.12864700	-1.69588300	1.51795800
H	1.09599100	-2.08770800	2.52280900
C	1.84379900	-0.56631100	1.15119000
C	1.80335400	-0.18096200	-0.18160300
N	1.20825900	-1.03026300	-1.12826200
H	1.12462700	-0.71707000	-2.08700100
C	0.38254700	-2.07984000	-0.79036500
O	-0.29479200	-2.66756100	-1.60861600
S	2.53721600	1.27738600	-0.82700100
H	-2.90664900	-0.07659900	2.13542200

H	-0.28267300	-3.09247900	0.81334500
C	2.66238900	0.23535500	2.12303700
H	3.72998900	0.12158400	1.92262100
H	2.41887200	1.29821300	2.04125200
H	2.47462000	-0.08529300	3.14853400

TS1-1^{TT}₆₄

N	-0.29828800	-0.76356200	1.54351900
C	-1.06139900	0.35054900	1.38312600
H	-0.81843200	1.18419500	2.02968700
C	-2.07115500	0.42836900	0.44595700
C	-3.12017400	1.50219800	0.49349100
H	-3.51256700	1.68901500	-0.50539700
H	-3.95527700	1.18370500	1.12347200
H	-2.70365800	2.42886100	0.88932000
C	-2.42904100	-0.82385100	-0.25848600
O	-3.40513400	-0.96030300	-0.95180800
N	-1.53997600	-1.88634600	-0.05490100
H	-1.74151600	-2.74558000	-0.55219900
C	-0.46498100	-1.93649100	0.81086400
O	0.25022200	-2.89329800	0.95059900
N	3.10323200	-0.15193400	0.33337500
C	2.66456900	1.09738100	0.77247500
H	3.29346800	1.59956400	1.49235600
C	1.52143500	1.66541300	0.23011600
C	0.80710200	0.93507400	-0.71316400
N	1.28580300	-0.33529000	-1.07193600
H	0.82921600	-0.82063700	-1.83312700
C	2.48870600	-0.88522800	-0.66392000
O	2.94336600	-1.90673700	-1.11678000
S	-0.72738800	1.39219400	-1.42684100
H	0.52264300	-0.74470600	2.13460200
H	3.98698000	-0.52783000	0.64246900
C	1.09921800	3.04870200	0.64484000
H	1.21172600	3.74812000	-0.18609500
H	0.04808300	3.07887400	0.93819900
H	1.70881800	3.40126500	1.47788300

IM1-1^{TT}₆₄

N	-0.42131800	-0.63172700	1.71000000
C	-1.25403100	0.43435800	1.45492500
H	-1.19893100	1.27604000	2.12745300
C	-1.97005100	0.50624900	0.18003300
C	-3.22210800	1.36811400	0.22588200

H	-3.64408300	1.47293400	-0.77367800
H	-3.97280000	0.89914100	0.86513100
H	-2.97626300	2.35600100	0.61779400
C	-2.27335100	-0.87153400	-0.38053400
O	-3.17773000	-1.09561800	-1.14208200
N	-1.39581700	-1.87424000	0.01235300
H	-1.51552400	-2.78221200	-0.42051200
C	-0.43011600	-1.81963100	1.01521600
O	0.30722200	-2.74126800	1.26402200
N	3.16375300	-0.13485900	0.15158100
C	2.75981200	1.11971700	0.59436100
H	3.45219900	1.63902200	1.24125000
C	1.56268100	1.65856500	0.19624000
C	0.75348100	0.89981600	-0.66623200
N	1.22999800	-0.35353800	-1.08159400
H	0.70591300	-0.86828500	-1.77658000
C	2.45592400	-0.90047400	-0.75637800
O	2.86465500	-1.94055900	-1.21140300
S	-0.84750500	1.34633900	-1.18425500
H	0.25978300	-0.59014800	2.45511700
H	4.06178900	-0.51353000	0.41074600
C	1.15802400	3.03427400	0.65031100
H	1.04833100	3.70533800	-0.20382800
H	0.19809900	3.01888100	1.16953700
H	1.91050100	3.44877700	1.32203300

TS2-1₆₄^{TT}

N	0.61435700	0.88639700	1.55154700
C	0.53620300	-0.41743800	1.05028300
H	0.27238500	-1.14026200	1.81709700
C	1.64509200	-0.86999900	0.12250400
C	2.57929400	-1.93256200	0.68274400
H	3.27181000	-2.26708800	-0.09027100
H	3.16120200	-1.52019000	1.51161600
H	1.99856100	-2.78368300	1.04047200
C	2.44580200	0.27168300	-0.48340400
O	3.39627600	0.08659800	-1.19805700
N	1.98699800	1.55048000	-0.20423300
H	2.50365100	2.31075500	-0.63173600
C	1.17606200	1.93878700	0.86913300
O	1.02669700	3.09511000	1.17009600
N	-3.24525300	0.57560800	0.06382300
C	-3.00262400	-0.60763900	0.73650200
H	-3.85967800	-1.08197200	1.19356200

C	-1.87724000	-1.41924200	0.22335700
C	-0.81089500	-0.69746600	-0.32029500
N	-1.10933700	0.59903300	-0.82551100
H	-0.45240500	1.03806600	-1.45536000
C	-2.32205600	1.24100300	-0.72650400
O	-2.56786900	2.29611500	-1.26484400
S	0.52424400	-1.53300900	-1.21815600
H	-0.03424400	1.17304000	2.27231500
H	-4.10993200	1.08181500	0.19349900
C	-1.77309100	-2.81508600	0.72432900
H	-2.68052600	-3.37779400	0.48343900
H	-0.91641700	-3.33930700	0.30384500
H	-1.68978000	-2.82069800	1.82318600

IM2-1₆₄^{TT}

N	0.52099100	1.07382500	1.36712700
C	0.44234300	-0.31953200	1.03098900
H	0.26036400	-0.89141600	1.94309300
C	1.68616200	-0.86678600	0.31211600
C	2.66174800	-1.67261900	1.14789600
H	3.44755600	-2.08360400	0.51379100
H	3.12732800	-1.02605400	1.89765800
H	2.13856100	-2.48595500	1.65160500
C	2.43025600	0.17731000	-0.50970300
O	3.38638000	-0.09760300	-1.18754300
N	1.92097200	1.46335200	-0.45560700
H	2.41080000	2.15972800	-1.00572500
C	1.06604900	2.00327000	0.52102600
O	0.88831100	3.19087700	0.60509500
N	-2.92805400	0.74796600	0.40426500
C	-2.61656700	-0.31646700	1.24006800
H	-3.23627700	-0.46665000	2.11161500
C	-1.84711700	-1.37886100	0.55755900
C	-0.61960400	-0.75789000	-0.03481800
N	-1.06833100	0.29560300	-0.93074500
H	-0.47070700	0.60016300	-1.68750000
C	-2.16629000	1.09984900	-0.70859200
O	-2.46402900	2.03341700	-1.41725400
S	0.62037800	-1.85479600	-0.84633900
H	-0.17668700	1.45519300	1.99195900
H	-3.68090100	1.39156000	0.60522900
C	-2.55740000	-2.44969100	-0.21104600
H	-1.86562800	-3.24612400	-0.49672200
H	-3.36766900	-2.88097900	0.37815400

