

Enantioselective Hydrosilylation of Unsaturated Carbon-Heteroatom Bonds (C=O, C=N) Catalyzed by [Ru-S] Complexes: A Theoretical Study

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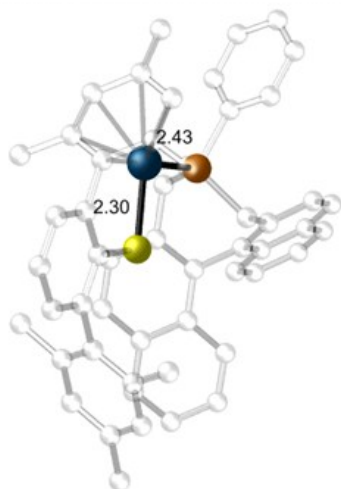
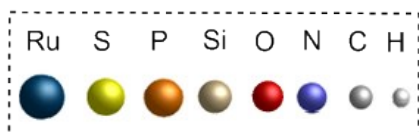
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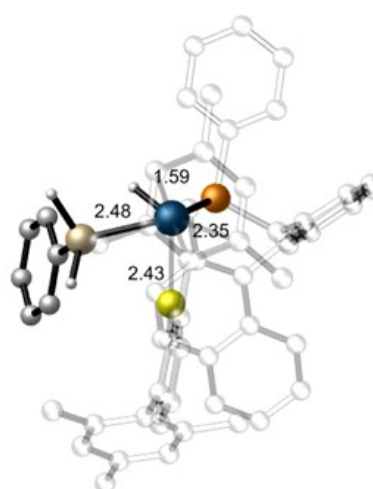
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Table S1. The ΔE_{gas} , ΔG_{gas} and ΔE_{sol} calculated for species involved in the hydrosilylation of imine and ketone.

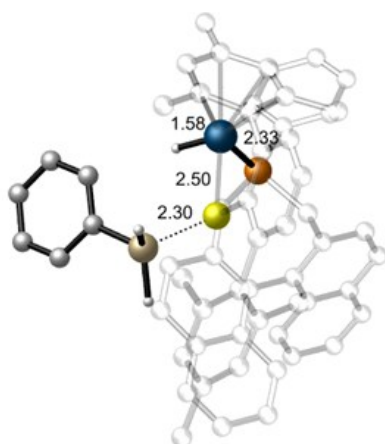
species	ΔG_{gas}	ΔE_{gas}	ΔE_{sol}
I1	0	0	0
I2	-7.87	-24.98	-22.92
I3	-11.17	-27.94	-24.50
I4	-18.45	-52.69	-42.35
I5	2.04	-11.36	-8.74
I6	5.50	-7.66	-6.87
I7	-16.60	-44.04	-36.15
TS_{I2-I3}	-0.58	-16.35	-14.09
TS_{I3-I4}	10.67	-25.48	-16.17
TS_{I4-I5}	6.57	-21.77	-17.60
TS_{I5-I6}	9.30	1.92	2.06
TS_{I6-I1}	7.57	-2.61	0.79
TS_{RI4-I1}	-1.42	-36.31	-25.92
TS_{SI4-I1}	2.47	-29.21	-22.98
TS_{I3-I7}	10.93	-22.22	-12.28
TS_{I7-I5}	7.29	-19.97	-15.19
TS_{RI7-I1}	8.20	-22.00	-21.59
TS_{SI7-I1}	9.07	-17.89	-17.42
I8	0	0	0
I9	-10.27	-42.10	-29.22
TS_{RI9-I1}	20.90	-14.42	-4.82
TS_{SI9-I1}	17.45	-13.72	-11.14
I10	-16.90	-49.06	-45.47
TS_{RI10-I1}	13.21	-15.67	-12.97
TS_{SI10-I1}	-5.60	-33.02	-34.68



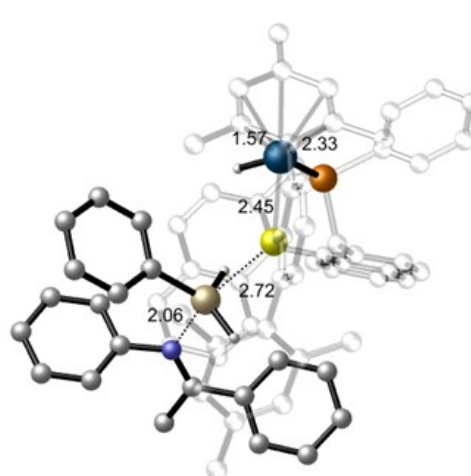
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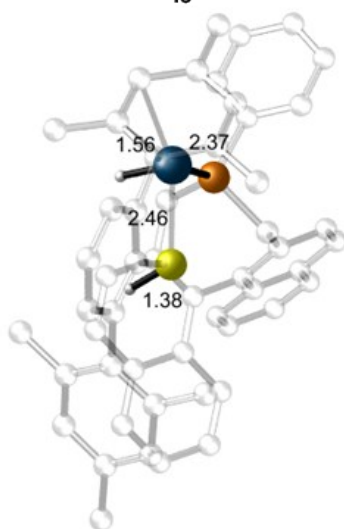
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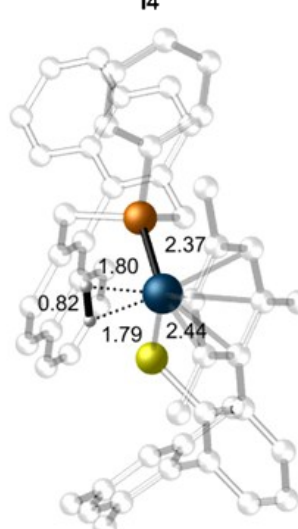
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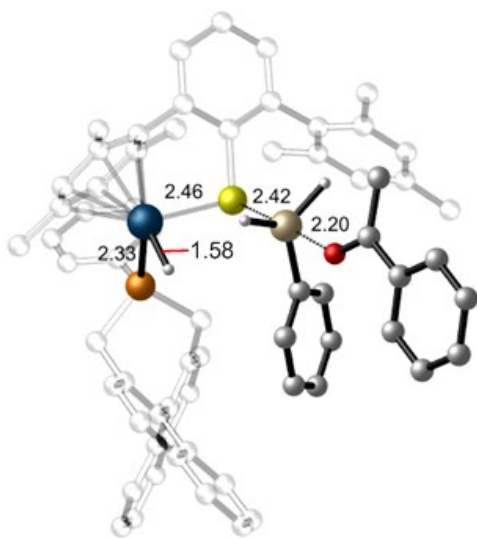
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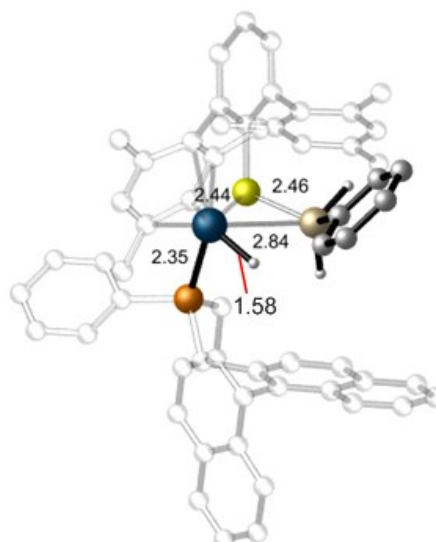
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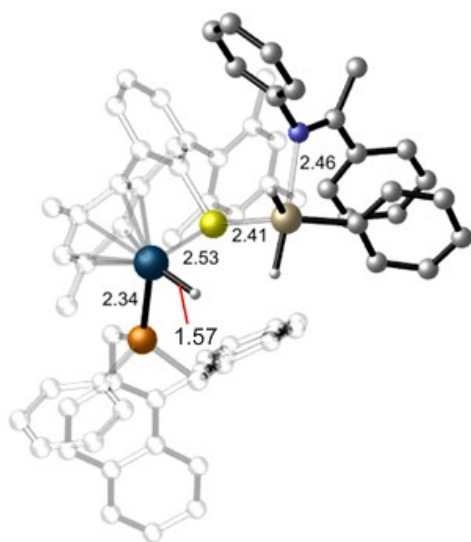
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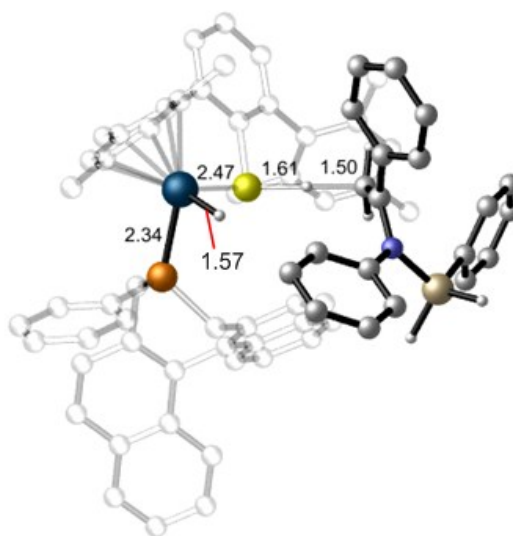
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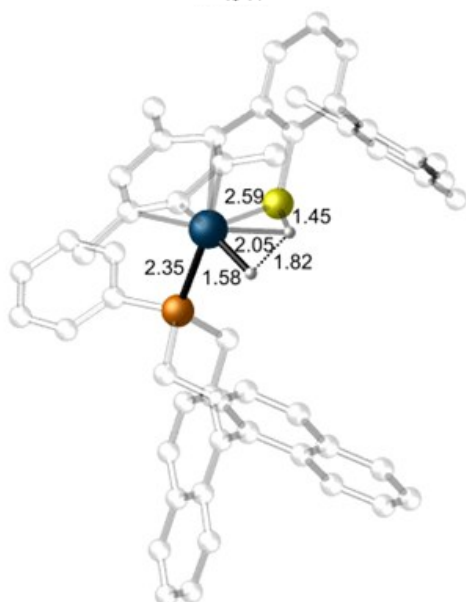
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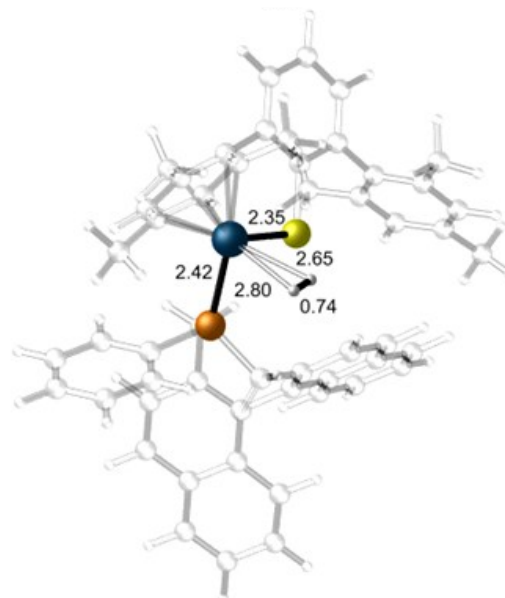
TS₁₃₋₁₄



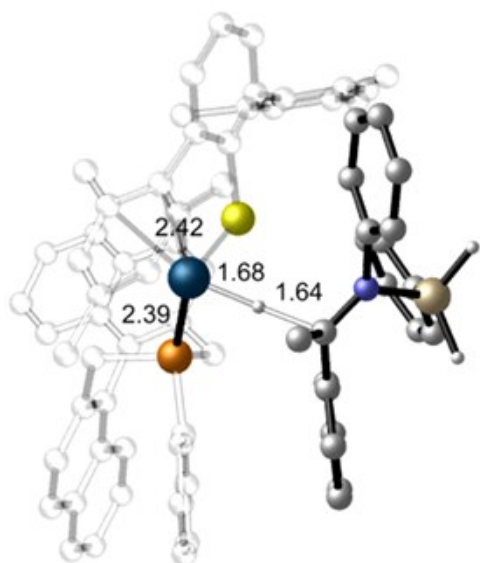
TS₁₄₋₁₅



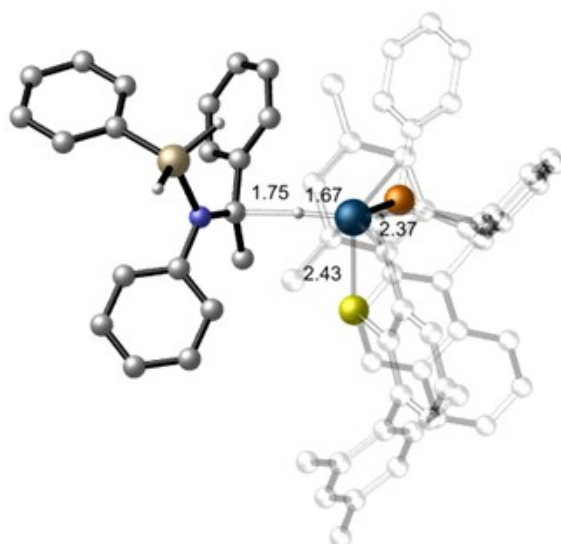
TS₁₅₋₁₆



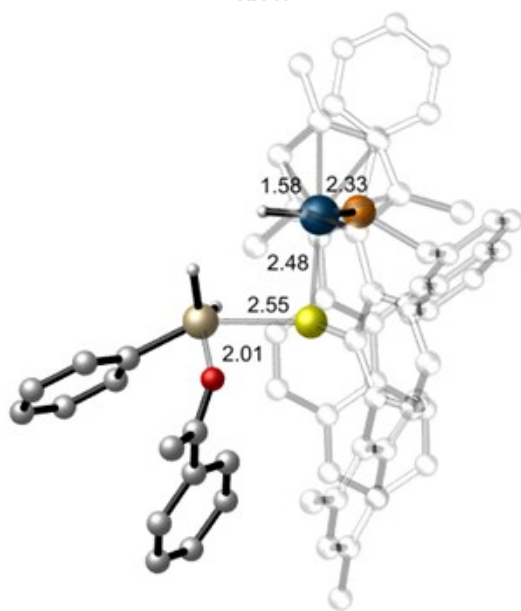
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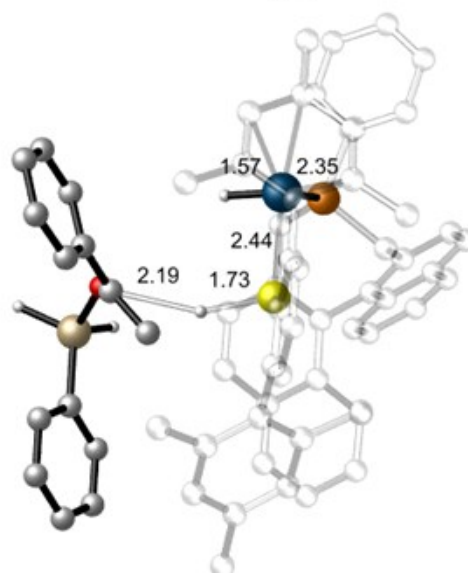
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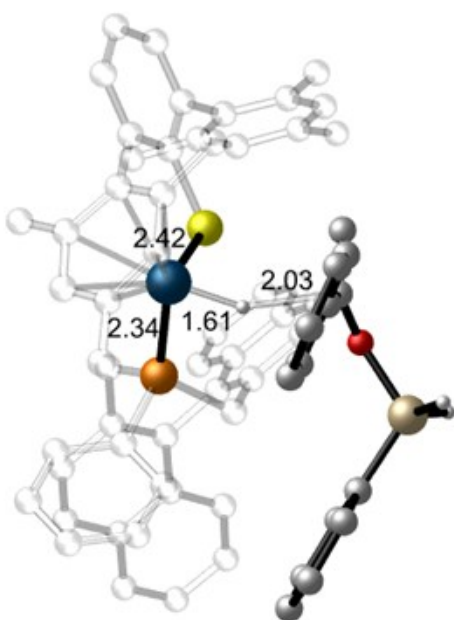
TS_{SI4-I1}



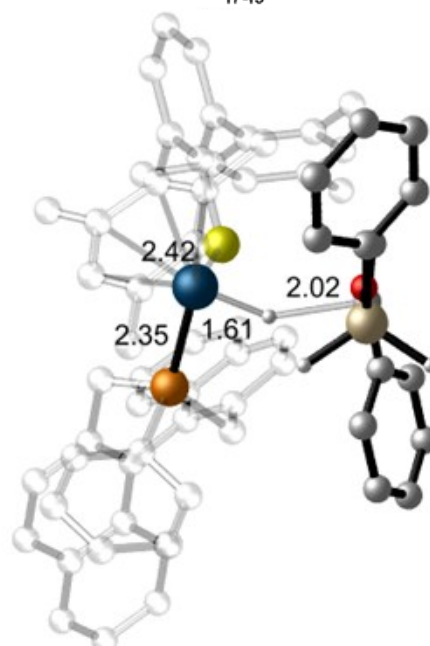
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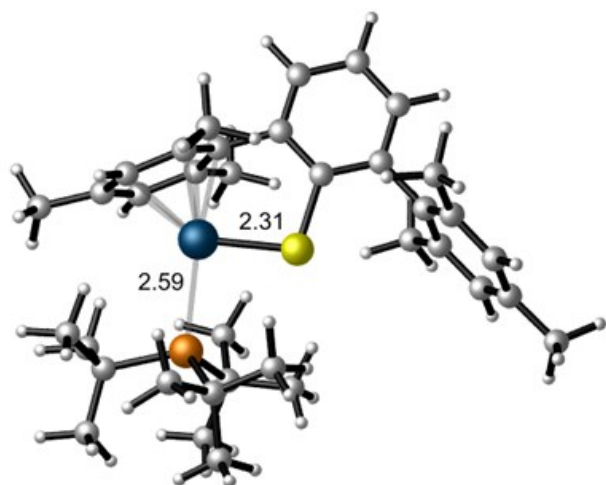
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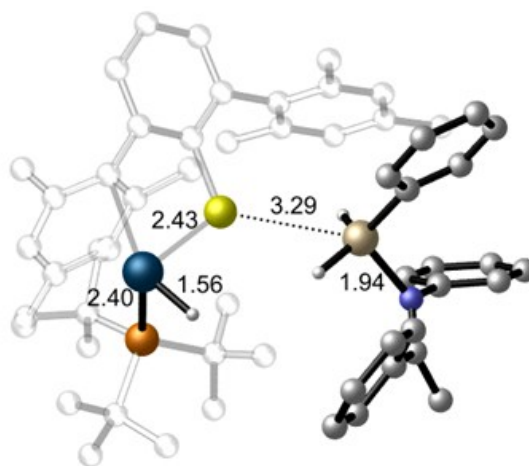
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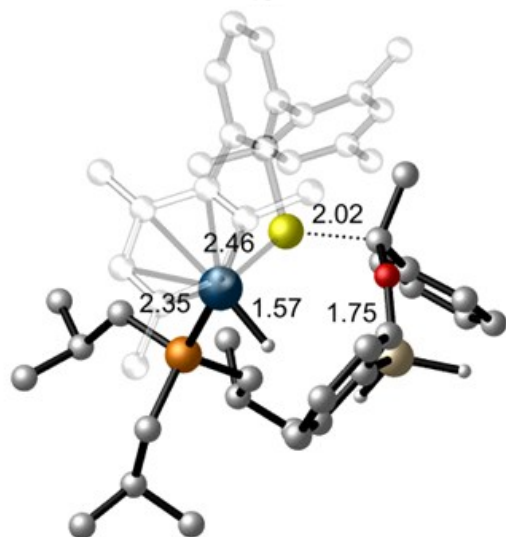
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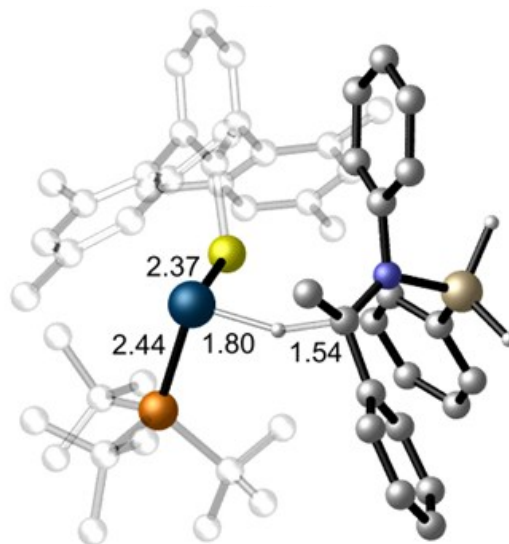
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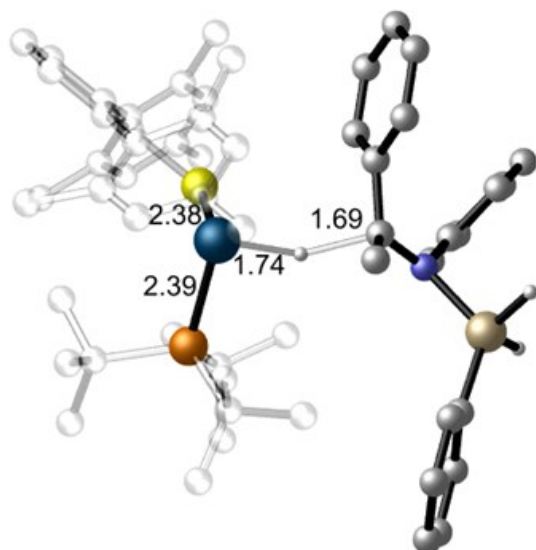
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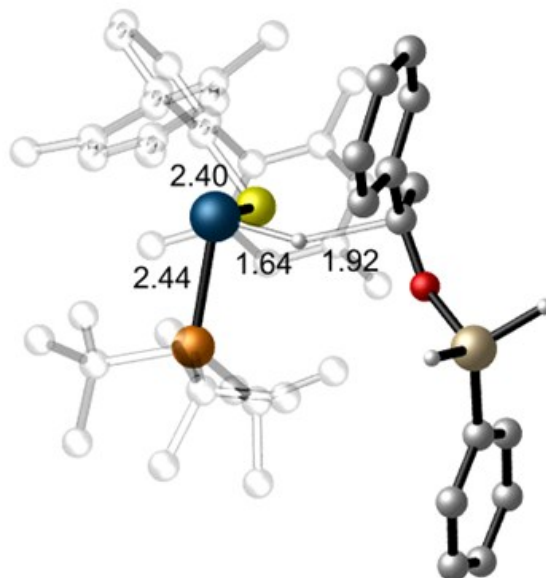
I10



TS_{RI9-I1}



TS_{SI9-I1}



TS_{RI10-I1}

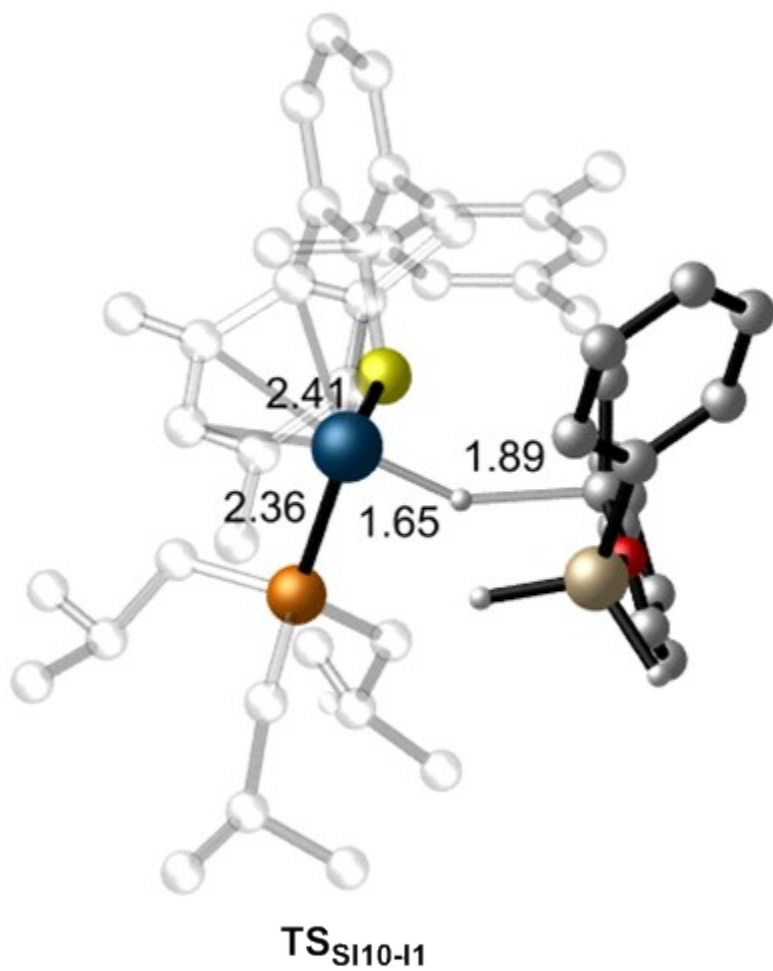


Figure S1. Optimized geometries with selected structural parameters (distances in Å) for the species involved in Table S1. Unimportant hydrogen and carbon atoms are transparent for clarity.

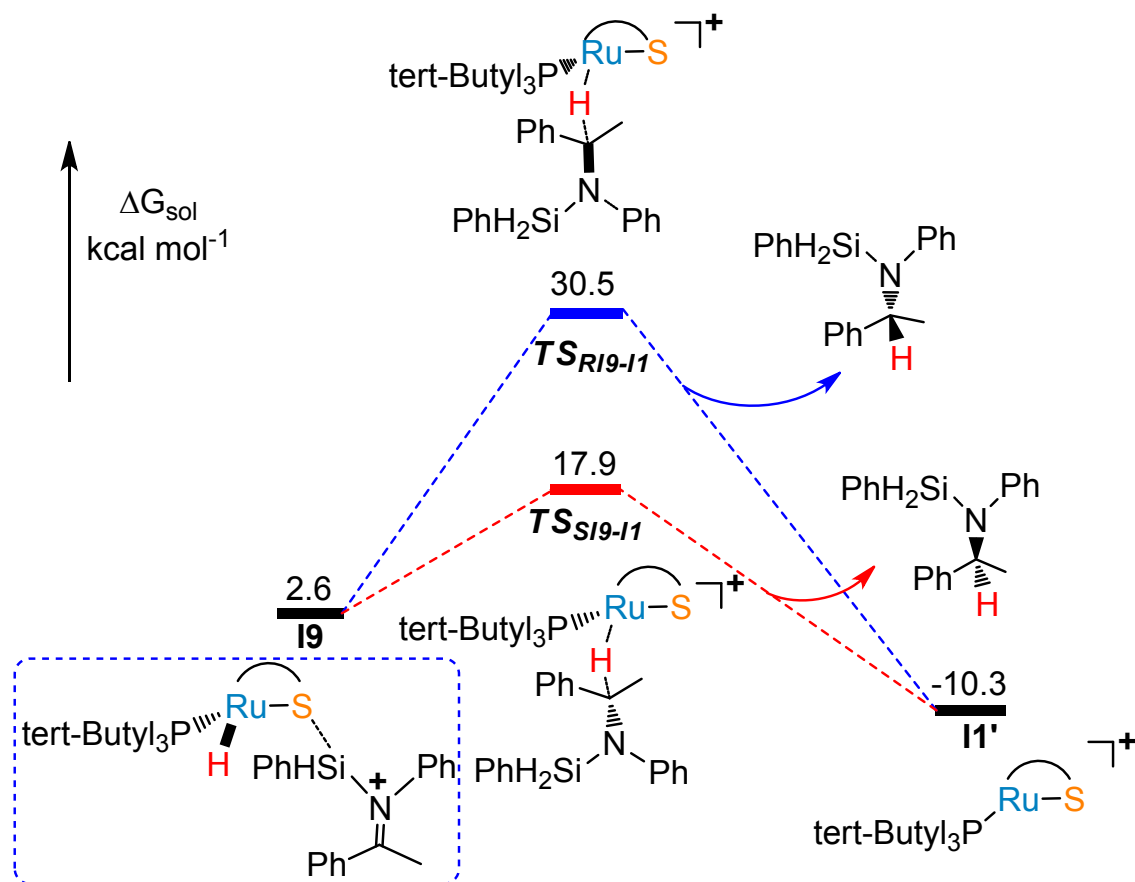


Figure S2. Free energy profile for [RuS]P(tBu)⁺ catalyzed hydrosilylation of imine.

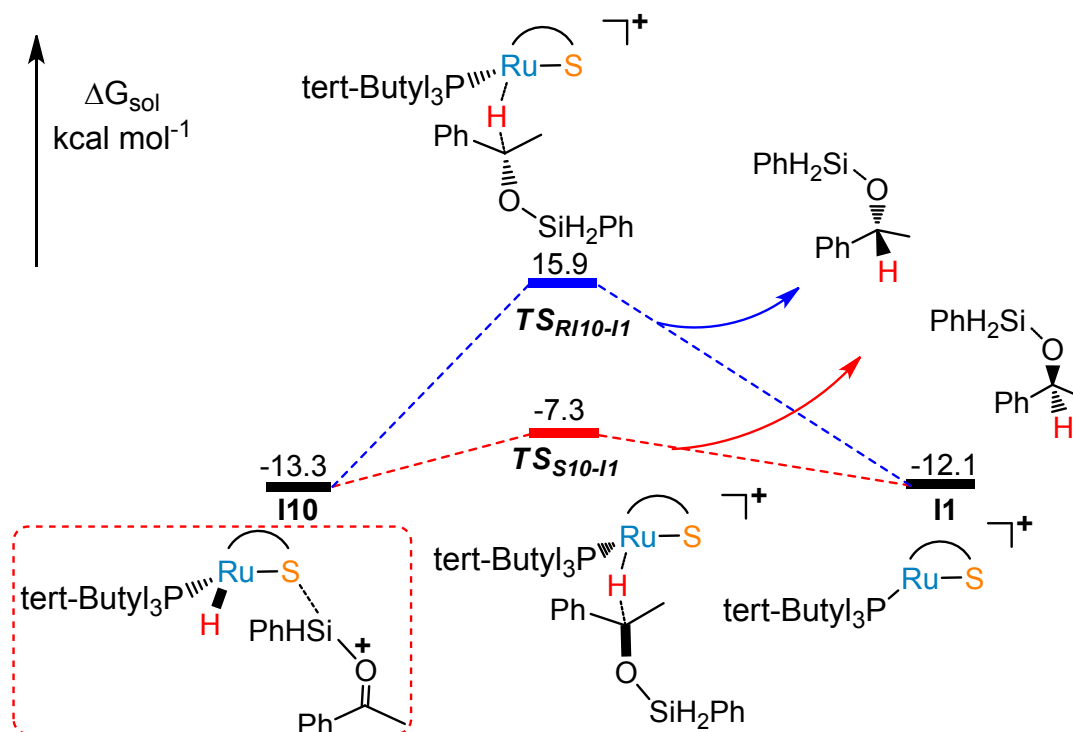


Figure S3. Free energy profile for [RuS]P(tBu)⁺ catalyzed hydrosilylation of ketone.

Cartesian coordinates for the complexes optimized in this study:

PhSiH₃

$G_{\text{gas}} = -522.616428$ a. u.

$E_{\text{gas}} = -522.703213166$ a. u.

Si	-2.35556900	-0.00000200	0.00434900
H	-2.89847600	-0.00283100	1.40005200
C	-0.45821400	0.00000300	-0.00717500
C	0.25878400	-1.20619500	-0.00816700
C	0.25878000	1.20619000	-0.00816700
C	1.65444100	-1.20775900	0.00256200
H	-0.27336800	-2.15284500	-0.02123700
C	1.65444900	1.20775100	0.00255100
H	-0.27338500	2.15282800	-0.02123800
C	2.35367300	0.00000100	0.00900300
H	2.19402100	-2.14815300	0.00174000
H	2.19402500	2.14814800	0.00171000
H	3.43776500	-0.00000300	0.01505400
H	-2.86694600	1.22335300	-0.68778600
H	-2.86714500	-1.22041600	-0.69281300

Imine

$G_{\text{gas}} = -595.472227$ a. u.

$E_{\text{gas}} = -595.669228579$ a. u.