H	-2.99460900	-2.03937800	-1.13237100
TS3-1 ₆₄ ^{TT}			
N	1.28936900	1.66548000	0.47407000
C	0.55543000	0.49718100	0.96298400
H	0.49905100	0.59577500	2.05101500
C	1.41775400	-0.74965700	0.66200800
C	2.72317400	-0.72809000	1.47056800
H	3.33598400	-1.58886100	1.20185900
H	3.28122800	0.18678100	1.26526700
H	2.50055200	-0.77089800	2.53858200
C	1.79843700	-0.77256500	-0.82835300
O	2.07255800	-1.76910300	-1.43794100
N	1.88182800	0.47889600	-1.42260900
H	2.20030400	0.49770300	-2.38370400
C	1.72427200	1.72928400	-0.82260100
O	1.98894800	2.75315800	-1.40551400
N	-3.39180100	-0.10446100	-0.53053600
C	-3.09902200	1.12980400	0.02014100
H	-3.91136700	1.83383500	0.11308400
C	-1.81178200	1.36522300	0.53752200
C	-0.85451300	0.38453200	0.40387400
N	-1.11846900	-0.70453700	-0.45104500
H	-0.38184900	-1.99847700	0.01973400
C	-2.43829400	-1.10025500	-0.67702400
O	-2.73047200	-2.22098000	-1.01818900
S	0.50038900	-2.25692200	1.10510400
H	1.09174000	2.57037300	0.87391000
H	-4.34716800	-0.40190600	-0.66695200
C	-1.53759100	2.68537200	1.20210700
H	-0.90940800	2.56298700	2.08787800
H	-1.03704500	3.37353100	0.51437400
H	-2.47019500	3.15268100	1.51991900
PT-1 ₆₄ ^{TT}			
N	-1.60427300	1.38603400	-0.70072600
C	-0.62395700	0.35607500	-1.04157100
H	-0.55814900	0.35234500	-2.13724700
C	-1.22688000	-0.99845400	-0.59470100
C	-2.49705600	-1.35751500	-1.37184300
H	-2.91225600	-2.29405000	-0.99839700
H	-3.23981200	-0.56554500	-1.26159300
H	-2.26676700	-1.47428600	-2.43229500
C	-1.57285600	-0.92248000	0.90125100

O	-1.57253200	-1.87874200	1.63376900
N	-1.97187600	0.32240000	1.32875100
H	-2.27377400	0.39594600	2.29286000
C	-2.05275900	1.51018200	0.58494800
O	-2.52179600	2.51351600	1.06096500
N	3.29326700	0.36147000	0.50504300
C	2.78389600	1.60085600	0.11940800
H	3.45847900	2.44090100	0.19754000
C	1.49744300	1.71125700	-0.35901400
C	0.73104400	0.54075900	-0.39645500
N	1.23695700	-0.61880200	0.17036400
H	-0.05699200	-2.83463700	0.38887900
C	2.55846200	-0.82168800	0.44911200
O	3.06141200	-1.90424200	0.66941700
S	0.04233600	-2.29441300	-0.84098400
H	-1.56441000	2.26565100	-1.19419700
H	4.27690100	0.24337100	0.69416900
C	0.98151200	3.04577400	-0.83284200
H	0.57479100	2.97887200	-1.84711400
H	0.20278500	3.43835900	-0.17354100
H	1.79352800	3.77310700	-0.86031400

TS1-2₆₄^{TT}

N	-0.66073200	1.39824700	-0.73233200
C	-0.35154100	0.05232000	-0.86617400
H	0.39938400	-0.14549100	-1.62896500
C	-1.46602300	-0.86361200	-0.78820000
C	-1.38714200	-2.26059600	-1.29281300
H	-1.61301600	-2.97292700	-0.49471200
H	-2.14357200	-2.41581000	-2.06832100
H	-0.40259600	-2.47659100	-1.70884300
C	-2.73613200	-0.40086800	-0.25642500
O	-3.71365900	-1.10816000	-0.12682600
N	-2.77978700	0.95090700	0.10487600
H	-3.63820800	1.28697800	0.52197900
C	-1.79854800	1.89479600	-0.10568000
O	-1.91447100	3.05748200	0.18891600
N	3.06210000	0.40964700	-0.88121400
C	2.86120400	-0.95502500	-0.68042600
H	3.57790200	-1.61048500	-1.15822300
C	1.84775500	-1.40701900	0.07365300
C	0.93917100	-0.38343500	0.63814900
N	1.58411200	0.86332800	0.82615000
H	1.11650000	1.55268300	1.40225000

C	2.51204400	1.37503900	-0.05616700
O	2.81145300	2.54587600	-0.11644000
S	-0.27698800	-0.80101500	1.80806700
H	0.05027700	2.10150000	-0.89080600
H	3.81887900	0.73750400	-1.46230400
C	1.66382900	-2.86091300	0.38825400
H	1.85102800	-3.03940800	1.45044200
H	0.64517300	-3.19412800	0.19273400
H	2.35593100	-3.46817900	-0.19690200

IM1-2₆₄^{TT}

N	-0.96480100	1.22224800	-1.23495600
C	-0.54253800	-0.15142800	-0.99375500
H	-0.18378500	-0.55011700	-1.94622200
C	-1.76286900	-0.90937000	-0.54637100
C	-2.21950100	-2.21028900	-1.10560600
H	-2.08142000	-3.02454500	-0.38647800
H	-3.29188000	-2.16389800	-1.30774900
H	-1.68820300	-2.46378100	-2.02304700
C	-2.66480800	-0.23436900	0.38087900
O	-3.58778800	-0.78333400	0.94370300
N	-2.39809000	1.12607200	0.58013600
H	-3.02687400	1.61997800	1.20162700
C	-1.71621500	1.93287500	-0.33110700
O	-1.79999500	3.13656600	-0.32217900
N	3.52439000	-0.21250100	0.05309100
C	2.83762400	-1.40699200	-0.03392600
H	3.45405100	-2.29754800	-0.04258300
C	1.50132600	-1.48378400	-0.11567200
C	0.70765400	-0.19887600	-0.01943100
N	1.55516400	0.92713000	-0.37779000
H	1.12548500	1.83747700	-0.26295500
C	2.90882900	1.01150900	-0.10812500
O	3.51194600	2.05698100	-0.06652600
S	0.22044400	-0.18988000	1.75950200
H	-0.43113400	1.79326000	-1.87428200
H	4.52410300	-0.18624200	0.17689400
C	0.80939100	-2.81083700	-0.21733300
H	0.04222600	-2.91528800	0.55269200
H	0.33477000	-2.94692600	-1.19181600
H	1.53226600	-3.61726900	-0.08877100