C	3.59046600	1.52368200	-0.39459100
C	2.24812500	1.18638200	-0.25897500
C	1.87205400	-0.12600700	0.06769300
C	2.87166800	-1.09118300	0.24831400
C	4.21828600	-0.75269500	0.10779800
C	4.58154100	0.55458100	-0.21176000
H	3.86736700	2.54164700	-0.64377400

H	1.46457100	1.92042600	-0.40065300
H	2.60854200	-2.11355800	0.49295900
H	4.98034700	-1.51071100	0.24758800
H	5.62763900	0.81803900	-0.31864800
C	0.42742800	-0.46564500	0.20027900
N	-0.42716400	0.45766300	-0.07164500
C	0.07395800	-1.85693900	0.67445300
H	-0.99015800	-1.93962900	0.89464900
H	0.32853200	-2.60732000	-0.08186800
H	0.63882500	-2.09689800	1.57973000
C	-1.82837200	0.28577000	-0.06738900
C	-2.60691100	1.17265700	0.68881700
C	-2.46283400	-0.68065400	-0.86188800
C	-3.99513400	1.06902200	0.67812200
H	-2.10382500	1.93401200	1.27288400
C	-3.85452900	-0.76628200	-0.88209900
H	-1.85990200	-1.34134800	-1.47590500
C	-4.62596300	0.10064000	-0.10741800
H	-4.58784400	1.75285400	1.27499900
H	-4.33557100	-1.51131100	-1.50575300
H	-5.70707700	0.03018800	-0.12282900

Ketone

$G_{\text{gas}} = -384.521598$ a. u.

$E_{\text{gas}} = -384.630357616$ a. u.

C	-1.81870700	-1.27585100	-0.00002800
C	-0.42656100	-1.19399800	-0.00005800
C	0.20498400	0.05564200	-0.00004300
C	-0.57195000	1.22220400	0.00005100
C	-1.96091700	1.13997200	0.00005500
C	-2.58617500	-0.11019000	0.00001200
H	-2.30290800	-2.24533300	-0.00009100
H	0.16207100	-2.10451400	-0.00012100

H	-0.06166000	2.17844700	0.00001600
H	-2.55732200	2.04476400	0.00012200
H	-3.66828600	-0.17508800	0.00002300
C	1.69012800	0.19371500	-0.00007200
O	2.21758200	1.31479100	-0.00008000
C	2.54039600	-1.05291200	0.00010100
H	3.58915400	-0.75889200	-0.00001500
H	2.33560200	-1.66434700	0.88443900
H	2.33550300	-1.66485700	-0.88383900

Silyl-amine (*R*)

G_{gas} = -1118.115155 a. u.

E_{gas} = -1118.4264547a. u.

C	-4.76220500	1.04695000	-0.62897000
C	-3.42974300	1.27212900	-0.29373200
C	-2.58447700	0.20869600	0.07740300
C	-3.14031200	-1.08523600	0.12470200
C	-4.48040100	-1.29755300	-0.19284000
C	-5.30172000	-0.23865500	-0.57909500
H	-5.38615200	1.88759500	-0.91162100
H	-3.04888300	2.28809500	-0.29041200
H	-2.51979500	-1.93382200	0.38856300
H	-4.87890100	-2.30520300	-0.14919100
H	-6.34085900	-0.41073900	-0.83146500
C	-0.54287600	-0.40344000	1.37739400
H	-1.31237500	-1.06788700	1.78808500
Si	-0.35352700	1.84520700	-0.34773300
C	1.50946100	1.54574800	-0.47115000
C	2.03854000	0.68128100	-1.44230600
C	2.39302000	2.19101000	0.40648900
C	3.40926900	0.43755200	-1.50792500
H	1.37454300	0.17402300	-2.13522900
C	3.76750000	1.95243200	0.34162100

H	2.00624000	2.88407000	1.14925600
C	4.27468700	1.06926900	-0.61136500
H	3.80015200	-0.24950800	-2.24984800
H	4.43796900	2.45438500	1.03018600
H	5.34069500	0.87697100	-0.65993800
N	-1.22780900	0.45041900	0.38215100
C	0.52614400	-1.28305300	0.73009500
C	0.23513400	-1.92495900	-0.48273400
C	1.79027500	-1.46981600	1.29818500
C	1.17812500	-2.74134900	-1.10416700
H	-0.72741100	-1.75315300	-0.95469100
C	2.74157500	-2.27735800	0.67041100
H	2.05345200	-0.96791500	2.22174300
C	2.43869200	-2.91920800	-0.52933400
H	0.93365400	-3.23012500	-2.04094200
H	3.72242500	-2.39499900	1.11740700
H	3.17734700	-3.54675000	-1.01511200
H	-0.95303100	2.03843500	-1.70211000
H	-0.54197300	3.09894500	0.46106600
C	-0.03507300	0.43915300	2.55461000
H	-0.85007300	1.07063100	2.91582400
H	0.29961000	-0.19765100	3.37821900
H	0.80372100	1.07721900	2.25966600

Silyl-amine (*S*)

G_{gas} = -1118.115155 a. u.

E_{gas} = -1118.4264547 a. u.

C	4.29636900	-1.82258800	-0.51779700
C	2.93234500	-1.85756400	-0.23947800
C	2.22510200	-0.68403100	0.08536100
C	2.94836300	0.52391100	0.14094600
C	4.31697100	0.54525400	-0.12005700
C	5.00280900	-0.62169100	-0.45750400

H	4.80999100	-2.74451000	-0.76694900	C	0.87846400	0.42820400	2.52174200
H	2.41767300	-2.81306100	-0.24310800	H	1.07205800	-0.55045400	2.96839500
H	2.43575000	1.44997900	0.36592300	H	1.82992400	0.94867200	2.40912000
H	4.84668100	1.49020600	-0.06973000	H	0.25497000	1.00443100	3.20955000
H	6.06530700	-0.59588000	-0.66657900				
C	0.15155300	0.23135400	1.17912900	Silyl-Ether (<i>R</i>)			
H	-0.81741700	-0.22206300	1.42766200	G_{gas} = -907.165519 a. u.			
Si	-0.14041800	-2.02712700	-0.49589600	E_{gas} = -907.387160225 a. u.			
C	-1.97782200	-1.61315900	-0.35176300	C	2.09605800	2.06941700	0.54368900
C	-2.54680100	-0.52578700	-1.03620200	C	1.43493800	0.91585800	0.97642900
C	-2.80679800	-2.40854400	0.45511600	C	1.88326000	-0.34776800	0.58038700
C	-3.90506900	-0.23634400	-0.90603900	C	3.00529700	-0.43702700	-0.25595200
H	-1.92783100	0.10557000	-1.66599900	C	3.66519100	0.70992600	-0.68897300
C	-4.16730900	-2.12238700	0.58353800	C	3.20925900	1.96949200	-0.28918000
H	-2.38708400	-3.25761800	0.98679400	H	1.73906000	3.04335800	0.85955400
C	-4.71596700	-1.03442300	-0.09590300	H	0.56607100	1.00950000	1.61830800
H	-4.32917200	0.60931500	-1.43517100	H	3.34400100	-1.41823600	-0.57521700
H	-4.79511900	-2.74556800	1.21029800	H	4.53080500	0.62575600	-1.33602100
H	-5.77188300	-0.80925300	0.00335400	H	3.72067100	2.86461000	-0.62426200
N	0.83291800	-0.75032000	0.31516100	C	1.15267600	-1.63071900	0.93719400
C	-0.18460200	1.54440200	0.46752300	O	0.49487700	-2.17920000	-0.24092900
C	0.12818600	1.75397100	-0.88059000	C	0.14366700	-1.50563900	2.07080200
C	-0.88617700	2.54504900	1.15405200	H	-0.31108500	-2.48223200	2.24803400
C	-0.23926900	2.93807500	-1.52365800	H	0.62967200	-1.16784800	2.99117000
H	0.66987500	0.98496300	-1.42217700	H	-0.65506300	-0.80340400	1.81464700
C	-1.25771600	3.72646600	0.51343300	H	1.89753400	-2.38815300	1.20298500
H	-1.15883700	2.39566800	2.19401700	Si	-0.35034000	-1.24767500	-1.43611200
C	-0.93314800	3.92881800	-0.82928600	C	-1.72165600	-0.16687700	-0.70729400
H	0.01933000	3.08445500	-2.56646500	C	-1.58540000	1.22922300	-0.68066600
H	-1.80329900	4.48684400	1.06098100	C	-2.88258200	-0.74174200	-0.16478100
H	-1.21956000	4.84770400	-1.32774200	C	-2.58203300	2.03295600	-0.12309600
H	0.32046300	-2.09077300	-1.91901900	H	-0.69062500	1.68896700	-1.09154400
H	0.04671800	-3.38051200	0.12788000	C	-3.87912900	0.05811100	0.39485300

H	-3.00773600	-1.82095000	-0.17832300	C	2.58203300	2.03295600	-0.12309600
C	-3.72808300	1.44678300	0.41613100	H	0.69062500	1.68896700	-1.09154400
H	-2.46557500	3.11087100	-0.11001900	C	3.87912900	0.05811100	0.39485300
H	-4.77070400	-0.39726800	0.81092000	H	3.00773600	-1.82095000	-0.17832300
H	-4.50280500	2.06910300	0.84986400	C	3.72808300	1.44678300	0.41613100
H	-0.92584800	-2.30150500	-2.31761200	H	2.46557500	3.11087100	-0.11001900
H	0.57859700	-0.34349100	-2.18674200	H	4.77070400	-0.39726800	0.81092000

Silyl-Ether (*S*)

$G_{\text{gas}} = -907.165519$ a. u.

$E_{\text{gas}} = -907.387160225$ a. u.

C	-2.09605800	2.06941700	0.54368900
C	-1.43493800	0.91585800	0.97642900
C	-1.88326000	-0.34776800	0.58038700
C	-3.00529700	-0.43702700	-0.25595200
C	-3.66519100	0.70992600	-0.68897300
C	-3.20925900	1.96949200	-0.28918000
H	-1.73906000	3.04335800	0.85955400
H	-0.56607100	1.00950000	1.61830800
H	-3.34400100	-1.41823600	-0.57521700
H	-4.53080500	0.62575600	-1.33602100
H	-3.72067100	2.86461000	-0.62426200
C	-1.15267600	-1.63071900	0.93719400
O	-0.49487700	-2.17920000	-0.24092900
C	-0.14366700	-1.50563900	2.07080200
H	0.31108500	-2.48223200	2.24803400
H	-0.62967200	-1.16784800	2.99117000
H	0.65506300	-0.80340400	1.81464700
H	-1.89753400	-2.38815300	1.20298500
Si	0.35034000	-1.24767500	-1.43611200
C	1.72165600	-0.16687700	-0.70729400
C	1.58540000	1.22922300	-0.68066600
C	2.88258200	-0.74174200	-0.16478100

Silyl enamine

$G_{\text{gas}} = -1116.924539$ a. u.

$E_{\text{gas}} = -1117.21255402$ a. u.

C	4.75745600	-0.97714200	-0.67401100
C	3.39623400	-1.21506900	-0.49089600
C	2.57077800	-0.24184400	0.09895200
C	3.15667100	0.97260900	0.50377800
C	4.51820400	1.19508300	0.32254700
C	5.33188600	0.22634800	-0.26889400
H	5.37093000	-1.74657300	-1.12950800
H	2.98439900	-2.17339600	-0.78860600
H	2.53768100	1.73600500	0.95900700
H	4.94464200	2.13984700	0.64138700
H	6.39064200	0.40658100	-0.40907600
C	0.39999700	0.34919900	1.11845700
Si	0.32777300	-1.73719700	-0.72592400
C	-1.52214500	-1.59025600	-0.39607900
C	-2.36907300	-0.97022400	-1.32658100
C	-2.06325900	-2.04081800	0.81751900
C	-3.72277100	-0.78749300	-1.04440100
H	-1.96481600	-0.60217300	-2.26489200
C	-3.41703600	-1.85732600	1.10291600

H	-1.42361000	-2.52473300	1.55031100	H	-2.60531800	-1.89515700	1.40199900
C	-4.24609200	-1.22774400	0.17270100	H	-2.43271300	1.64124700	-1.01403800
H	-4.36376300	-0.29398000	-1.76607500	H	-4.79394100	1.28058100	-1.70615300
H	-3.82374500	-2.20460900	2.04615900	H	-6.05978700	-0.66685800	-0.82501700
H	-5.29719800	-1.08152100	0.39545600	C	-0.96805800	0.17306500	0.67404600
N	1.18211300	-0.46423300	0.23073700	O	-0.34423600	1.09600500	-0.15056800
C	-0.60012300	1.23613200	0.46918700	C	-0.35643000	-0.39569700	1.72195200
C	-0.33292700	1.77176100	-0.79902300	H	0.68335700	-0.20543900	1.95892100
C	-1.83055100	1.51101500	1.08069200	H	-0.88466800	-1.07382900	2.37601300
C	-1.27478100	2.57781500	-1.43713400	Si	1.22705100	1.80682300	0.05436300
H	0.61627300	1.54709700	-1.27604800	C	2.53461700	0.46262800	-0.13962000
C	-2.77316200	2.31132100	0.43904900	C	2.23917900	-0.69540700	-0.87429200
H	-2.06427900	1.04966600	2.03440200	C	3.80165900	0.59400600	0.44529500
C	-2.49870000	2.84691800	-0.82156300	C	3.19921300	-1.69549800	-1.03184200
H	-1.05551900	2.99248100	-2.41464500	H	1.25288900	-0.81725400	-1.31253900
H	-3.73081600	2.49853800	0.91165500	C	4.76470500	-0.40324700	0.28320200
H	-3.23648200	3.46280100	-1.32315000	H	4.04138400	1.47451400	1.03551900
H	0.63615300	-1.54571700	-2.17834400	C	4.46294800	-1.54770700	-0.45667100
H	0.81049800	-3.09002100	-0.29684600	H	2.96178600	-2.58856300	-1.59852300
C	0.59086200	0.30818700	2.44424700	H	5.74274000	-0.29119200	0.73715300
H	0.05818700	0.97673800	3.10983000	H	5.20862500	-2.32496000	-0.57986900
H	1.31840300	-0.36747100	2.87797500	H	1.34556500	2.43883800	1.40678100
				H	1.26535200	2.83802900	-1.01813700

Silyl ketene

$$G_{\text{gas}} = -905.973488 \text{ a. u.}$$

$$E_{\text{gas}} = -906.170387183 \text{ a. u.}$$

C	-4.40799900	-1.39053000	0.35604000
C	-3.08631300	-1.18310000	0.74139800
C	-2.36899500	-0.07749000	0.26137500
C	-2.99664700	0.80069700	-0.63185700
C	-4.31975700	0.59031500	-1.01773300
C	-5.03169300	-0.50249700	-0.52338900
H	-4.94867400	-2.25073500	0.73393400

I1

$$G_{\text{gas}} = -2840.33736 \text{ a. u.}$$

$$E_{\text{gas}} = -2841.0992708 \text{ a. u.}$$

Ru	1.19126400	-2.06380500	-0.20472400
S	1.71737600	0.13522200	0.18918100
P	-1.19108600	-1.58666200	-0.05295500
C	3.32857300	-2.48726400	-0.13645000
C	2.89399400	-2.79138600	-1.46730400
C	1.83452600	-3.73882100	-1.65929800