TS2-2₆₄^{TT}

N	1.25721000	0.89041900	1.53298200
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C	0.61856500	-0.33325700	1.09789600
H	0.49487500	-0.96898200	1.97712500
C	1.44202100	-1.07607000	0.05298400
C	2.00148700	-2.43810400	0.35264200
H	1.25360700	-3.09867500	0.79165000
H	2.35622300	-2.88298400	-0.57751600
H	2.85186000	-2.37284800	1.04116200
C	2.30304000	-0.23934700	-0.78686500
O	2.97911100	-0.66753100	-1.69878200
N	2.25960900	1.14429400	-0.53398400
H	2.84163400	1.71345200	-1.13651900
C	1.94216400	1.72599400	0.68338100
O	2.22759400	2.86844400	0.96131500
N	-3.26316200	0.47649200	-0.45186300
C	-3.03900900	-0.74213300	0.11844400
H	-3.87808500	-1.42495200	0.13754700
C	-1.81889100	-1.06683300	0.65951800
C	-0.76042600	-0.11915700	0.45220400
N	-1.14954100	1.18968200	0.16530800
H	-0.43345700	1.89703200	0.04991800
C	-2.33827900	1.52199800	-0.44614700
O	-2.58931800	2.60395200	-0.90683100
S	-0.27272900	-1.28081400	-1.38247500
H	0.95362800	1.33536000	2.38703900
H	-4.14494200	0.69574900	-0.89278100
C	-1.64505400	-2.34988800	1.42341300
H	-0.78691600	-2.91764400	1.07030600
H	-1.51731500	-2.15065500	2.49148500
H	-2.52906500	-2.97619100	1.30263200

IM2-2₆₄^T

N	-0.87429000	-0.79157700	1.24857500
C	-0.37963900	0.36088400	0.49184800
H	-0.60222900	1.28936900	1.03467000
C	-1.21045000	0.44262900	-0.81625600
C	-0.79796600	1.62797200	-1.68621200
H	0.24158300	1.52277300	-2.00056500
H	-1.44784300	1.70157500	-2.55630100
H	-0.90448500	2.55032100	-1.10910200
C	-2.68668800	0.56978500	-0.42573000
O	-3.48606900	1.23315800	-1.03077800
N	-3.04290000	-0.16929200	0.68936500
H	-4.02841900	-0.20375800	0.92050900
C	-2.20928300	-0.92830700	1.52455900

O	-2.66449200	-1.62819700	2.39377500
N	3.79859100	-0.12486900	0.04051800
C	3.33404000	1.10434100	0.49853400
H	4.08591500	1.84708700	0.71918200
C	1.98588400	1.32697700	0.65535900
C	1.10436700	0.28991200	0.33778500
N	1.64172100	-0.93260900	-0.09148800
H	1.01801300	-1.65401800	-0.43106100
C	2.98146800	-1.18631800	-0.29397900
O	3.40361600	-2.23631600	-0.71924900
S	-1.09631700	-1.06575400	-1.83914100
H	-0.27033100	-1.19160500	1.95445400
H	4.78376500	-0.29224900	-0.09368600
C	1.51060500	2.66251400	1.16748500
H	0.86531600	3.16720600	0.44525600
H	0.95567300	2.55953400	2.10322000
H	2.36378500	3.31277400	1.36054000

TS3-2₆₄^{TT}

N	-1.00647400	-0.06372600	1.53025400
C	-0.41330400	0.67326300	0.42852500
H	-0.60443500	1.74678300	0.54735100
C	-1.07951300	0.26338900	-0.91043100
C	-0.65027900	1.18803500	-2.04290000
H	0.42714600	1.11232100	-2.19713300
H	-1.16288500	0.90870700	-2.96170000
H	-0.91640200	2.22393500	-1.80915200
C	-2.60267700	0.32324900	-0.75210700
O	-3.34319500	0.54903400	-1.67499200
N	-3.08013000	0.09189800	0.52243500
H	-4.08243500	-0.02018600	0.61346300
C	-2.33862100	-0.30598800	1.64601700
O	-2.87319300	-0.79601900	2.61062500
N	3.65764900	-0.31829300	-0.00182800
C	3.38881600	1.01006600	0.23023000
H	4.20945500	1.70801000	0.17918500
C	2.03276800	1.40946400	0.38739600
C	1.06673000	0.43465800	0.39860100
N	1.41445000	-0.91991700	0.46376000
H	0.27163400	-1.62532800	-0.25418700
C	2.68490500	-1.31625800	0.07097700
O	2.96368600	-2.46598100	-0.17514900
S	-0.68835200	-1.49373000	-1.32589500
H	-0.42039900	-0.43336600	2.26386800

H	4.56967500	-0.62775800	-0.30657600
C	1.72822100	2.87386500	0.51439400
H	1.20712400	3.23465500	-0.37715800
H	1.09017200	3.07339600	1.37747100
H	2.64585400	3.45003700	0.62846200

PT-2₆₄^{TT}

N	0.91292400	-1.14162300	-1.02911100
C	0.39569600	0.17539900	-0.71321300
H	0.61609300	0.85021500	-1.54947000
C	1.15740600	0.76278000	0.50243500
C	0.78458700	2.21468300	0.77645500
H	-0.26982600	2.28857800	1.04552600
H	1.39115600	2.60209400	1.59435100
H	0.98736600	2.83050300	-0.10360000
C	2.65982300	0.68323200	0.20646800
O	3.45703600	1.48289100	0.62548500
N	3.04895800	-0.38275900	-0.58333200
H	4.04549700	-0.54473800	-0.66207100
C	2.23891400	-1.43805100	-1.03623400
O	2.71650300	-2.48653000	-1.39602900
N	-3.71920900	-0.16001200	0.21449000
C	-3.37961500	0.93785600	-0.53054300
H	-4.12306000	1.69459900	-0.72143400
C	-1.98078700	1.10073600	-0.85612600
C	-1.10027100	0.08966600	-0.51159300
N	-1.53505600	-1.10871700	-0.01481600
H	0.71283400	-1.38691200	1.48034600
C	-2.83332000	-1.23023600	0.41190600
O	-3.24738500	-2.22946700	0.96440600
S	0.84179300	-0.17754100	2.05307900
H	0.26571400	-1.91017100	-1.13956500
H	-4.66039600	-0.30695500	0.55087500
C	-1.62769700	2.37077400	-1.55426700
H	-1.71158700	3.20730700	-0.85095300
H	-0.62470400	2.37669400	-1.97109800
H	-2.34875000	2.55504100	-2.35540900