H	1. 47280700	-3. 91151800	-2. 66597100	C	3. 51446100	3. 11145400	1. 66812700
C	1. 23553100	-4. 43344000	-0. 58152200	C	3. 47687100	2. 45158300	-2. 10483000
C	1. 66346900	-4. 10378800	0. 72996300	H	3. 29957500	3. 15530700	-2. 92187200
H	1. 16348200	-4. 55787900	1. 57749000	H	2. 75535600	1. 62907500	-2. 20437500
C	2. 71436000	-3. 16075700	0. 97739100	H	4. 47914200	2. 02992800	-2. 23167300
C	3. 47248100	-2. 07122200	-2. 65147600	C	2. 02214900	6. 45896500	0. 60754600
H	4. 45321000	-2. 49350700	-2. 89635700	H	2. 74282200	7. 15474100	1. 04880700
H	3. 61630200	-1. 00911100	-2. 44072400	H	1. 12007200	6. 47850200	1. 22693300
H	2. 82662800	-2. 17569400	-3. 52489200	H	1. 75942000	6. 83426500	-0. 38502300
C	0. 15068200	-5. 44264100	-0. 81975400	C	3. 89165100	2. 40263500	2. 94666300
H	0. 59549800	-6. 43196600	-0. 97110900	H	4. 96747400	2. 20484800	2. 99734900
H	-0. 43266700	-5. 19408400	-1. 70916000	H	3. 38108900	1. 43568300	3. 02449100
H	-0. 53506600	-5. 50321700	0. 02857100	H	3. 61758700	3. 00183000	3. 81713700
C	3. 11946400	-2. 84121400	2. 38692700	C	-2. 19704600	-3. 13013500	0. 15620300
H	4. 04277200	-3. 37714500	2. 63321400	C	-2. 91748900	-3. 67856900	-0. 90824200
H	2. 34663200	-3. 14757700	3. 09406300	H	-2. 94546100	-3. 17935100	-1. 87131500
H	3. 31211800	-1. 77405300	2. 51321000	C	-3. 61063800	-4. 88025500	-0. 73714000
C	3. 56396700	-0. 02727800	0. 21498900	H	-4. 17031500	-5. 30012700	-1. 56447800
C	4. 18692700	-1. 28621600	0. 09135400	C	-3. 59222800	-5. 53064100	0. 49670000
C	5. 57738100	-1. 38426800	0. 14074000	H	-4. 13655500	-6. 45785800	0. 62926800
H	6. 04950300	-2. 35632900	0. 04368200	C	-2. 87757400	-4. 98084000	1. 56518500
C	6. 35123500	-0. 23399300	0. 30671600	H	-2. 87029800	-5. 47903700	2. 52764700
H	7. 43091600	-0. 30895600	0. 34710500	C	-2. 17640000	-3. 78706600	1. 39418400
C	5. 73122400	1. 00876600	0. 40515300	H	-1. 61477400	-3. 37001200	2. 22594400
H	6. 32458400	1. 91035200	0. 51390800	C	-1. 73079800	-0. 45562600	1. 37001900
C	4. 33345700	1. 13450200	0. 35516100	H	-1. 57917400	-1. 00492200	2. 30248100
C	3. 70277200	2. 48600400	0. 42152400	H	-1. 03184000	0. 38601900	1. 35496800
C	3. 32169700	3. 13310300	-0. 76655400	C	-3. 15919400	-0. 02431800	1. 19154100
C	2. 77897800	4. 41943700	-0. 69001100	C	-4. 18134900	-0. 66100100	1. 94526300
H	2. 51090400	4. 93302900	-1. 60978900	H	-3. 90450900	-1. 42125500	2. 66849800
C	2. 59266500	5. 06513600	0. 53387500	C	-5. 49705100	-0. 31636000	1. 77149600
C	2. 95804500	4. 39069100	1. 70389000	H	-6. 27489500	-0. 79545100	2. 35664600
H	2. 81009900	4. 87531700	2. 66493500	C	-5. 86832100	0. 66677000	0. 81552000

C	-4.85413200	1.30501000	0.03866400	Ru	-0.91187900	-2.25378400	0.10541600
C	-3.48157200	0.95351600	0.25832000	S	-1.48563700	0.06538400	-0.33365200
C	-7.23075800	1.01668500	0.60597100	P	1.30754800	-1.48451600	0.26418700
H	-7.98969500	0.52882900	1.20871300	C	-2.46151400	-2.61992400	-1.57604900
C	-7.57911700	1.94782900	-0.34118200	C	-2.85916700	-3.54141300	-0.56091700
H	-8.61919900	2.20900800	-0.49519600	C	-1.88811000	-4.45882800	-0.07227600
C	-6.57594500	2.56807800	-1.12841500	H	-2.15310700	-5.09839900	0.76394400
H	-6.86124200	3.29343900	-1.88109000	C	-0.60703400	-4.59021600	-0.65586900
C	-5.24992700	2.25602800	-0.94612500	C	-0.29587800	-3.75508100	-1.76262400
H	-4.49025100	2.73337000	-1.55364600	H	0.67450900	-3.86284100	-2.23984100
C	-1.93407700	-0.66841700	-1.53857000	C	-1.19127300	-2.77408900	-2.23694400
H	-1.50436200	-1.08874300	-2.45048100	C	-4.25606300	-3.56968500	-0.00679900
H	-3.01081700	-0.86435800	-1.52102100	H	-4.84601900	-4.30456300	-0.56628300
C	-1.64361800	0.80552700	-1.41492200	H	-4.75121600	-2.60322700	-0.10072100
C	-0.58591600	1.38069400	-2.16812800	H	-4.25972000	-3.86878000	1.04446500
H	-0.01678700	0.74885900	-2.84340400	C	0.34914600	-5.64270000	-0.16695500
C	-0.28424400	2.71354700	-2.04752800	H	0.11358400	-6.60488000	-0.63425000
H	0.52262700	3.15256300	-2.62581600	H	0.27632800	-5.76568200	0.91614200
C	-1.01637200	3.54322400	-1.15761200	H	1.38285700	-5.39087200	-0.41050100
C	-2.07329400	2.97707400	-0.38253000	C	-0.83494900	-1.87534000	-3.38850700
C	-2.38773500	1.58793000	-0.54014200	H	-1.61016600	-1.91894700	-4.15879200
C	-0.71927300	4.92712500	-1.02148700	H	0.11566700	-2.17205000	-3.83640400
H	0.07681600	5.34708500	-1.62732600	H	-0.76205100	-0.83135800	-3.06113400
C	-1.42529700	5.71572200	-0.14676700	C	-2.97633400	-0.18902200	-1.38794000
H	-1.19689300	6.77141900	-0.05624900	C	-3.31423500	-1.44609400	-1.91611500
C	-2.45603800	5.14936900	0.64572400	C	-4.43758700	-1.58871900	-2.73749900
H	-2.99859600	5.77590700	1.34366500	H	-4.68676900	-2.56692200	-3.13691800
C	-2.77135400	3.81663500	0.53366900	C	-5.22638000	-0.48037800	-3.03654800
H	-3.56018100	3.39143400	1.14258900	H	-6.09320200	-0.58598800	-3.67703300
				C	-4.90063200	0.76204500	-2.49320500
I2				H	-5.52070000	1.62800300	-2.70020200
G _{gas} = -3362.957404 a. u.				C	-3.78583000	0.92713700	-1.66109300
E _{gas} = -3363.83349989 a. u.				C	-3.51562800	2.25496000	-1.03234700

C	-4.24914100	2.62540900	0.11256400	C	3.29439500	-0.15801100	-1.28063000
C	-4.00185800	3.86657100	0.70470300	C	4.36658900	-0.79712000	-1.96307900
H	-4.56795000	4.15196900	1.58798800	H	4.15384500	-1.65330100	-2.59553400
C	-3.06849400	4.75957900	0.16790600	C	5.64785300	-0.32101400	-1.87168200
C	-2.37103600	4.37968400	-0.98074000	H	6.45635500	-0.80384800	-2.41029600
H	-1.65595000	5.06563900	-1.42368400	C	5.94077200	0.81179000	-1.06643100
C	-2.56429900	3.13186600	-1.58084200	C	4.87405700	1.48423000	-0.39834600
C	-5.30086200	1.70637000	0.68952800	C	3.52960000	1.00186100	-0.55395200
H	-5.61883700	2.05184900	1.67627300	C	7.27136300	1.29032300	-0.91955000
H	-4.92943400	0.67994600	0.78654900	H	8.06969200	0.77177300	-1.44010400
H	-6.18769700	1.66374200	0.04755700	C	7.54062700	2.38242600	-0.13176100
C	-2.81720500	6.09602500	0.82253300	H	8.55696700	2.74121900	-0.02233300
H	-3.74748700	6.54332500	1.18282300	C	6.48623400	3.04240100	0.54807000
H	-2.35446800	6.79750100	0.12342400	H	6.70903800	3.89615500	1.17687200
H	-2.14874100	5.99592000	1.68690000	C	5.18832400	2.60850700	0.41837200
C	-1.75515500	2.74531000	-2.79452100	H	4.39013100	3.11820500	0.94423300
H	-2.39501300	2.40506700	-3.61491900	C	1.85506500	-0.19226400	1.53425100
H	-1.06281800	1.93000400	-2.55194500	H	1.30839000	-0.38973400	2.46022100
H	-1.16039800	3.59099200	-3.14700500	H	2.91925400	-0.39482400	1.69411100
C	2.36821700	-2.95701900	0.66005400	C	1.61593700	1.21281100	1.05163600
C	2.24333000	-3.52782300	1.93375400	C	0.57789800	1.96863400	1.65412300
H	1.55350600	-3.10246900	2.65765200	H	0.00881500	1.51949200	2.45686500
C	2.99793400	-4.64968100	2.27541700	C	0.30563800	3.24567300	1.24050200
H	2.90180700	-5.08336800	3.26373700	H	-0.49589900	3.81416000	1.70258300
C	3.87779900	-5.21077400	1.34595700	C	1.05552300	3.83695700	0.18957800
H	4.46540000	-6.08091900	1.61270600	C	2.09664100	3.08691500	-0.43591000
C	4.00320800	-4.64515000	0.07697700	C	2.39197200	1.76475300	0.04238900
H	4.69050700	-5.07208300	-0.64380200	C	0.79561400	5.16533300	-0.24665700
C	3.24833400	-3.51997500	-0.26748700	H	0.02260900	5.73153600	0.26379800
H	3.36154900	-3.08521700	-1.25198900	C	1.50261600	5.71805500	-1.28610400
C	1.90624500	-0.73599000	-1.36825400	H	1.29964900	6.73189400	-1.61071400
H	1.83447700	-1.51269300	-2.13564200	C	2.50584300	4.95871300	-1.94026200
H	1.15226100	0.02862100	-1.58890300	H	3.04907700	5.39418800	-2.77055300

C	2.79908400	3.68179800	-1.52490300	H	-4.55572200	-3.61182200	-0.37658600
H	3.57296300	3.11484100	-2.02807900	H	-3.99584900	-2.08371600	0.29317500
Si	-2.34927100	-1.54392900	1.99192400	H	-4.07693200	-3.52263700	1.32736700
H	-0.50743300	-2.30471100	1.64661700	C	0.53134300	-5.55972500	1.32875200
C	-1.84789500	-0.15783000	3.16236600	H	0.30318100	-6.62014700	1.17824400
C	-2.42274400	1.11460400	3.01222500	H	0.34033400	-5.31613200	2.37656300
C	-0.94854100	-0.37685400	4.21756900	H	1.59553700	-5.40904400	1.13069800
C	-2.10641100	2.14474300	3.89965600	C	-0.04495800	-3.13575000	-3.10495900
H	-3.09419300	1.31211900	2.18277100	H	-0.47249800	-3.75974200	-3.89706800
C	-0.61746200	0.65769700	5.09564100	H	1.03896700	-3.27729600	-3.12013600
H	-0.51156700	-1.36222500	4.36660100	H	-0.26938500	-2.09456100	-3.35002000
C	-1.19948100	1.91846500	4.93773900	C	-2.57264100	-0.65303700	-1.64225300
H	-2.55976900	3.12157900	3.77130200	C	-2.59675000	-1.99484300	-2.06364200
H	0.08021200	0.48010700	5.90580000	C	-3.32389300	-2.34432900	-3.20569400
H	-0.94760300	2.71897300	5.62348900	H	-3.34030800	-3.38160500	-3.52328100
H	-3.64081500	-1.19713000	1.32579300	C	-4.01911400	-1.37225900	-3.92201700
H	-2.56889600	-2.80257200	2.79252300	H	-4.57237100	-1.64460300	-4.81241400

I3

$$G_{\text{gas}} = -3362.971586 \text{ a. u.}$$

$$E_{\text{gas}} = -3363.84700635 \text{ a. u.}$$

Ru	-0.40419200	-2.36177900	0.29287900	C	-4.60613600	2.23944700	-1.39299300
S	-1.50389100	-0.17134900	-0.18842600	C	-4.67566500	3.54424200	-0.90301700
P	1.72004300	-1.40441300	0.14255800	H	-5.62396800	3.91319600	-0.52175100
C	-1.86154800	-3.04650400	-1.30282000	C	-3.55905500	4.38820300	-0.89433300
C	-2.43457500	-3.53950300	-0.06265100	C	-2.35620700	3.89747700	-1.40224700
C	-1.64667900	-4.34942400	0.76919300	H	-1.47988100	4.53931300	-1.41870200
H	-2.04885300	-4.68364600	1.71983100	C	-2.24010100	2.59472500	-1.89978700
C	-0.30707800	-4.70651900	0.41811500	C	-5.85724500	1.38917600	-1.39187500
C	0.17371200	-4.29876900	-0.85013000	H	-6.58003700	1.77772200	-0.67061200
H	1.18501100	-4.57449400	-1.13372200	H	-5.64942000	0.34521000	-1.14069300
C	-0.60540600	-3.51974400	-1.76169500	H	-6.34098300	1.39170400	-2.37491500
C	-3.84053700	-3.16609800	0.32281500	C	-3.66691600	5.80159800	-0.38146000

H	-4.12607600	6.45437400	-1.13155900	C	5.83924100	4.10241800	0.88619000
H	-2.68041300	6.20791100	-0.14649000	H	5.94780200	4.87979300	1.63321300
H	-4.28580800	5.85211000	0.51875500	C	4.65134000	3.41958300	0.77759300
C	-0.90629100	2.17540300	-2.47125200	H	3.82864500	3.65740500	1.44094700
H	-0.92370900	1.16045500	-2.87417900	C	2.28465100	-0.28628200	1.55690100
H	-0.13150200	2.22942000	-1.69835800	H	2.01751000	-0.78253700	2.49123300
H	-0.61283100	2.85575700	-3.27718500	H	3.37303500	-0.20443300	1.48493000
C	3.06784300	-2.67900800	0.03228100	C	1.61807900	1.05626800	1.43866500
C	3.49619700	-3.29814600	1.21296400	C	0.50920300	1.36018700	2.27440500
H	3.07574500	-2.99982900	2.16903900	H	0.16661700	0.61694900	2.98960600
C	4.45715800	-4.30961700	1.16604600	C	-0.09767100	2.58922800	2.20724600
H	4.79039100	-4.77901100	2.08421000	H	-0.91145200	2.83682500	2.88030200
C	4.98916200	-4.71315800	-0.06048200	C	0.34226400	3.56946500	1.27783900
H	5.73557300	-5.49746800	-0.09645400	C	1.42472800	3.25993800	0.39995400
C	4.56156000	-4.10098000	-1.23957700	C	2.07867300	1.98649900	0.51515500
H	4.97740200	-4.40698800	-2.19235600	C	-0.25576700	4.85908300	1.22352500
C	3.60424400	-3.08458900	-1.19395300	H	-1.06569400	5.08448500	1.91076200
H	3.28662500	-2.61122000	-2.11718700	C	0.18723100	5.80168500	0.32729800
C	1.94883000	-0.24335900	-1.33855300	H	-0.25643900	6.79068100	0.30588200
H	1.93482500	-0.84990200	-2.24854100	C	1.22428000	5.47868000	-0.58521200
H	1.03998700	0.36590500	-1.33531500	H	1.55103600	6.21861300	-1.30631000
C	3.19196700	0.59721600	-1.23919800	C	1.82330200	4.24103700	-0.55470700
C	4.31000900	0.28860200	-2.06057500	H	2.61994400	4.00535200	-1.25034600
H	4.22732000	-0.52176400	-2.77703600	Si	-3.03875500	0.73854800	1.26242800
C	5.47177300	1.01032700	-1.97236500	H	-4.33003800	0.21492500	0.73131700
H	6.31634200	0.77765800	-2.61235300	H	-0.13941400	-1.99645600	1.80531100
C	5.59646700	2.06732000	-1.03240800	H	-2.90574000	2.21539800	1.12993400
C	4.48666400	2.38986200	-0.19425300	C	-2.69287300	0.16836800	3.02076500
C	3.26189300	1.65384900	-0.33772200	C	-2.69569300	1.11746800	4.05629300
C	6.80909300	2.79860800	-0.90126900	C	-2.47462800	-1.18059200	3.33844300
H	7.63943700	2.54533400	-1.55218100	C	-2.46795500	0.72922500	5.37731600
C	6.92972000	3.79713200	0.03325200	H	-2.88399600	2.16448900	3.83568700
H	7.85721000	4.34865100	0.12931100	C	-2.24107000	-1.56876600	4.65808100