RS₅₄^{TT}

C	-1.23929400	1.99607100	-0.28862200
C	-1.58449800	-0.43586800	-0.53129800
C	-0.67959500	-0.43782900	-1.67107800
C	-0.14256300	0.74054600	-2.04958300
O	-1.37456300	2.99888800	0.36870400

S	-2.29844300	-1.79321100	0.09608900
C	0.28082700	-0.23296800	2.13091100
O	-0.58234200	-0.05663400	2.95449700
C	1.84592700	0.69706800	0.43663300
C	2.11614200	-0.67233300	-0.01745000
C	1.54652900	-1.68815400	0.64938500
H	0.55450200	0.82502200	-2.87441600
H	1.70764900	-2.72568600	0.38213700
N	-0.43284400	1.91887200	-1.40715800
H	0.13772600	2.73735900	-1.57276700
N	0.94628600	0.80282900	1.49454700
H	0.67119200	1.73964400	1.77514300
N	0.70911500	-1.48261500	1.72531500
H	0.14800900	-2.24444200	2.08012100
N	-1.87931800	0.80108800	0.00170100
H	-2.44417500	0.81173900	0.84584300
O	2.30856600	1.69246100	-0.08310100
C	3.04449100	-0.74451300	-1.18884000
H	2.61263000	-0.22264400	-2.04618100
H	3.98723900	-0.24638500	-0.95714200
H	3.24651800	-1.77839400	-1.47342200
C	-0.37852300	-1.76267100	-2.29795200
H	0.05335500	-2.44029800	-1.55951000
H	-1.29333300	-2.23216600	-2.66300500
H	0.32114000	-1.64742500	-3.12851000

STS1-1₅₄^{TT}

C	-0.74492400	0.22426700	1.49419100
C	-2.65364600	-0.11437800	-0.05447700
N	-2.13114400	-1.38539300	-0.30055100
C	-0.90472900	-1.84949200	0.11872900
C	-0.17120200	-1.01333600	1.04869300
O	-3.67362900	0.25658600	-0.58103600
H	-2.67918200	-1.92629700	-0.95519600
H	-0.85383000	-2.92528000	0.23180000
C	0.90142200	-0.28307000	-0.75656100
N	0.17132400	0.78330100	-1.21623900
C	0.27609000	2.09378100	-0.75388200
N	1.42799400	2.29730000	-0.02749100
C	2.36598600	1.32476200	0.20355900
C	2.18898500	0.04001400	-0.18554600
H	-0.62821800	0.59764500	-1.81189000
O	-0.53796900	2.94820300	-0.99264500
H	1.52519300	3.21843700	0.37509000

H	3.27139100	1.65914400	0.69427700
S	0.53974200	-1.82258500	-1.58650700
N	-1.92350400	0.63008600	0.83546900
H	-2.28241500	1.55255300	1.04893100
O	-0.25057000	0.96261200	2.33306000
C	0.80737800	-1.66607700	1.98343000
H	1.62558500	-0.98258400	2.22352300
H	0.32716400	-1.93154100	2.93046000
H	1.21852000	-2.57572500	1.54103200
C	3.27662500	-0.98792200	-0.07246400
H	4.08661300	-0.61501100	0.55643400
H	2.90527900	-1.92145500	0.34368100
H	3.68075900	-1.21608300	-1.06140100

SIM1-1₅₄^{TT}

C	-0.85339200	0.49171400	1.32877900
C	-2.86723800	0.20321800	-0.11048200
N	-2.32511400	-0.94426500	-0.62117000
C	-1.17628300	-1.65079900	-0.11936800
C	-0.25829700	-0.78724000	0.76668400
O	-3.91545900	0.66763300	-0.48442200
H	-2.91217600	-1.39446700	-1.30918100
H	-1.46671900	-2.59901700	0.33457000
C	0.78500500	-0.43961900	-0.38038600
N	0.45230300	0.78645900	-1.07845600
C	0.94828800	2.03177100	-0.75194600
N	2.13206000	1.97346100	-0.04930000
C	2.80671400	0.78224700	0.16807200
C	2.24538600	-0.41837200	-0.01394200
H	-0.41009700	0.81498600	-1.60658500
O	0.42190100	3.06840700	-1.08740000
H	2.54663700	2.86233100	0.18009500
H	3.84023600	0.88529400	0.47523500
S	0.16949200	-1.89262300	-1.36607100
N	-2.10905100	0.83371700	0.88084800
H	-2.48362200	1.72001600	1.19950800
O	-0.24519300	1.18184700	2.10852000
C	0.31065200	-1.60329200	1.92244600
H	1.13183800	-1.06304400	2.39329300
H	-0.46771500	-1.76864300	2.67085300
H	0.65908300	-2.57346100	1.56783800
C	3.04619100	-1.68456000	0.09084100
H	4.07346400	-1.45056100	0.37404800
H	2.64271800	-2.38256800	0.82493500

H	3.07095700	-2.20802200	-0.86870500
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STS2-1₅₄^{TT}

C	-1.17317400	1.32271500	-0.95988100
N	-2.25374200	0.55314800	-1.31524300
C	-2.68526300	-0.66464700	-0.74239300
N	-1.96644900	-1.03085100	0.36557400
C	-1.35801700	0.00001100	1.24623700
C	-0.50369100	0.96617100	0.38674600
H	-2.70480800	0.78635000	-2.19248400
O	-3.55993200	-1.30374900	-1.26699300
H	-2.35276900	-1.82025400	0.87270200
H	-2.17360400	0.60362500	1.65617800
C	0.82421400	0.29977200	0.01404600
N	0.73553100	-0.99943900	-0.29459800
C	1.77248900	-1.87121500	-0.60533000
N	2.99387000	-1.21160700	-0.65588400
C	3.12845200	0.11458700	-0.46581400
C	2.08077600	0.94193300	-0.15631500
O	1.63442300	-3.04165400	-0.81097200
H	3.79405000	-1.79710900	-0.86059400
H	4.13463300	0.50146700	-0.57646000
S	-0.38799000	-0.74580800	2.57271800
H	-0.16449500	-1.46536000	-0.10039900
O	-0.77240100	2.22732000	-1.65336300
C	-0.35666600	2.26631600	1.19068500
H	0.01669100	3.08548500	0.58626500
H	-1.34825600	2.54551700	1.55013500
H	0.27179700	2.08571700	2.06200100
C	2.34848000	2.42209100	-0.05543800
H	1.67638900	2.97788500	-0.70911300
H	2.24025400	2.78989300	0.96346700
H	3.37117300	2.61920400	-0.37877600