H	-2.46292600	-1.92757000	2.55099900	C	-0.04579500	4.50531000	0.83669400
C	-2.23349100	-0.61376100	5.67712000	C	-0.32536400	5.74081600	1.42710500
H	-2.47325500	1.47037900	6.16770100	H	0.20089400	6.62473900	1.08033500
H	-2.06618300	-2.61273000	4.89237300	C	-1.27491400	5.83554800	2.44268200
H	-2.05149100	-0.91569300	6.70185100	H	-1.48445700	6.79117800	2.90733500
I4				C	-1.96660900	4.69336800	2.83968700
				H	-2.72885100	4.75716400	3.60981400
				C	-1.71188500	3.44402400	2.25696700
				C	-2.56501600	2.27625800	2.63221600
				C	-3.86635800	2.20332100	2.09121500
				C	-4.67948200	1.11441300	2.42078800
				H	-5.68862500	1.06815800	2.01664700
				C	-4.23889100	0.10498600	3.28346800
				C	-2.95359900	0.20470700	3.82090300
				H	-2.59853600	-0.56499900	4.50066800
				C	-2.10823300	1.27864900	3.51157800
				C	-4.38905000	3.29503000	1.18682400
				H	-5.36989200	3.03021100	0.78450100
				H	-3.71212500	3.47260600	0.34435500
				H	-4.49000700	4.24223100	1.72590900
				C	-5.14707600	-1.05061100	3.62587800
				H	-4.72898600	-1.65587700	4.43391000
				H	-5.29695700	-1.70683500	2.75817200
				H	-6.13365500	-0.69741900	3.94026100
				C	-0.72989300	1.35732600	4.11915600
				H	0.03765400	1.25813300	3.34278900
				H	-0.58475400	0.56145800	4.85374800
				H	-0.57282300	2.31974400	4.61651100
				C	4.52523500	0.96007000	0.14546600
				C	5.66336900	0.81309600	-0.65249700
				H	5.59356200	0.35955000	-1.63576900
				C	6.90667200	1.25244100	-0.18773100
				H	7.78558000	1.13443700	-0.81060500
G_{gas} = -3958.455414 a. u.							
E_{gas} = -3959.555686 a. u.							
Ru	1.51660400	2.34794700	-1.00973200				
S	-0.22919000	1.71115900	0.58683800				
P	2.82770700	0.50389200	-0.46805600				
C	0.94845400	4.41023600	-0.27252200				
C	0.46810300	4.33580400	-1.62989400				
C	1.40119300	4.04175200	-2.65208100				
H	1.04604200	3.93323800	-3.67127600				
C	2.77841900	3.83051800	-2.37386800				
C	3.22044500	4.00113900	-1.03077300				
H	4.27064100	3.83861100	-0.80324300				
C	2.34573800	4.36489100	0.02206800				
C	-0.99611200	4.51286100	-1.92994700				
H	-1.33799200	5.50447400	-1.61651900				
H	-1.59962200	3.76704200	-1.40134700				
H	-1.18691200	4.39954300	-2.99919100				
C	3.75736300	3.49620600	-3.46713000				
H	4.17389400	4.40673500	-3.91064700				
H	3.27486300	2.92317900	-4.26262800				
H	4.58913900	2.90538500	-3.07297900				
C	2.85643400	4.59064700	1.41974000				
H	2.78063300	5.64829800	1.69348900				
H	3.90445100	4.29326400	1.49807400				
H	2.27210000	4.02345800	2.15021800				
C	-0.71513100	3.34490300	1.26988200				

C	7. 01734400	1. 83386100	1. 07509200	C	-0. 25156700	-3. 37002900	-2. 40079100
H	7. 98228900	2. 17002100	1. 43526200	C	0. 60308300	-3. 56852600	-1. 27431900
C	5. 88125100	1. 98213200	1. 87545800	C	1. 74582600	-2. 71693200	-1. 09751700
H	5. 96326300	2. 43344000	2. 85778400	C	-1. 35159900	-4. 25139400	-2. 60616700
C	4. 63865700	1. 55215600	1. 40980600	H	-1. 97225100	-4. 11250700	-3. 48574100
H	3. 75322700	1. 69310300	2. 02481200	C	-1. 61647300	-5. 26615500	-1. 71921500
C	2. 14623300	-0. 63446200	0. 88469800	H	-2. 44522500	-5. 94319200	-1. 89381000
H	2. 16833100	-0. 07020100	1. 82075100	C	-0. 79460200	-5. 43969900	-0. 57516400
H	1. 09466700	-0. 76583900	0. 61969100	H	-1. 01211900	-6. 23772000	0. 12599800
C	2. 89051900	-1. 93315200	0. 97804300	C	0. 28601800	-4. 61770000	-0. 36066400
C	3. 82529800	-2. 11629600	2. 03428000	H	0. 91184100	-4. 75924400	0. 51295900
H	3. 95863300	-1. 31608900	2. 75541100	H	0. 91044400	1. 26554500	-1. 98002900
C	4. 54944200	-3. 27520900	2. 14164700	Si	-2. 04343300	-0. 18863300	-0. 10508600
H	5. 25513700	-3. 41239500	2. 95429400	H	-2. 33771700	-0. 12659900	1. 33678000
C	4. 40672200	-4. 30931100	1. 17824200	H	-0. 77067200	-0. 74406300	-0. 65257000
C	3. 48882500	-4. 13631000	0. 09805400	C	-2. 92658400	0. 84087500	-1. 40914700
C	2. 70424200	-2. 93482300	0. 03057800	C	-2. 21570300	1. 18645500	-2. 56960300
C	5. 17968800	-5. 50048800	1. 25650300	C	-4. 27884500	1. 19339700	-1. 31114800
H	5. 86662500	-5. 61755800	2. 08827400	C	-2. 85162600	1. 85480700	-3. 61657200
C	5. 06858400	-6. 47561200	0. 29628900	H	-1. 16163900	0. 93153400	-2. 64974600
H	5. 66319700	-7. 37889500	0. 36087100	C	-4. 91609900	1. 86174100	-2. 35744600
C	4. 18120700	-6. 29458100	-0. 79414700	H	-4. 84330100	0. 93022000	-0. 42106800
H	4. 11335700	-7. 05886700	-1. 55934300	C	-4. 20363300	2. 18937900	-3. 51309400
C	3. 41384400	-5. 15834900	-0. 89287600	H	-2. 29543400	2. 11163800	-4. 51178500
H	2. 74790700	-5. 02904200	-1. 73734800	H	-5. 96523500	2. 12211200	-2. 27332200
C	3. 16828700	-0. 77519800	-1. 82316600	H	-4. 70040100	2. 70311700	-4. 32827700
H	3. 38348500	-0. 22497900	-2. 74222600	C	-0. 12184900	-2. 50057500	2. 95158000
H	4. 05207000	-1. 34758000	-1. 52564700	C	-0. 88093200	-2. 48995600	1. 78321400
C	1. 97857500	-1. 67987000	-1. 99568100	C	-2. 22021000	-2. 90539800	1. 80010500
C	1. 09652300	-1. 47365800	-3. 09027000	C	-2. 76897800	-3. 37409400	3. 00601200
H	1. 30172700	-0. 65814200	-3. 77577400	C	-2. 01413100	-3. 37038400	4. 17657400
C	0. 02444000	-2. 30404000	-3. 29963800	C	-0. 68994400	-2. 92810900	4. 15311000
H	-0. 61680500	-2. 16644900	-4. 16541400	H	0. 91875300	-2. 19798100	2. 91495200

H	-0.41625200	-2.21385600	0.84569200	C	1.11311800	-4.16109900	1.16373800
H	-3.79328600	-3.72733000	3.03734900	H	0.55964400	-4.49412000	2.03516500
H	-2.45643200	-3.71981800	5.10209000	C	2.21052600	-3.31636100	1.32324100
H	-0.09876400	-2.93581200	5.06126100	C	3.36392300	-2.98567800	-2.37892000
C	-3.07938700	-2.92318300	0.59044400	H	4.26514500	-3.60403900	-2.45045600
N	-3.10129500	-1.94347500	-0.27432200	H	3.67784100	-1.94028500	-2.35226100
C	-3.96320700	-4.13814600	0.43551500	H	2.76808900	-3.14484600	-3.27953800
H	-4.90168300	-4.01453200	0.98797400	C	-0.48919500	-5.52924300	-0.27223300
H	-4.21358400	-4.31206100	-0.61070000	H	-0.15695300	-6.56205300	-0.11981200
H	-3.44765200	-5.01066700	0.83820400	H	-0.93876000	-5.45893300	-1.26491400
C	-4.06231900	-1.94321000	-1.35633800	H	-1.26472000	-5.31068100	0.46524400
C	-5.42777400	-1.91462800	-1.06509700	C	2.65548800	-2.84664700	2.68172700
C	-3.61572400	-1.81943900	-2.67119500	H	3.68576000	-3.16118100	2.87573800
C	-6.35154500	-1.78157400	-2.10110800	H	2.01516200	-3.25824200	3.46340800
H	-5.76035600	-1.95711500	-0.03275700	H	2.63348300	-1.75446100	2.75828500
C	-4.54321900	-1.68154900	-3.70193400	C	3.50302800	-0.39799900	0.30674100
H	-2.55118600	-1.78889700	-2.86881700	C	3.90238400	-1.74197800	0.25307600
C	-5.91098700	-1.66427700	-3.41997100	C	5.26934400	-2.03642500	0.26087800
H	-7.41076400	-1.75418400	-1.87559900	H	5.58570400	-3.07329800	0.22203000
H	-4.19686500	-1.56787100	-4.72217400	C	6.21129700	-1.00887500	0.29734600
H	-6.62871300	-1.54753900	-4.22279800	H	7.26851000	-1.24434000	0.29981600

I5

$$G_{\text{gas}} = -2841.49823 \text{ a. u.}$$

$$E_{\text{gas}} = -2842.27725787 \text{ a. u.}$$

Ru	0.79565100	-2.17870100	-0.33536200	C	5.79205500	0.31932700	0.31410600
S	1.68524700	-0.01434700	0.42415600	H	6.51669000	1.12621400	0.31895500
P	-1.46805100	-1.51492800	-0.16195400	C	4.42801200	0.64880200	0.32280400
C	2.88761700	-2.83064900	0.13287900	C	4.00267400	2.07875400	0.30729100
C	2.57308600	-3.35394000	-1.15271000	C	3.78470700	2.71981500	-0.92607100
C	1.44365000	-4.22929300	-1.26198400	C	3.45742600	4.07921500	-0.92926000
H	1.15698200	-4.59557300	-2.24080200	H	3.31562900	4.58512900	-1.88110400
C	0.68079600	-4.59460400	-0.13715300	C	3.33342800	4.80550300	0.25823900
				C	3.52014200	4.13589600	1.47174000
				H	3.41086500	4.68368900	2.40324000
				C	3.85783300	2.78207700	1.51726400
				C	3.90677100	1.95936500	-2.22680200

H	3. 74572500	2. 62239300	-3. 07978500	C	-6. 99649700	2. 10604000	0. 63793300
H	3. 17138400	1. 14482100	-2. 29298500	H	-7. 83625200	1. 74106500	1. 22006200
H	4. 89589600	1. 50297500	-2. 33486200	C	-7. 16084100	3. 12526200	-0. 26724100
C	3. 03378300	6. 28289500	0. 24430900	H	-8. 13357300	3. 58075600	-0. 40846100
H	3. 93457100	6. 86282200	0. 47143100	C	-6. 05532900	3. 58048300	-1. 02947800
H	2. 28011100	6. 53695300	0. 99475900	H	-6. 19679500	4. 37579200	-1. 75168200
H	2. 66991100	6. 60991500	-0. 73341900	C	-4. 81125100	3. 02045100	-0. 86325100
C	4. 06347200	2. 08262300	2. 83852600	H	-3. 97480300	3. 37250900	-1. 45514000
H	5. 08248800	1. 69291100	2. 93099100	C	-2. 08269000	-0. 43029400	-1. 58813000
H	3. 37967300	1. 23235300	2. 94449100	H	-1. 73064500	-0. 88087700	-2. 51779400
H	3. 88489000	2. 76530800	3. 67124500	H	-3. 17605800	-0. 44109300	-1. 56671000
C	-2. 69970100	-2. 90040800	-0. 06357300	C	-1. 53847200	0. 96243900	-1. 40891300
C	-3. 22445100	-3. 44146300	-1. 24229000	C	-0. 40348700	1. 38319500	-2. 15679100
H	-2. 95905200	-3. 01728500	-2. 20585000	H	0. 02761700	0. 69864300	-2. 88155500
C	-4. 09271100	-4. 53353900	-1. 18645100	C	0. 12108900	2. 64351900	-1. 99061200
H	-4. 49922600	-4. 94538700	-2. 10259500	H	0. 97159800	2. 97256700	-2. 58092100
C	-4. 44257300	-5. 08764900	0. 04595600	C	-0. 45430600	3. 54893700	-1. 05695800
H	-5. 12050100	-5. 93157900	0. 08855400	C	-1. 57771300	3. 13135800	-0. 28107600
C	-3. 92221300	-4. 54890500	1. 22455600	C	-2. 12698300	1. 82302700	-0. 48976800
H	-4. 19652100	-4. 97290300	2. 18347900	C	0. 05415400	4. 86599400	-0. 89103100
C	-3. 04925400	-3. 46060800	1. 17042900	H	0. 89012500	5. 17795700	-1. 50744800
H	-2. 64161700	-3. 05938600	2. 09298600	C	-0. 50587900	5. 72629100	0. 02139500
C	-1. 87007300	-0. 39947800	1. 32237600	H	-0. 12101200	6. 73353200	0. 13051800
H	-1. 83513600	-1. 01676600	2. 22339600	C	-1. 59400100	5. 29937300	0. 82374400
H	-1. 04142900	0. 31202100	1. 38271200	H	-2. 01927600	5. 97903200	1. 55254600
C	-3. 19328300	0. 29483900	1. 16407200	C	-2. 11666200	4. 03668000	0. 67820800
C	-4. 32136000	-0. 16826900	1. 89275400	H	-2. 95309500	3. 71951400	1. 28923100
H	-4. 19720600	-0. 99657300	2. 58226900	H	0. 61576700	-1. 51082700	-1. 73039300
C	-5. 54785900	0. 42496100	1. 73970000	H	1. 57381500	0. 90345700	-0. 59941100
H	-6. 40436800	0. 07521300	2. 30629900				
C	-5. 72390600	1. 50055700	0. 82892600	I6			
C	-4. 60364400	1. 97191500	0. 07946400	$G_{\text{gas}} = -2841.492706 \text{ a. u.}$			
C	-3. 32178300	1. 36106300	0. 28224600	$E_{\text{gas}} = -2842.271362 \text{ a. u.}$			