PS₅₄^{TT}

C	-1.22897300	1.59439000	-0.44254700
N	-1.74141000	0.91806800	-1.52368600
C	-1.88678600	-0.47783300	-1.67853200
N	-1.85510100	-1.15367100	-0.50473200
C	-1.64377400	-0.49778000	0.77382400
C	-0.64702800	0.68834500	0.66956300
H	-1.99534500	1.47183600	-2.33242700
O	-2.05676800	-0.96348600	-2.76953500
H	-1.73369100	-2.15322000	-0.57269000

H	-2.59063500	-0.04382000	1.09017300
C	0.76925300	0.26158200	0.23733900
N	0.92104300	-1.01471000	0.02850100
C	2.12524700	-1.56599600	-0.36817100
N	3.13176700	-0.63667600	-0.64411200
C	2.99848800	0.68680000	-0.40062700
C	1.84060000	1.22170200	0.07545600
O	2.32534200	-2.75105500	-0.48659300
H	4.00328700	-1.01985100	-0.98536200
H	3.87055000	1.29773600	-0.60316000
S	-1.34569100	-1.70980800	2.09495600
H	-0.20340300	-2.18836500	1.57429200
O	-1.22783700	2.80041400	-0.39669600
C	-0.61948900	1.45532800	1.99658200
H	-0.30927100	2.48515100	1.84632200
H	-1.62112100	1.47258900	2.43154500
H	0.04546900	0.96178600	2.70573500
C	1.80771200	2.69471100	0.40219000
H	0.92230900	3.19469100	0.01611200
H	1.84543100	2.85686500	1.48160900
H	2.68598500	3.17597200	-0.03109700

STS1-2₃₄^{TT}

C	1.27412600	-1.36934700	0.54646900
C	3.04366000	-0.06613400	-0.63014600
N	2.62628800	1.03026800	0.08839000
C	1.61113500	1.01725500	1.00827100
C	0.59601400	-0.06138600	0.98427700
O	3.94376200	-0.04483900	-1.43052200
H	3.16484700	1.86870300	-0.08173400
H	1.55188400	1.85288000	1.68522200
C	-0.60594000	0.19810900	-0.08078700
N	-1.45431400	-0.98189600	-0.04566400
C	-2.75638800	-1.03467500	-0.47337000
N	-3.37356500	0.20385900	-0.51655400
C	-2.75970900	1.34926000	-0.05205600
C	-1.45047500	1.42425400	0.23375700
H	-1.00139000	-1.88763300	-0.07707500
O	-3.33944800	-2.05939100	-0.74327300
H	-4.35737500	0.18843100	-0.73334300
H	-3.40977200	2.20722400	0.06892500
S	0.03355600	0.58630100	-1.74947800
N	2.36415600	-1.23618900	-0.28840200
H	2.73615000	-2.08776100	-0.69206300

O	0.86370600	-2.46119200	0.85774900
C	-0.02037500	-0.25932100	2.37378400
H	-0.73132900	-1.08170900	2.35897900
H	0.76352500	-0.48710900	3.09728200
H	-0.53953600	0.64819800	2.68614600
C	-0.85803100	2.72514700	0.69762300
H	-0.51786000	2.68466000	1.73564800
H	-0.01205900	3.01893400	0.07239300
H	-1.61350800	3.50978800	0.63464700

SIM1- 2_{54}^{TT}

C	1.31348700	-1.37759500	0.53925800
C	3.09215700	-0.05996900	-0.61305500
N	2.68495900	1.02361300	0.12079700
C	1.64567000	1.01426500	1.02163000
C	0.63613900	-0.07851300	1.00781600
O	3.99113400	-0.03840700	-1.41614300
H	3.21684400	1.86595700	-0.04851500
H	1.60171400	1.82826800	1.72557700
C	-0.58139600	0.17279000	-0.00891100
N	-1.44520500	-0.99347000	0.05477100
C	-2.73391400	-1.03891100	-0.40795800
N	-3.32712300	0.21161400	-0.50826000
C	-2.71288400	1.35598900	-0.05296800
C	-1.40705400	1.41902800	0.26858500
H	-1.00195100	-1.90494800	0.07457600
O	-3.33333500	-2.05816200	-0.65911600
H	-4.30355100	0.20560300	-0.75768800
H	-3.35455900	2.22403400	0.03828700
S	-0.01118500	0.57588700	-1.70606400
N	2.39808800	-1.23146700	-0.29734500
H	2.76751900	-2.07778100	-0.71433200
O	0.89885000	-2.47524500	0.82840200
C	0.06798700	-0.29246600	2.41704600
H	-0.61797900	-1.13582200	2.43018400
H	0.88072500	-0.48984800	3.11740500
H	-0.46943000	0.60072400	2.74103300
C	-0.81887200	2.71562500	0.75154200
H	-0.49493200	2.66194700	1.79405500
H	0.03700300	3.01633700	0.14449400
H	-1.57416300	3.50035200	0.68543000

RT $_{54}^{TT}$

C	1.12472200	2.09245500	0.14233000
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C	1.47213300	-0.26594000	0.70367100
C	0.49307900	-0.23631700	1.66941600
C	-0.13539600	0.99715700	1.93629100
O	1.25559600	3.01845500	-0.62697200
S	2.42754300	-1.67248700	0.28994700
C	0.05350900	-0.60965600	-1.92575600
O	1.07199600	-0.57652300	-2.57729900
C	-1.76621900	0.58526600	-0.72740700
C	-2.15488100	-0.69177400	-0.11972100
C	-1.50960600	-1.80460500	-0.50253400
H	-0.92562900	1.12117100	2.65985200
H	-1.75835300	-2.78402400	-0.11173800
N	0.19886700	2.10472000	1.17282500
H	-0.42895100	2.89743200	1.14157200
N	-0.69343700	0.50992100	-1.61895000
H	-0.34253300	1.39082500	-1.98629600
N	-0.47628900	-1.77886000	-1.41336400
H	0.08425300	-2.60262800	-1.57846200
N	1.87821500	0.94201800	0.08964800
H	2.47887200	0.87409900	-0.72297700
O	-2.29219000	1.64968700	-0.48373000
C	-3.28671500	-0.62529700	0.85685500
H	-3.03692900	0.05013200	1.67852500
H	-4.18145000	-0.22242400	0.37823500
H	-3.51470900	-1.61176600	1.26361300
C	0.07939800	-1.47048100	2.41620100
H	0.24014300	-2.36032400	1.80807800
H	0.66475800	-1.58608300	3.33215400
H	-0.97502700	-1.40900500	2.69511800

TS1-1₅₄^{TT}

C	1.35229200	0.29649100	-1.37720700
C	-0.11051700	2.11725700	-0.51047800
N	0.73655900	2.17658900	0.58668900
C	1.76281600	1.28796900	0.82279100
C	2.17658600	0.41832800	-0.17500900
O	-1.06846600	2.83523100	-0.63375600
H	0.43375500	2.80715900	1.31478900
H	2.41951000	1.54210100	1.64422700
C	-0.46797200	-0.86082900	0.95648000
N	-1.59460400	-0.01570000	1.02629800
C	-2.70815400	-0.08771900	0.21454200
N	-2.56470300	-0.99863300	-0.81541000
C	-1.49695100	-1.88306400	-0.93138500

C	-0.43900900	-1.83558000	-0.03128000
H	-1.67812700	0.62107700	1.80619200
O	-3.70022000	0.58158100	0.37653600
H	-3.37208000	-1.08179900	-1.41466500
H	-1.55218600	-2.60304400	-1.73399100
S	0.78930400	-0.52629400	2.12942800
O	1.57590900	-0.48327900	-2.27989700
N	0.27013800	1.17651500	-1.44889300
H	-0.32964700	1.09537200	-2.26071500
C	3.41316600	-0.40708300	-0.07187200
H	4.12184700	-0.11730700	-0.85279900
H	3.88362300	-0.28301600	0.90350800
H	3.18508500	-1.46296600	-0.22425000
C	0.68247100	-2.82712800	-0.18311700
H	1.27103200	-2.60193100	-1.07553100
H	1.33516400	-2.81191800	0.68823200
H	0.27527400	-3.83454200	-0.29048800

IM1-1₅₄^T

C	-1.39886500	0.22724900	1.43041900
C	-0.10847700	2.13647800	0.48997000
N	-0.92614900	2.07847900	-0.61744700
C	-1.68987700	0.92322400	-0.98349700
C	-2.18071300	0.18726000	0.20316900
O	0.74505900	2.97531300	0.63784300
H	-0.64201500	2.71219600	-1.35152300
H	-2.51341000	1.21235100	-1.63988200
C	0.57019200	-0.73689200	-0.97712400
N	1.68443400	0.12050200	-0.94464500
C	2.77721900	-0.00892500	-0.11185400
N	2.65406100	-1.05449500	0.78392500
C	1.60084100	-1.96054500	0.78113100
C	0.54724700	-1.82309500	-0.08829600
H	1.75183100	0.87480400	-1.61378300
O	3.74159500	0.71593700	-0.15685800
H	3.44790700	-1.18314300	1.39246700
H	1.66246700	-2.76344700	1.50122300
S	-0.71089700	-0.29653400	-2.07890200
O	-1.60135300	-0.49836100	2.38612200
N	-0.37003100	1.16548900	1.44929100
H	0.19138300	1.21709000	2.28942500
C	-3.38601900	-0.67184600	0.10326200
H	-3.51564600	-1.25117200	1.01616700
H	-4.27903300	-0.05621700	-0.05409100

H	-3.30373600	-1.35141300	-0.75141300
C	-0.59225500	-2.80569700	-0.03390200
H	-1.35919400	-2.47461600	0.67086500
H	-1.05029100	-2.93037600	-1.01500500
H	-0.23028100	-3.77771000	0.30359100

TS2-1^{TT}₅₄

C	-0.81096700	0.71460100	1.17794000
C	-2.92160800	0.45484000	-0.11282400
N	-2.68388000	-0.89844800	-0.13681700
C	-1.40857900	-1.51324800	0.06713500
C	-0.44655700	-0.68603700	0.90147400
O	-3.93022000	0.95986700	-0.54214700
H	-3.39680700	-1.41510200	-0.63191300
H	-1.56171700	-2.50820000	0.48213300
C	0.78574200	-0.50592100	-0.55942700
N	0.69238800	0.82346500	-1.08689000
C	1.48030500	1.87623600	-0.68137800
N	2.61617600	1.48905700	0.01709200
C	3.03121400	0.19344700	0.20846200
C	2.09052000	-0.88241200	-0.17819200
H	-0.18612100	1.10799200	-1.49704600
O	1.23440800	3.03342300	-0.92679700
H	3.16590300	2.26378500	0.36106300
H	3.77633200	0.02480900	0.97510600
S	-0.29746200	-1.67214200	-1.43508000
O	-0.13425700	1.44256500	1.87444600
N	-1.91499700	1.20618800	0.48610600
H	-2.11798200	2.19252100	0.59839900
C	0.20081500	-1.40141700	2.05608400
H	0.58099800	-2.37481300	1.74221500
H	1.01884200	-0.80264800	2.45813700
H	-0.53034800	-1.56299200	2.85455000
C	2.57920100	-2.27151400	0.00053300
H	1.83077400	-3.01331500	-0.27035500
H	3.46814000	-2.41862000	-0.62613600
H	2.90360800	-2.43927100	1.03584700

IM2-1^{TT}₅₄

C	-0.89662100	1.08512300	0.80486300
C	-3.03545500	0.46199500	-0.29687000
N	-2.79827800	-0.83726800	0.07323400
C	-1.49874600	-1.37396700	0.33283900
C	-0.47486200	-0.37128000	0.90164500

O	-4.05824900	0.84075000	-0.80773100
H	-3.52804100	-1.47005700	-0.22389000
H	-1.60916500	-2.24822400	0.97102900
C	0.64877500	-0.61469400	-0.20822700
N	0.97529400	0.50788600	-1.07046200
C	1.94550700	1.45948000	-0.80269100
N	2.80348400	1.13344500	0.23380800
C	2.72292800	-0.04142600	0.96269600
C	1.96614000	-1.12461700	0.31535900
H	0.28951500	0.80893700	-1.75060100
O	2.05040300	2.48390200	-1.43857300
H	3.41728000	1.88668200	0.50984900
H	3.03128600	-0.02600600	1.99849300
S	-0.42760400	-1.80316000	-1.12093200
O	-0.24474800	1.96706500	1.30299500
N	-2.00619200	1.35248900	0.02627500
H	-2.23795200	2.33047500	-0.10695700
C	-0.08268900	-0.69679700	2.33821600
H	0.38069800	-1.68447200	2.38722800
H	0.61018600	0.04916400	2.72411500
H	-0.97720700	-0.69788100	2.96664000
C	2.70148000	-2.16173300	-0.47581500
H	3.60354800	-2.47417300	0.05068900
H	2.07437600	-3.03448100	-0.66834400
H	3.00898800	-1.75150300	-1.44895600