Ru	0.88520100	-2.30719900	-0.64867900	C	4.31083000	2.62097700	-0.79954200
S	1.67766500	-0.02841300	-0.30826500	C	4.07451600	3.95740300	-1.13011200
P	-1.31276600	-1.47106300	-0.39341200	H	4.49195300	4.35522300	-2.05127000
C	2.72093500	-2.78180100	0.62461900	C	3.33619900	4.79803300	-0.29149800
C	2.89365500	-3.56813600	-0.54822800	C	2.78653500	4.25988700	0.87499600
C	1.85380800	-4.47574400	-0.91542300	H	2.18171400	4.89208900	1.51891600
H	1.95386300	-5.02875400	-1.84406800	C	2.99865400	2.92689500	1.23690500
C	0.70424800	-4.68388100	-0.11904000	C	5.11352600	1.73400500	-1.72053300
C	0.58154100	-3.90793200	1.06762800	H	5.37823100	2.26506200	-2.63728100
H	-0.31023200	-4.02790100	1.67524800	H	4.54187100	0.83948400	-1.99468900
C	1.56043700	-2.96572300	1.46429500	H	6.04023600	1.39385800	-1.24656100
C	4.10842000	-3.40269800	-1.42084300	C	3.17337500	6.26124200	-0.62072100
H	4.97387200	-3.89320500	-0.96395100	H	4.05665000	6.82885800	-0.30844000
H	4.36025700	-2.34704800	-1.54694400	H	2.30882300	6.68792300	-0.10545100
H	3.94575700	-3.84829500	-2.40414000	H	3.04946600	6.41990100	-1.69636700
C	-0.33907700	-5.69871900	-0.49452200	C	2.38478300	2.37164800	2.49878700
H	-0.05696400	-6.68475100	-0.11025100	H	3.13549100	1.89239400	3.13525500
H	-0.44316900	-5.77729800	-1.57915700	H	1.62604500	1.61710100	2.25537900
H	-1.31414000	-5.43955300	-0.07500200	H	1.90024900	3.16228700	3.07540700
C	1.40164400	-2.15709600	2.72148000	C	-2.51354200	-2.88547500	-0.34126300
H	2.24731300	-2.33075900	3.39351400	C	-2.90933700	-3.47168900	-1.54976400
H	0.48309600	-2.43026700	3.24563300	H	-2.55320500	-3.07303600	-2.49539800
H	1.37737900	-1.08510200	2.49704300	C	-3.76586900	-4.57337900	-1.54703700
C	3.27261000	-0.36508000	0.54755300	H	-4.07516600	-5.01773900	-2.48554500
C	3.65158000	-1.66152000	0.92499200	C	-4.22837000	-5.09704000	-0.33760200
C	4.87259400	-1.89211600	1.56493500	H	-4.89694000	-5.94936300	-0.33613300
H	5.14891300	-2.90327000	1.84712300	C	-3.83465700	-4.51595500	0.86931500
C	5.72023700	-0.82121800	1.84010300	H	-4.19970100	-4.91354700	1.80891800
H	6.66628600	-0.98926600	2.33947400	C	-2.97826300	-3.41199000	0.86845900
C	5.34241000	0.46746700	1.46365600	H	-2.68705700	-2.96360900	1.81248500
H	5.99713000	1.30898300	1.66512100	C	-1.59248600	-0.43254000	1.15959900
C	4.12518300	0.71731500	0.81476400	H	-1.46748200	-1.08254300	2.03030100
C	3.78664700	2.11308000	0.40381400	H	-0.76380100	0.28353800	1.15395800

C	-2.93904200	0.24017000	1.13918900
C	-3.98382100	-0.25189300	1.96734300
H	-3.77890700	-1.07622800	2.64218300
C	-5.22965300	0.31917000	1.94273000
H	-6.01930000	-0.05080000	2.58809300
C	-5.51225500	1.40071600	1.06676800
C	-4.47438200	1.90908900	0.22856000
C	-3.16540200	1.32515300	0.30041700
C	-6.80886000	1.98127400	1.00419800
H	-7.58479100	1.58849900	1.65294000
C	-7.07446300	3.01308400	0.13809400
H	-8.06473600	3.45028200	0.09491900
C	-6.05151000	3.50714900	-0.71038100
H	-6.27310300	4.31372000	-1.39907600
C	-4.78633500	2.97186400	-0.66815000
H	-4.01243700	3.35489300	-1.32232100
C	-1.98620500	-0.33168800	-1.74846700
H	-1.66959700	-0.72660300	-2.71652800
H	-3.07646600	-0.39727600	-1.67914700
C	-1.49378500	1.07492300	-1.53737200
C	-0.43930600	1.57526900	-2.34484900
H	-0.01695500	0.93850100	-3.11606500
C	0.04339000	2.84491000	-2.15826900
H	0.85323700	3.22512500	-2.77158100
C	-0.49619500	3.67948800	-1.14469600
C	-1.53846900	3.18183900	-0.30610400
C	-2.05010100	1.86301600	-0.53792700
C	-0.02185400	5.00598000	-0.95341100
H	0.75733100	5.37395800	-1.61243600
C	-0.53510000	5.79966000	0.04253800
H	-0.17643100	6.81409000	0.17552700
C	-1.53903900	5.29230500	0.90628200
H	-1.92600900	5.91862800	1.70141900

C	-2.02868500	4.01924500	0.73810900
H	-2.79997800	3.64299500	1.39935400
H	0.45007500	-2.10989400	-2.38152600
H	1.13120600	-1.65764000	-2.29982900

I7

$$G_{\text{gas}} = -3747.501838 \text{ a. u.}$$

$$E_{\text{gas}} = -3748.50302295 \text{ a. u.}$$

Ru	-0.02710300	-1.64822700	-1.78879000
S	1.28053100	-1.39295000	0.27475000
P	-1.98771400	-1.17742400	-0.63068500
C	1.38667400	-3.38506100	-2.08552900
C	1.76789400	-2.43076500	-3.09770000
C	0.77903300	-1.98419900	-4.00059700
H	1.03617900	-1.22328000	-4.72962600
C	-0.55434500	-2.47502400	-3.95614800
C	-0.86077700	-3.48567300	-3.00230100
H	-1.87436800	-3.87375600	-2.95762300
C	0.10006200	-4.00624900	-2.09715000
C	3.18131200	-1.92130800	-3.18161000
H	3.83377000	-2.68204500	-3.62444000
H	3.58356800	-1.68471000	-2.19289100
H	3.23164700	-1.02201300	-3.79933300
C	-1.58575400	-1.99993900	-4.94320900
H	-1.52185000	-2.57298900	-5.87436700
H	-1.43872900	-0.94503200	-5.18702000
H	-2.59708400	-2.12511400	-4.54778100
C	-0.26955500	-5.08824600	-1.11828100
H	0.14535600	-6.05281000	-1.43075500
H	-1.35618200	-5.18843200	-1.04538400
H	0.11651900	-4.86947000	-0.11909400
C	2.41902900	-2.84757000	0.13846500
C	2.34882200	-3.68985600	-0.98367800

C	3.17832800	-4.81289700	-1.05950500	H	-3.90174900	-6.14365500	1.51317100
H	3.11740700	-5.45861100	-1.92945800	C	-2.53663100	-4.49402000	1.75654000
C	4.06988500	-5.09810000	-0.02674600	H	-2.07580200	-4.89926800	2.65046900
H	4.70874200	-5.97083800	-0.08657700	C	-2.10034500	-3.27207100	1.24467600
C	4.12758500	-4.26341300	1.08733200	H	-1.28988500	-2.73859100	1.73352700
H	4.80840100	-4.48518500	1.90237800	C	-1.88463800	0.02543400	0.82270300
C	3.30665800	-3.13172600	1.19140300	H	-1.24645700	-0.42776800	1.58511400
C	3.37621300	-2.25968300	2.40247600	H	-1.35735700	0.90183800	0.43233300
C	4.46183400	-1.38333700	2.58234800	C	-3.25087700	0.36502800	1.34853100
C	4.46562400	-0.52326800	3.68702100	C	-3.71303400	-0.25634600	2.54030400
H	5.29803600	0.16260300	3.81812400	H	-3.04831800	-0.93391600	3.06611900
C	3.43288000	-0.53106100	4.62644500	C	-4.97181700	-0.00661900	3.02289700
C	2.39205500	-1.45194900	4.45959200	H	-5.31612100	-0.47737400	3.93786000
H	1.60059800	-1.49925600	5.20248400	C	-5.85512700	0.86122700	2.32679500
C	2.34973800	-2.32068000	3.36747400	C	-5.41315600	1.48561500	1.12133200
C	5.63379100	-1.37446000	1.62745800	C	-4.07984800	1.23916000	0.65424400
H	6.17823700	-0.42840300	1.69597600	C	-7.17459800	1.10756000	2.79698200
H	5.31877400	-1.52240000	0.58993400	H	-7.49350300	0.63040700	3.71796700
H	6.33935600	-2.17889200	1.86462300	C	-8.02895200	1.92500100	2.09883700
C	3.42787600	0.43656000	5.78328200	H	-9.03317500	2.10634300	2.46285100
H	2.97147500	-0.00903800	6.67073600	C	-7.60048600	2.52961300	0.88991500
H	2.85611000	1.33795900	5.53429000	H	-8.28522600	3.16266600	0.33794100
H	4.44177300	0.75021700	6.04276800	C	-6.32931100	2.31621100	0.41260300
C	1.24631500	-3.34469200	3.25632800	H	-6.01205600	2.77838500	-0.51488200
H	0.78160200	-3.33016600	2.26636100	C	-3.42146500	-0.41756100	-1.60717100
H	0.47190300	-3.16250000	4.00591300	H	-3.42528500	-0.86870500	-2.60244500
H	1.63907700	-4.35547900	3.41498600	H	-4.34759500	-0.68042200	-1.08729400
C	-2.69227800	-2.73877400	0.09340300	C	-3.24362000	1.07471800	-1.68546400
C	-3.72155700	-3.43885900	-0.54330900	C	-2.69633300	1.65269900	-2.86135100
H	-4.19501200	-3.03421000	-1.43296900	H	-2.44271000	1.00091300	-3.69134300
C	-4.15390800	-4.66624100	-0.03249500	C	-2.49166000	3.00556400	-2.95134100
H	-4.95591200	-5.20268600	-0.52609400	H	-2.07984400	3.44440500	-3.85428200
C	-3.56260800	-5.19416500	1.11641600	C	-2.81197100	3.85726600	-1.86052800

C	-3.35613800	3.29150100	-0.66825000	H	5.49769900	8.20468000	-1.00264500
C	-3.57190600	1.87594600	-0.59909900	C	4.81799600	2.91048400	-0.70651400
C	-2.57792800	5.25976000	-1.92334700	C	5.99101600	1.97148600	-0.73045300
H	-2.17215600	5.67626100	-2.83978200	H	5.65354200	0.94222000	-0.61283800
C	-2.85901500	6.06982100	-0.84970600	H	6.52825700	2.06273100	-1.67968200
H	-2.68077800	7.13711900	-0.90700500	H	6.69439600	2.21266800	0.07179500
C	-3.38847100	5.50868200	0.34126000	O	3.64724000	2.46747500	-0.61313400
H	-3.60478100	6.15351300	1.18509800	H	3.78736300	0.16583900	0.53937900
C	-3.63028000	4.15806800	0.43021300	H	2.54390400	0.49212300	-1.65896000
H	-4.02900300	3.73608500	1.34508500				
H	-0.06929200	-0.06907100	-1.90780500	TS_{I2-I3}			
Si	2.56556200	0.60179800	-0.18095600	G_{gas} = -3362.954717 a. u.			
C	1.31674100	1.69855400	0.69508000	E_{gas} = -3363.82853637 a. u.			
C	1.01718300	1.47888400	2.04766900	Ru	-0.96394000	-1.44034500	0.74180100
C	0.65351400	2.72021300	-0.00140800	S	-1.52781300	0.13164000	-1.03841000
C	0.06075300	2.26740500	2.69201500	P	1.24575400	-1.52149700	-0.04127000
H	1.51546300	0.68028900	2.59413200	C	-3.13114500	-2.07120000	0.44065000
C	-0.30175100	3.50794800	0.64384300	C	-3.03103800	-1.93227300	1.85585500
H	0.88122000	2.90043300	-1.04794600	C	-1.98447400	-2.64046100	2.51429200
C	-0.60258000	3.27547300	1.98904500	H	-1.82385600	-2.46165100	3.57244800
H	-0.17016800	2.09040500	3.73648200	C	-1.15263800	-3.55682600	1.82783600
H	-0.81521300	4.29463000	0.10153700	C	-1.43949200	-3.83145600	0.45280500
H	-1.35464400	3.88139600	2.48177000	H	-0.83623400	-4.56813400	-0.07061600
C	4.09331000	6.59555800	-0.72342400	C	-2.41554400	-3.12161800	-0.25299300
C	3.92256600	5.21768500	-0.64985400	C	-3.98180800	-1.06486200	2.63299200
C	5.02944300	4.36475500	-0.79463400	H	-4.91238100	-1.61713600	2.80803400
C	6.30568100	4.90751700	-1.01118200	H	-4.23545900	-0.15141400	2.09217500
C	6.47066300	6.28754400	-1.08862700	H	-3.56283900	-0.78344600	3.60101700
C	5.36604700	7.13054900	-0.94476300	C	-0.06215200	-4.31151200	2.53883500
H	3.24134400	7.25380400	-0.60607400	H	-0.43644700	-5.27230200	2.90748800
H	2.94641500	4.78105800	-0.46997900	H	0.31345800	-3.74570900	3.39487700
H	7.16837800	4.26082600	-1.12336200	H	0.77152300	-4.51757300	1.86112100
H	7.45489600	6.70577000	-1.25931300	C	-2.67012700	-3.36955400	-1.71378300

H	-3.72122500	-3.62274600	-1.88268900	C	2.40615700	-4.08641600	-0.53585000
H	-2.04842500	-4.18864400	-2.08002500	H	2.97714300	-3.95030000	0.37676600
H	-2.45527600	-2.47391400	-2.30868900	C	2.54106400	-5.27602400	-1.25952500
C	-3.37064500	-0.07964900	-1.06361100	H	3.21041700	-6.04931300	-0.90183600
C	-3.97611400	-1.13224900	-0.35535600	C	1.82577800	-5.46169800	-2.44200000
C	-5.36403800	-1.29082500	-0.40683400	H	1.93626600	-6.38162700	-3.00342100
H	-5.82663100	-2.10615600	0.13976500	C	0.97086100	-4.45722700	-2.90720900
C	-6.14155000	-0.40831900	-1.15517100	H	0.42107000	-4.59617700	-3.83111800
H	-7.21648200	-0.53452000	-1.19719400	C	0.82723000	-3.27408800	-2.18391400
C	-5.53184900	0.63555300	-1.84662400	H	0.14715500	-2.50099700	-2.53559000
H	-6.12901000	1.33121400	-2.42608000	C	1.73628900	-0.14204200	-1.24336800
C	-4.14148900	0.82145700	-1.81314000	H	1.22227700	-0.34395100	-2.18635600
C	-3.52641300	1.96924500	-2.54173800	H	1.32570500	0.78368800	-0.83009600
C	-3.66506200	3.27208100	-2.02666000	C	3.22571700	-0.06008400	-1.41649300
C	-3.06795900	4.33554300	-2.71079200	C	3.82345600	-0.57129400	-2.59911500
H	-3.16243100	5.33978200	-2.30722600	H	3.18610700	-0.99985900	-3.36569100
C	-2.36308800	4.14097200	-3.90026100	C	5.18223900	-0.51564400	-2.77564600
C	-2.25949300	2.84124300	-4.40539400	H	5.63664500	-0.89679700	-3.68406600
H	-1.72661200	2.67460400	-5.33740300	C	6.02198000	0.03556100	-1.77090900
C	-2.82969300	1.75040100	-3.74689200	C	5.43801100	0.53463800	-0.56684200
C	-4.46668300	3.55187200	-0.77553600	C	4.01333300	0.48852400	-0.41280200
H	-4.11298500	4.46528800	-0.29032000	C	7.43403100	0.08474900	-1.93320800
H	-4.40218500	2.73233400	-0.05485000	H	7.86279800	-0.29190400	-2.85602200
H	-5.52786300	3.69304600	-1.01209400	C	8.23785600	0.59384800	-0.94320600
C	-1.75882400	5.30663700	-4.64224700	H	9.31270100	0.62820400	-1.07441900
H	-0.83774300	5.01628700	-5.15391300	C	7.66239500	1.07178300	0.26138700
H	-1.52751100	6.13097500	-3.96349300	H	8.30526000	1.46166400	1.04165900
H	-2.45154800	5.68688300	-5.40084700	C	6.30095100	1.04207900	0.44742500
C	-2.70092800	0.36522400	-4.33601200	H	5.87120900	1.40663800	1.37286100
H	-3.64335100	-0.18732800	-4.27305200	C	2.62735400	-1.41365500	1.24324100
H	-1.93736300	-0.22050700	-3.80878600	H	2.36616800	-2.06939800	2.07774200
H	-2.40917600	0.42158300	-5.38706100	H	3.54639000	-1.77193300	0.77056300
C	1.54582900	-3.08606300	-0.99521800	C	2.74915400	0.02337600	1.67766600

C	2.16368800	0.43216600	2.90436800	E_{gas} = -3959.51232369 a. u.			
H	1.73339400	-0.32573500	3.55144200	Ru	0.66837300	-2.57043900	0.28243500
C	2.15697300	1.75215200	3.27861000	S	-0.81991900	-0.56069100	-0.11613000
H	1.70349200	2.05825600	4.21604100	P	2.70286300	-1.42984600	0.52176500
C	2.73703300	2.74097900	2.43885000	C	-0.64324600	-3.41273900	-1.33436200
C	3.35563800	2.34244100	1.21429300	C	-1.05379300	-4.14454000	-0.16395100
C	3.36758200	0.95519700	0.85309700	C	-0.06741300	-4.82178700	0.58181500
C	2.71527100	4.11848100	2.79221800	H	-0.35461400	-5.31417900	1.50473400
H	2.24730400	4.40641000	3.72785700	C	1.29263700	-4.85963200	0.17495800
C	3.27400900	5.06346200	1.96723300	C	1.62611400	-4.24962100	-1.06594500
H	3.25455400	6.11086400	2.24349100	H	2.65709600	-4.30385600	-1.40337200
C	3.87788500	4.67179500	0.74532500	C	0.67550600	-3.57472200	-1.87346800
H	4.30935500	5.42587800	0.09789600	C	-2.49411900	-4.20601800	0.24207900
C	3.91818000	3.34836800	0.37673800	H	-3.01938700	-4.96365900	-0.35125700
H	4.37872800	3.05601100	-0.55963100	H	-2.99771700	-3.25682700	0.06760600
Si	-1.21484500	1.37525400	1.06060700	H	-2.59803800	-4.46535200	1.29807400
H	-2.13298400	2.42163700	0.49773000	C	2.31341500	-5.62174200	0.97457200
H	-0.18839300	-0.43170700	1.67101900	H	2.21980600	-6.69555000	0.77913500
H	0.20871800	1.78315800	0.87149800	H	2.17313100	-5.45708400	2.04569800
C	-1.82584300	1.33145900	2.86653900	H	3.33025000	-5.31791800	0.71623500
C	-2.90711000	2.17344800	3.17290700	C	1.07252000	-3.00172100	-3.20849200
C	-1.25534300	0.57327400	3.90135800	H	0.65901600	-3.60378300	-4.02491500
C	-3.41275300	2.24834200	4.47384700	H	2.15992800	-2.99613800	-3.31529600
H	-3.36134200	2.77368700	2.38926400	H	0.70338000	-1.98198500	-3.34133300
C	-1.74573100	0.65787100	5.20460100	C	-1.60298500	-1.09863400	-1.72235200
H	-0.42772400	-0.09251900	3.68444700	C	-1.55713400	-2.47245200	-2.05797900
C	-2.83274300	1.49074600	5.49081200	C	-2.19540600	-2.93761800	-3.20846500
H	-4.25316200	2.89731400	4.69069400	H	-2.16072800	-3.99770700	-3.43905200
H	-1.28610900	0.07691000	5.99666200	C	-2.80788700	-2.04007900	-4.08152500
H	-3.22022600	1.54936100	6.50127600	H	-3.28455000	-2.39476600	-4.98761800
TS_{I3-I4}				C	-2.72723500	-0.67817900	-3.81958000
				H	-3.10730500	0.03269700	-4.54431600
				C	-2.13046900	-0.16887900	-2.64717800
G_{gas} = -3958.40902 a. u.							

C	-2.03047500	1.32513100	-2.56500000	H	2.46647300	0.00900300	-1.38797300
C	-3.19662200	2.11855300	-2.70394500	C	4.53999000	0.27914400	-0.83988200
C	-3.08533600	3.50942400	-2.74395800	C	5.79706000	-0.15913000	-1.33936000
H	-3.99157200	4.10391400	-2.82168800	H	5.84347400	-1.08250800	-1.90639200
C	-1.85229300	4.15664800	-2.65104600	C	6.93451800	0.57774000	-1.14032500
C	-0.71039100	3.36656500	-2.53522300	H	7.88663100	0.24263700	-1.53810200
H	0.26660300	3.84082400	-2.48077400	C	6.89006300	1.78787000	-0.39899600
C	-0.77438100	1.96912600	-2.49775800	C	5.63817700	2.24831800	0.10911600
C	-4.59067900	1.53308900	-2.75592000	C	4.44744200	1.48715400	-0.15859300
H	-5.30491400	2.24467000	-2.33091900	C	8.07002100	2.54014900	-0.14659500
H	-4.66448100	0.60267300	-2.19093000	H	9.01054000	2.17777700	-0.54843700
H	-4.91383900	1.32142300	-3.78127900	C	8.02247100	3.69382500	0.59606400
C	-1.76022000	5.65974200	-2.61686000	H	8.92560200	4.26093100	0.78692000
H	-2.57816700	6.12375300	-3.17342800	C	6.78654400	4.14033600	1.12696400
H	-0.81349500	6.00811600	-3.03742500	H	6.75853500	5.04114700	1.72858800
H	-1.81650900	6.02240700	-1.58209800	C	5.62740500	3.43988600	0.89157100
C	0.54175300	1.24302100	-2.39184700	H	4.69258400	3.78897100	1.31228400
H	0.47456100	0.19709700	-2.70119500	C	2.93147300	-0.05009800	1.79739600
H	0.88385200	1.26686900	-1.35078300	H	2.40035000	-0.35840200	2.70027100
H	1.29977700	1.74078600	-3.00469400	H	4.00489900	-0.00930900	2.00779500
C	4.04853900	-2.62110000	1.01009800	C	2.42332000	1.27211100	1.29422400
C	4.13154500	-3.01117700	2.35254100	C	1.23125600	1.80739300	1.85286400
H	3.44384900	-2.59627300	3.08365700	H	0.72020600	1.23229800	2.61864800
C	5.08431300	-3.94772000	2.75444400	C	0.76706600	3.04079900	1.47786600
H	5.14499000	-4.24135900	3.79580700	H	-0.11248800	3.46833400	1.94867000
C	5.95679000	-4.50589800	1.81729800	C	1.43206600	3.78549100	0.46569200
H	6.69772600	-5.23177300	2.13014600	C	2.60225700	3.23896800	-0.14292700
C	5.87381600	-4.12462200	0.47741200	C	3.12664700	1.98778400	0.33367300
H	6.55147000	-4.55178400	-0.25261100	C	0.96823000	5.06826700	0.05932300
C	4.92108000	-3.18480800	0.07454600	H	0.10435000	5.49200300	0.56376500
H	4.86894200	-2.89699000	-0.96964200	C	1.60478600	5.76421600	-0.94026000
C	3.32341400	-0.57812300	-1.05305300	H	1.24935200	6.74389400	-1.23810200
H	3.49650200	-1.35641900	-1.80203400	C	2.72984900	5.19597600	-1.58998700

H	3.21511600	5.73964600	-2.39192900	H	-6.90659300	0.52414500	1.21794500
C	3.21802200	3.96994900	-1.19989300	H	-6.74536900	1.66892500	-0.12613400
H	4.08907700	3.55099700	-1.69005600	C	-4.78283400	-1.57584600	0.17297200
Si	-2.15675400	-0.64179300	1.89090600	C	-4.82868600	-1.99272100	-1.16188500
H	-0.78240900	-0.63973000	2.51348200	C	-5.31484600	-2.40051800	1.17049400
H	0.65466200	-2.27249800	1.82890400	C	-5.40857300	-3.21698900	-1.49391800
H	-2.72181000	-2.01282200	2.00633700	H	-4.39496900	-1.37186300	-1.93489600
C	-2.99652600	0.61486800	3.05016200	C	-5.88720500	-3.62771300	0.83299000
C	-4.26124100	0.37303400	3.60566000	H	-5.27697700	-2.09296900	2.20789900
C	-2.28761200	1.74370700	3.48231200	C	-5.93947700	-4.04008000	-0.49968500
C	-4.80813400	1.23840000	4.55393200	H	-5.43682300	-3.52450400	-2.53310800
H	-4.83247100	-0.49713700	3.30067100	H	-6.29689200	-4.25773800	1.61379200
C	-2.84061200	2.63060400	4.40651600	H	-6.39025400	-4.99052300	-0.75878100
H	-1.29982800	1.94256400	3.07862800	TS_{I4-I5} G_{gas} = -3958.415548 a. u. E_{gas} = -3959.50639925 a. u.			
C	-4.10277600	2.37716600	4.94616700				
H	-5.77998200	1.02517400	4.98493700				
H	-2.28639100	3.51201000	4.70873600	Ru	1.22184400	-2.38639600	-0.60146300
H	-4.53018500	3.05809300	5.67309100	S	-0.50644300	-0.69709300	-1.13050200
C	-2.49825900	3.68435300	0.58471200	P	2.72924800	-0.72854800	0.07642600
C	-3.01102700	2.40385900	0.38527500	C	0.32740400	-3.39797900	-2.40155900
C	-4.31156700	2.09035000	0.79208300	C	0.13853300	-4.33953100	-1.33818200
C	-5.07581600	3.07008600	1.44895500	C	1.28127400	-4.74997800	-0.60364800
C	-4.54428600	4.33373200	1.69103300	H	1.14560600	-5.40258400	0.25236600
C	-3.25875800	4.65023800	1.24220900	C	2.58722100	-4.32179200	-0.93918200
H	-1.51397000	3.91698900	0.19660400	C	2.74120000	-3.48991800	-2.09052300
H	-2.41155400	1.66373200	-0.12765800	H	3.74343200	-3.17618200	-2.36857200
H	-6.07633800	2.83754100	1.79640300	C	1.64679600	-3.05440700	-2.86459600
H	-5.13487000	5.07310300	2.21870600	C	-1.21483500	-4.88898000	-0.98643600
H	-2.85947700	5.64627100	1.40119600	H	-1.34513700	-5.87878300	-1.43923900
C	-4.89843200	0.76003900	0.51508800	H	-2.01460100	-4.24784600	-1.35985400
N	-4.16790600	-0.31748100	0.51474800	H	-1.32636600	-4.99026400	0.09561800
C	-6.38968900	0.71774900	0.26869900	C	3.77923000	-4.80792600	-0.16075500
H	-6.66249400	-0.08220700	-0.41996800				

H	3. 53231000	-4. 92339200	0. 89744300	H	-0. 43106400	0. 66128700	-4. 03815800
H	4. 61709900	-4. 11129500	-0. 23532200	H	0. 01371200	1. 72657100	-2. 69415300
H	4. 11060300	-5. 77998200	-0. 54187700	H	-0. 47227600	2. 42021800	-4. 24732200
C	1. 83845500	-2. 17881300	-4. 07459600	C	4. 31268900	-1. 46590100	0. 70914800
H	1. 48607600	-2. 68251500	-4. 98026000	C	4. 32085300	-1. 98810300	2. 00878700
H	2. 89460300	-1. 93511300	-4. 21003200	H	3. 43462500	-1. 90715400	2. 63250000
H	1. 27648000	-1. 24413600	-3. 98306600	C	5. 46095000	-2. 62236200	2. 50215000
C	-1. 32530100	-1. 50429100	-2. 58190000	H	5. 46312000	-3. 02094900	3. 50990500
C	-0. 84905600	-2. 74388800	-3. 04990500	C	6. 59894700	-2. 74100400	1. 70057000
C	-1. 45032900	-3. 34799300	-4. 15728100	H	7. 48511100	-3. 23113000	2. 08561100
H	-1. 07374200	-4. 30337900	-4. 50817000	C	6. 59350300	-2. 22421000	0. 40451600
C	-2. 51661200	-2. 72446600	-4. 80234400	H	7. 47575000	-2. 31019000	-0. 21904600
H	-2. 98216600	-3. 19156700	-5. 66158400	C	5. 45105500	-1. 59046000	-0. 09186700
C	-2. 96411200	-1. 48732900	-4. 34978500	H	5. 45728800	-1. 19827200	-1. 10234000
H	-3. 77219000	-0. 97912300	-4. 86478500	C	3. 20933900	0. 44649900	-1. 33292000
C	-2. 37831800	-0. 84887200	-3. 24357900	H	3. 71446800	-0. 14643100	-2. 10130200
C	-2. 89248900	0. 50500000	-2. 86854200	H	2. 24565900	0. 76759500	-1. 74479600
C	-4. 22990200	0. 64182800	-2. 43753600	C	4. 04446500	1. 60949000	-0. 87147000
C	-4. 75249600	1. 91974800	-2. 21250800	C	5. 43067700	1. 65293500	-1. 18471400
H	-5. 78070900	2. 01595000	-1. 87525500	H	5. 85345400	0. 87422000	-1. 81019300
C	-3. 99720800	3. 07048900	-2. 44435100	C	6. 22613300	2. 67449600	-0. 73560100
C	-2. 67355900	2. 91622400	-2. 86206700	H	7. 28002900	2. 70667800	-0. 99122300
H	-2. 06947200	3. 79848600	-3. 05347700	C	5. 68772400	3. 70554100	0. 07910400
C	-2. 10205700	1. 65870000	-3. 07143600	C	4. 29593700	3. 68742900	0. 39409100
C	-5. 13644100	-0. 55291000	-2. 22843200	C	3. 47230600	2. 63308600	-0. 12655200
H	-5. 86277500	-0. 34027000	-1. 43811000	C	6. 50669800	4. 75109500	0. 58718400
H	-4. 58241600	-1. 45549700	-1. 95469900	H	7. 56146900	4. 75329300	0. 33255200
H	-5. 70120700	-0. 79015300	-3. 13704100	C	5. 97623500	5. 73288400	1. 38720700
C	-4. 60082900	4. 44708700	-2. 32346300	H	6. 60636200	6. 52552500	1. 77244300
H	-4. 69643500	4. 91137000	-3. 31070800	C	4. 59813200	5. 70736100	1. 71886300
H	-3. 97597500	5. 10861100	-1. 71384500	H	4. 18998200	6. 47831500	2. 36170400
H	-5. 59517600	4. 40683600	-1. 87382600	C	3. 77939600	4. 71423100	1. 23651400
C	-0. 66878000	1. 60654200	-3. 54415200	H	2. 72879200	4. 70095600	1. 50073400

C	2.26321600	0.50389800	1.44027500	C	-4.35857900	2.25900600	2.27355300
H	1.72681700	-0.05498900	2.21180300	C	-5.50024300	1.50867100	1.94611600
H	3.20690500	0.87332400	1.85321200	C	-4.25499400	3.57752700	1.80573400
C	1.42346600	1.62753400	0.89509600	C	-6.51279200	2.06461400	1.16609300
C	0.02794600	1.64673900	1.16356900	H	-5.60289200	0.48658800	2.30226000
H	-0.39690600	0.85568900	1.77789600	C	-5.27356100	4.13833500	1.03149000
C	-0.76409900	2.65505800	0.67706000	H	-3.38453000	4.17833200	2.05766800
H	-1.82805800	2.69160700	0.89138700	C	-6.40102100	3.38206400	0.71217700
C	-0.21600800	3.68795100	-0.12592800	H	-7.39278800	1.47957600	0.92386100
C	1.17842100	3.67258800	-0.42446400	H	-5.18973100	5.16279600	0.68694900
C	2.00040000	2.63423200	0.13087700	H	-7.19686700	3.81869800	0.11853800
C	-1.03181600	4.73589300	-0.63279100	N	-2.46634000	-0.07544000	2.94714100
H	-2.08942500	4.72702700	-0.38321900	C	-3.39629300	-2.14177400	1.98197300
C	-0.49812400	5.71831200	-1.43034900	C	-3.92386200	-2.57135200	3.21064200
H	-1.12434100	6.51591000	-1.81375000	C	-3.39607700	-3.02250600	0.89101300
C	0.88026000	5.68481800	-1.76361300	C	-4.45743500	-3.85076300	3.33689300
H	1.29193900	6.45298400	-2.40747800	H	-3.92250000	-1.89369500	4.05743100
C	1.69695200	4.69233000	-1.27507700	C	-3.93397900	-4.30151600	1.02015700
H	2.74886100	4.67954900	-1.53334400	H	-2.95882600	-2.70380500	-0.05119300
H	0.86298700	-2.32203600	0.92228600	C	-4.46762200	-4.71772500	2.24146800
C	-0.41619000	-1.14962200	5.89947000	H	-4.87036800	-4.17051600	4.28596100
C	-1.41399100	-0.51869700	5.15422300	H	-3.93621000	-4.97510400	0.17041800
C	-1.49685200	-0.73628200	3.77333200	H	-4.88762100	-5.71164900	2.34000300
C	-0.56878900	-1.58839700	3.15857800	H	-3.65869400	1.40143900	4.79428000
C	0.41288100	-2.22673000	3.91139200	H	-1.87282400	2.49940900	3.54004500
C	0.49825100	-2.00727500	5.28822100	C	-3.01384900	-0.13354600	0.57976100
H	-0.36428300	-0.97374400	6.96736600	H	-1.75363100	-0.54854200	-0.12622400
H	-2.12809100	0.11881200	5.66040900	H	-3.70410000	-0.54164200	-0.15071000
H	-0.61565400	-1.74705400	2.08591700	H	-2.81775500	0.92918400	0.47753900
H	1.11006700	-2.89137400	3.41071200				
H	1.26315200	-2.49829200	5.87720600				
C	-2.93954400	-0.74134100	1.81996500				
Si	-3.04819500	1.58667600	3.44394400				

TS_{I5-I6}

G_{gas} = -2841.486661 a. u.