TS3-1₅₄^{TT}

C	-1.81080000	1.11408300	0.34981200
C	-2.16001800	-0.50782800	-1.51144700
N	-1.53222400	-1.43515200	-0.74563300
C	-1.21087700	-1.24585600	0.65976000
C	-0.69472300	0.19819800	0.89878900
O	-2.56191700	-0.68379800	-2.63589500
H	-1.37706900	-2.33742800	-1.17037100
H	-2.10764500	-1.36933800	1.27808700
C	0.63352200	0.45729400	0.18203300
N	1.28622800	-0.65674900	-0.36491000
C	2.66725400	-0.66126600	-0.53636700
N	3.24931100	0.58053500	-0.71924300
C	2.52337400	1.74348700	-0.58926200
C	1.20323200	1.69446200	-0.06535200
H	0.87057500	-1.95717500	0.26840200
O	3.31181300	-1.68336800	-0.55990100
H	4.25543500	0.58889400	-0.80875900

H	3.03656100	2.67265500	-0.77993200
S	-0.05907500	-2.54169700	1.20400800
N	-2.34029300	0.72634500	-0.86096400
H	-2.99585300	1.35772700	-1.30402000
O	-2.19980600	2.10618200	0.91498400
C	-0.54470100	0.46243700	2.40104700
H	-0.28942700	1.50561100	2.57814900
H	-1.48332400	0.25761000	2.92164200
H	0.23762400	-0.17610800	2.80881200
C	0.51785700	3.01611100	0.13031100
H	-0.25109700	3.17149500	-0.63211700
H	0.01980900	3.08408800	1.09571600
H	1.24302200	3.82541700	0.04606100

PT-1₅₄^{TT}

C	1.59134900	1.35760600	-0.18299000
C	1.60557800	-0.03318300	1.89494900
N	1.34599300	-1.10518200	1.10509400
C	1.49433100	-1.04351500	-0.34073100
C	0.77720900	0.23619200	-0.86135800
O	1.66654200	-0.03926700	3.10070500
H	1.19778300	-1.99227000	1.56225900
H	2.55512100	-0.90530300	-0.58851200
C	-0.68494700	0.30504000	-0.40588900
N	-1.27825300	-0.90827100	-0.20820500
C	-2.54092700	-0.99459400	0.30611700
N	-3.25490700	0.18552700	0.56883000
C	-2.79557600	1.40431600	0.15199300
C	-1.42537700	1.48199900	-0.30176400
H	-0.17555400	-2.62510900	-0.86372100
O	-3.07371600	-2.05870100	0.55727800
H	-4.18598100	0.06194100	0.94067800
H	-3.42188500	2.27233400	0.27642600
S	1.14308600	-2.64177100	-1.12336200
N	1.83626200	1.14895100	1.16006800
H	2.26828500	1.90419300	1.67717400
O	1.99048900	2.34658600	-0.74732600
C	0.90254800	0.34957600	-2.38042000
H	0.59308300	1.33662900	-2.72108100
H	1.93826500	0.19769900	-2.69376900
H	0.27942100	-0.40989800	-2.85172700
C	-0.94123700	2.85787400	-0.61548900
H	-0.43515900	3.27617700	0.26351300
H	-0.22307900	2.88326800	-1.43087300

H	-1.78756800	3.50469100	-0.84883400
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TS1-2₅₄^{TT}

C	1.06495900	-1.21499800	0.69446400
C	3.23229400	-0.33877100	-0.18414100
N	2.87090700	0.87991800	0.33709400
C	1.67325000	1.13495100	0.98292800
C	0.63310800	0.17121600	1.03226600
O	4.27170700	-0.53924800	-0.76551300
H	3.54389600	1.61748600	0.18940400
H	1.58698300	2.10343700	1.45267400
C	-0.74685500	0.42651200	-0.53199800
N	-1.31992500	-0.82081000	-0.86036700
C	-2.54540800	-1.30870200	-0.45566000
N	-3.32539700	-0.36524100	0.18706400
C	-2.94861600	0.96098700	0.31413500
C	-1.72709700	1.40194000	-0.03333400
H	-0.72357400	-1.53151800	-1.26523500
O	-2.91616800	-2.43735300	-0.66851200
H	-4.25770200	-0.66906600	0.42080400
H	-3.70327100	1.62195500	0.72116300
S	0.42424100	0.98972800	-1.75875900
N	2.28671800	-1.33069900	0.03985800
H	2.55904100	-2.26290500	-0.24722000
O	0.40315800	-2.19848600	0.93293500
C	-0.31025800	0.22467500	2.21164100
H	-1.17412500	-0.41917900	2.04455400
H	0.20505700	-0.13591600	3.10579700
H	-0.65152600	1.24450700	2.39428000
C	-1.34397000	2.84297200	0.12239600
H	-0.43963200	2.94718800	0.72813100
H	-1.13011000	3.30239100	-0.84436000
H	-2.14704200	3.39978400	0.60714500

IM1-2₅₄^{TT}

C	1.31116400	-1.37710100	0.49978400
C	3.09266100	-0.01681700	-0.59911500
N	2.68217300	1.04271200	0.16245000
C	1.62650100	1.00971200	1.04881500
C	0.62817300	-0.09833900	1.01514200
O	3.98850700	0.02858900	-1.40574400
H	3.20271000	1.89463500	0.00796900
H	1.59077000	1.78567100	1.79543400
C	-0.59493700	0.14893600	0.03016600

N	-1.47920600	-1.00016100	0.12526200
C	-2.75893600	-1.03809800	-0.35048900
N	-3.33183400	0.22485000	-0.49928200
C	-2.70125200	1.37262000	-0.11150200
C	-1.38541900	1.42326600	0.22327000
H	-1.04298600	-1.91501700	0.17301900
O	-3.38499000	-2.04658100	-0.57330200
H	-4.29943200	0.22588800	-0.78321600
H	-3.31867800	2.26230500	-0.08364000
S	-0.10879000	0.59395300	-1.67967200
N	2.40378400	-1.20037700	-0.31709600
H	2.77109700	-2.02991200	-0.76817300
O	0.88930400	-2.48495200	0.74046000
C	0.09066900	-0.34414800	2.43219400
H	-0.56464900	-1.21125000	2.45639300
H	0.92111100	-0.51148500	3.11962000
H	-0.47329500	0.52964200	2.76708500
C	-0.79808900	2.72402000	0.70006900
H	-0.53278600	2.68237000	1.75995500
H	0.09216100	2.99509200	0.13302600
H	-1.53556800	3.51887800	0.57662900

TS2-2₃₄^{TT}

C	1.30179300	-1.29544900	0.45357300
C	3.27609100	-0.11083700	-0.51012600
N	2.68213900	1.05913200	-0.14833200
C	1.31723700	1.18972500	0.15910700
C	0.63687100	0.03345500	0.86193000
O	4.37631300	-0.21752700	-0.99568300
H	3.20043900	1.88170800	-0.42082700
H	1.11295900	2.17246500	0.55898300
C	-0.78123200	0.09338400	0.27695900
N	-1.49827500	-1.11019600	0.20511800
C	-2.75672400	-1.25955800	-0.31482200
N	-3.41271200	-0.04755600	-0.52479700
C	-2.89208600	1.15509400	-0.14645800
C	-1.60460100	1.28741300	0.33711300
H	-0.97747900	-1.97626600	0.31014000
O	-3.28149500	-2.31876200	-0.54887800
H	-4.34667100	-0.12369300	-0.89946000
H	-3.55346800	2.00702200	-0.22557100
S	-0.11238400	0.92515400	-1.60850100
N	2.49514500	-1.23585100	-0.21192200
H	2.92481400	-2.12645600	-0.43340400

O	0.82678400	-2.37075900	0.75554800
C	0.66608800	0.05939900	2.40338400
H	0.13875200	-0.80929000	2.80131000
H	1.69861300	0.02996000	2.75906400
H	0.19601000	0.96392500	2.78710400
C	-1.22708400	2.64412000	0.89013900
H	-0.67057800	2.57015700	1.82354300
H	-0.64073100	3.22404800	0.17792500
H	-2.13952300	3.20115400	1.10405600

IM2-2_{s4}^{TT}

C	1.11202800	-1.38351900	0.35052900
C	3.27555200	-0.27870400	-0.23999400
N	2.67354900	0.92576600	0.01329000
C	1.24191700	1.09796700	-0.02830100
C	0.49863500	-0.02496300	0.73358300
O	4.44077400	-0.41874200	-0.50795000
H	3.26077300	1.72542400	-0.17921400
H	1.03396900	2.04920200	0.44880200
C	-1.00080900	0.07627500	0.44700000
N	-1.67171100	-1.08662500	0.03380000
C	-2.97658200	-1.17211300	-0.38942900
N	-3.63166800	0.04205200	-0.41477500
C	-3.05926000	1.22164700	0.03607900
C	-1.74396000	1.26686000	0.45867000
H	-1.20199500	-1.97961900	0.12563500
O	-3.50635600	-2.21047500	-0.71267100
H	-4.59519500	0.00384000	-0.70829000
H	-3.69983900	2.09068000	0.04018700
S	0.71275800	1.18688000	-1.78790000
N	2.41177100	-1.36567700	-0.10656200
H	2.83438300	-2.27303100	-0.26418900
O	0.56589100	-2.44679600	0.53565500
C	0.78856400	0.08252900	2.25376500
H	0.30662500	-0.74995300	2.76704300
H	1.86245000	0.05107100	2.45280300
H	0.38676800	1.01248100	2.65310800
C	-1.24526900	2.62985600	0.88950200
H	-0.61609800	2.59310700	1.77823700
H	-0.69560600	3.13219300	0.08916700
H	-2.10131100	3.25900200	1.13414500

TS3-2_{s4}^{TT}

C	1.06884600	0.82275300	1.09741400
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C	3.21391200	-0.10283600	0.22692700
N	2.63182500	-0.16079300	-1.01578400
C	1.20015400	-0.34207000	-1.16499300
C	0.46360600	0.74037600	-0.31817900
O	4.37407100	-0.34375400	0.44728700
H	3.22483900	-0.62513900	-1.69035200
H	0.95814700	-0.15564700	-2.21096700
C	-1.01266700	0.43015100	-0.16554100
N	-1.22645300	-0.75841300	0.57100800
C	-2.42415700	-1.45859300	0.45886700
N	-3.52023900	-0.68090400	0.12017800
C	-3.39603700	0.66695200	-0.11504000
C	-2.12225100	1.24960400	-0.30347600
H	-0.03991000	-1.77228300	0.29972700
O	-2.51712200	-2.64136100	0.67939500
H	-4.40641100	-1.15900400	0.04777600
H	-4.30903600	1.22941200	-0.23577300
S	0.71086500	-2.09340700	-0.84338500
N	2.35029900	0.32509100	1.23821000
H	2.77691800	0.42491700	2.15164500
O	0.49104300	1.34363800	2.01512500
C	0.77775600	2.09418900	-0.98145200
H	0.44512300	2.92211100	-0.36012100
H	1.85443400	2.18522200	-1.12499400
H	0.29899900	2.15361500	-1.95995200
C	-2.13145500	2.73273500	-0.57512600
H	-1.60715700	3.27019800	0.21697000
H	-1.66843300	2.98500500	-1.52753900
H	-3.15955700	3.09348100	-0.59839000

PT-2₅₄^{TT}

C	1.10651400	1.01488000	0.92189400
C	3.20961100	-0.13580700	0.21072800
N	2.57606000	-0.47194300	-0.96379100
C	1.14608800	-0.56267000	-1.04813700
C	0.47235200	0.69451300	-0.44463100
O	4.37493600	-0.34553900	0.43049400
H	3.13479900	-1.06414500	-1.56278500
H	0.85420800	-0.63421200	-2.09658500
C	-1.00276600	0.42857500	-0.27333000
N	-1.23724500	-0.85973000	0.19235400
C	-2.45510300	-1.46275500	0.29203800
N	-3.50699000	-0.55848800	0.18956000
C	-3.31976300	0.81176700	0.04098200

C	-2.07634800	1.34097500	-0.20630200
H	0.93274200	-1.96501400	0.92325400
O	-2.63522500	-2.65021700	0.47411500
H	-4.42852300	-0.95238600	0.29993600
H	-4.20954800	1.42130100	0.10252200
S	0.52436600	-2.16927700	-0.34147900
N	2.38077000	0.49646100	1.13838600
H	2.84094600	0.78002300	1.99610600
O	0.57295300	1.70194300	1.74974600
C	0.80790400	1.87811800	-1.37300400
H	0.56824500	2.82401900	-0.89363400
H	1.87131200	1.87807900	-1.61734100
H	0.22976400	1.79177900	-2.29514100
C	-1.95136400	2.83671700	-0.35058700
H	-1.23501100	3.23698500	0.36959700
H	-1.64255700	3.13104500	-1.35519200
H	-2.91845800	3.30147100	-0.15538300