E_{gas} = -2842.25609313 a. u.

Ru	1. 00398900	-1. 44443400	-0. 94460800	C	4. 05781900	3. 57526500	0. 20120100
S	2. 08794900	0. 51102500	0. 36263700	C	3. 74827000	4. 71719400	0. 94274400
P	-1. 06822300	-1. 31512800	0. 16025700	H	3. 45188900	5. 62173700	0. 41948500
C	3. 15033300	-1. 98125100	-1. 26108000	C	3. 81118500	4. 72382000	2. 33975700
C	2. 53797700	-2. 03459200	-2. 54548600	C	4. 18268600	3. 54666500	2. 99508900
C	1. 37744600	-2. 86363700	-2. 69195000	H	4. 22888000	3. 53382400	4. 08018200
H	0. 83784400	-2. 84869200	-3. 63168500	C	4. 49891300	2. 38357000	2. 28835000
C	0. 89293500	-3. 65711400	-1. 62501700	C	3. 96852300	3. 59034300	-1. 30569600
C	1. 66781900	-3. 73533100	-0. 41423500	H	3. 65066300	4. 57056700	-1. 66582600
H	1. 32507700	-4. 38594400	0. 38410500	H	3. 24642500	2. 84765700	-1. 66719900
C	2. 78648900	-2. 93103000	-0. 21618000	H	4. 93259700	3. 35464900	-1. 76826900
C	3. 01314600	-1. 18865700	-3. 69513200	C	3. 50732200	5. 97918700	3. 11810800
H	3. 82899600	-1. 69269700	-4. 22415800	H	4. 40146600	6. 60496600	3. 21145800
H	3. 38702100	-0. 22171300	-3. 35298200	H	3. 16088100	5. 74574400	4. 12765200
H	2. 20282000	-1. 01482600	-4. 40570600	H	2. 73818800	6. 57642700	2. 62205000
C	-0. 33861000	-4. 50619300	-1. 77633300	C	4. 88281700	1. 12138400	3. 02325600
H	-0. 06107000	-5. 54271400	-1. 99459300	H	5. 85865300	0. 74649400	2. 69837000
H	-0. 96691800	-4. 14694900	-2. 59465700	H	4. 15332100	0. 32108800	2. 84528800
H	-0. 92721200	-4. 50656100	-0. 85333900	H	4. 92800100	1. 29799000	4. 09960000
C	3. 54162200	-2. 94621900	1. 08315500	C	-1. 15502500	-2. 55980700	1. 53933900
H	4. 59547300	-3. 18821300	0. 91493300	C	-2. 20895700	-3. 46487500	1. 68861300
H	3. 11766700	-3. 68403000	1. 76677500	H	-3. 04677500	-3. 46194600	1. 00048900
H	3. 51075500	-1. 96417800	1. 56798200	C	-2. 19115000	-4. 38870700	2. 73881800
C	3. 83196600	0. 21419400	-0. 22576600	H	-3. 00977300	-5. 08971200	2. 84972500
C	4. 17339500	-0. 93983800	-0. 94984900	C	-1. 13053000	-4. 40282600	3. 64333700
C	5. 49750500	-1. 11055200	-1. 36734200	H	-1. 12316300	-5. 11620500	4. 45869300
H	5. 76287300	-1. 99779400	-1. 93266900	C	-0. 07804300	-3. 49315600	3. 50052400
C	6. 46407300	-0. 15699000	-1. 05092200	H	0. 74338900	-3. 49698800	4. 20775100
H	7. 48841900	-0. 29733200	-1. 37375700	C	-0. 08663100	-2. 57886600	2. 44883200
C	6. 11081900	0. 97241700	-0. 31691800	H	0. 73818200	-1. 87963300	2. 32771000
H	6. 85472500	1. 71984900	-0. 06383800	C	-1. 42546900	0. 35078200	0. 98921100
C	4. 78936500	1. 18001500	0. 10710700	H	-0. 74817700	0. 43229800	1. 84398700
C	4. 43850500	2. 40584400	0. 88399500	H	-1. 15105400	1. 11418900	0. 25469400

C	-2.86752900	0.45400200	1.39955300	C	-4.18058100	3.21530400	-1.06170800
C	-3.21914500	0.26764200	2.76323600	H	-4.45383300	3.16580000	-0.01432000
H	-2.43142500	0.08726300	3.48750600	H	0.23031000	-0.42411400	-1.87207900
C	-4.53015700	0.32272800	3.16166300	H	1.44480600	0.55293800	-0.93630500
H	-4.79537800	0.19201400	4.20549500				
C	-5.56671200	0.54244400	2.21535800	TS_{I6-II}			
C	-5.23158800	0.71019200	0.83710000	G_{gas} = -2841.489415 a. u.			
C	-3.85249200	0.67911100	0.44516800	E_{gas} = -2842.26331602 a. u.			
C	-6.93244600	0.58020900	2.61061100	Ru	1.02427200	-2.22327100	-0.44971400
H	-7.17086600	0.45940200	3.66221900	S	1.69099300	0.01473600	-0.20503400
C	-7.92786400	0.76120900	1.68232600	P	-1.28562800	-1.51179100	-0.30335900
H	-8.96592500	0.78906300	1.99109400	C	2.96333700	-2.70984300	0.47179500
C	-7.59975100	0.90545300	0.31036000	C	2.99243600	-3.33862500	-0.80321100
H	-8.39246900	1.03559800	-0.41679000	C	1.93453600	-4.24591600	-1.15734000
C	-6.28933800	0.87932700	-0.10309100	H	1.92718900	-4.65693700	-2.16099400
H	-6.04944700	0.98735600	-1.15411300	C	0.90595400	-4.61026000	-0.26250500
C	-2.61828800	-1.54192400	-0.89157500	C	0.87705900	-3.94340800	0.99458900
H	-2.45049700	-2.38470200	-1.56608500	H	0.04665100	-4.13161000	1.66633800
H	-3.44929100	-1.77589400	-0.22091500	C	1.88535800	-3.00795000	1.39409300
C	-2.88404700	-0.26418700	-1.64424100	C	4.04590200	-2.98758200	-1.81721200
C	-2.50321400	-0.16070700	-3.00837000	H	4.98682900	-3.49058800	-1.57107700
H	-2.06031100	-1.02471200	-3.49464800	H	4.24151500	-1.91264300	-1.82784900
C	-2.70202600	1.00386800	-3.70526400	H	3.74350500	-3.30147500	-2.81797300
H	-2.42516900	1.07618400	-4.75185300	C	-0.14832500	-5.60924700	-0.64215000
C	-3.27091800	2.13957400	-3.06863400	H	0.19984700	-6.62111200	-0.40889000
C	-3.64799400	2.05467800	-1.69390600	H	-0.36804900	-5.56672800	-1.71152600
C	-3.46293700	0.81795400	-0.99273800	H	-1.07786300	-5.43716000	-0.09457100
C	-3.46263800	3.36215500	-3.76962200	C	1.81961700	-2.35287000	2.74326800
H	-3.17992200	3.40982000	-4.81614500	H	2.54380300	-2.82281400	3.41764600
C	-3.99123800	4.45954200	-3.13574900	H	0.82445900	-2.46438200	3.17911100
H	-4.13477900	5.38735400	-3.67641500	H	2.06126000	-1.28978100	2.68308800
C	-4.34746400	4.38414000	-1.76522800	C	3.38763600	-0.25932700	0.47433500
H	-4.75410200	5.25837000	-1.27089100	C	3.86325400	-1.55429800	0.75036900

C	5.15307400	-1.74273700	1.24885600	H	-4.65993100	-6.14537800	-0.10960800
H	5.50811600	-2.74741300	1.45413500	C	-3.55584700	-4.70306300	1.04750000
C	5.97235200	-0.63835600	1.48377400	H	-3.81394300	-5.14936700	2.00068300
H	6.97187800	-0.77750800	1.87669600	C	-2.75314900	-3.56074900	1.00958400
C	5.49849100	0.64251200	1.20868600	H	-2.39342800	-3.13144700	1.93964600
H	6.12952100	1.50786600	1.38209300	C	-1.66560800	-0.44565700	1.21335000
C	4.20713100	0.85462900	0.70070100	H	-1.52557900	-1.06461900	2.10382200
C	3.75911900	2.24684300	0.39563900	H	-0.88234200	0.31948500	1.21163500
C	4.13673400	2.84106400	-0.82233900	C	-3.04775300	0.14157500	1.13796600
C	3.80064300	4.17727800	-1.05604300	C	-4.09393900	-0.41417000	1.92239200
H	4.10881300	4.64380300	-1.98791700	H	-3.86739900	-1.22871300	2.60237100
C	3.10257200	4.93176900	-0.10873800	C	-5.37051400	0.07914300	1.84060500
C	2.69261200	4.30518600	1.07163900	H	-6.16403300	-0.33907300	2.45083500
H	2.11900100	4.86952300	1.80144300	C	-5.68047200	1.14136600	0.94998500
C	3.01209800	2.97219300	1.34138200	C	-4.64209000	1.70752000	0.15002600
C	4.89227700	2.04922200	-1.86267700	C	-3.30629000	1.20126100	0.27707100
H	5.04769300	2.64388900	-2.76522600	C	-7.00527800	1.64479300	0.83228900
H	4.34071600	1.14331300	-2.14106500	H	-7.78242600	1.20933500	1.45170300
H	5.87310800	1.73041000	-1.49478500	C	-7.29583700	2.65681700	-0.04908500
C	2.83860800	6.39963800	-0.33436700	H	-8.30753600	3.03490900	-0.13390600
H	1.94838900	6.72805400	0.20819900	C	-6.27055100	3.20810500	-0.85879500
H	2.70146300	6.62528200	-1.39602100	H	-6.51138700	3.99886100	-1.55929600
H	3.68199400	7.00217800	0.02016200	C	-4.97910300	2.74759900	-0.76396200
C	2.56078100	2.32142800	2.62594000	H	-4.20255800	3.17322900	-1.38821000
H	3.40228200	1.87967600	3.16965200	C	-1.98208200	-0.43013900	-1.70052600
H	1.84193900	1.51836800	2.41959700	H	-1.61673200	-0.82057200	-2.65269000
H	2.07519300	3.04837000	3.28009800	H	-3.06942100	-0.54844400	-1.65882400
C	-2.42796200	-2.97054300	-0.21749400	C	-1.56359000	1.00235100	-1.49609200
C	-2.91003800	-3.53274000	-1.40526400	C	-0.49884100	1.53594600	-2.26872100
H	-2.66632600	-3.08349300	-2.36345600	H	-0.02818900	0.91061500	-3.02056800
C	-3.71091200	-4.67557100	-1.36525500	C	-0.06598000	2.82229300	-2.07199300
H	-4.08716300	-5.10177900	-2.28763900	H	0.75551800	3.22555000	-2.65460400
C	-4.03364700	-5.26202300	-0.13997000	C	-0.67289900	3.64454300	-1.08714900

C	-1.73881400	3.12075200	-0.29501100	H	0.95053700	-3.87399700	-4.79498800
C	-2.19013000	1.78135700	-0.53112300	H	0.50689200	-4.69325900	-3.29169600
C	-0.24208700	4.98319500	-0.87746800	C	-0.55683400	1.13888400	-3.93632500
H	0.55989900	5.36886200	-1.49795600	H	-1.35582800	1.59587100	-4.52705100
C	-0.82608300	5.76655600	0.08713600	H	0.37446800	1.19179000	-4.50408400
H	-0.50187700	6.79070300	0.23266700	H	-0.44220600	1.73174600	-3.02292000
C	-1.86195000	5.23783800	0.89900800	C	-2.73145200	1.28523900	-1.52918000
H	-2.30747800	5.85835700	1.66756800	C	-3.08878000	0.48831700	-2.63839500
C	-2.30684100	3.95077000	0.71523000	C	-4.22125900	0.79273700	-3.39843200
H	-3.10060200	3.55630000	1.33823200	H	-4.47509400	0.16895200	-4.24991000
H	0.68130900	-2.00636500	-3.21843800	C	-4.99765300	1.90583500	-3.08251500
H	1.04311500	-1.40533300	-2.97227000	H	-5.87113700	2.15030900	-3.67451600
TS_{RI4-II} G_{gas} = -3958.428274 a. u. E_{gas} = -3959.52956984 a. u.				C	-4.61343100	2.72606400	-2.02270500
				H	-5.17917900	3.62550000	-1.80091500
				C	-3.48408100	2.44319400	-1.23758200
				C	-3.09293500	3.43767600	-0.18688700
				C	-3.90326700	3.64787300	0.95048600
				C	-3.56716200	4.65882700	1.85521400
				H	-4.19185200	4.80828700	2.73140900
				C	-2.45580300	5.48367700	1.66064000
				C	-1.67897200	5.27837200	0.51890000
				H	-0.83860400	5.93966000	0.32448900
Ru	-0.73155600	-1.32918700	-1.45428800	C	-1.97890100	4.27498300	-0.41112700
S	-1.32942900	0.79500000	-0.45030300	C	-5.13763800	2.81735500	1.21317500
P	1.45159400	-1.14360800	-0.49410200	H	-5.56280300	3.06449400	2.18840500
C	-2.18552200	-0.63103000	-3.03381000	H	-4.91744000	1.74641300	1.20724100
C	-2.54074600	-1.99688900	-2.86835400	H	-5.91227900	2.98868800	0.45834300
C	-1.52782000	-2.99374800	-3.04380000	C	-2.10314800	6.54826700	2.66859100
H	-1.78645100	-4.03202600	-2.86107600	H	-2.99057100	7.10229300	2.98641000
C	-0.22987700	-2.67342300	-3.46658500	H	-1.38543600	7.26200000	2.25775000
C	0.05142600	-1.30253800	-3.77104600	H	-1.65733300	6.10307500	3.56560700
H	1.03138000	-1.04364400	-4.15771900	C	-1.13204600	4.14335800	-1.65260600
C	-0.89268200	-0.28628000	-3.60099200	H	-1.74738900	3.95127900	-2.53699300
C	-3.95716200	-2.41911600	-2.59556900				
H	-4.52163900	-2.41262600	-3.53541100				
H	-4.45927100	-1.74281800	-1.90637400				
H	-4.00715500	-3.43600600	-2.20007200				
C	0.80861300	-3.73376900	-3.71834000				
H	1.77653900	-3.46438700	-3.28478500				

H	-0.42219100	3.31525800	-1.54826500	H	0.95285600	0.34510600	1.40087000
H	-0.55675500	5.05653300	-1.82617100	H	2.61488400	-0.26103400	1.48028400
C	2.19410800	-2.74981800	0.11955900	C	2.33850700	1.50311800	0.26841200
C	1.61747200	-3.93993600	-0.33941100	C	1.50032100	2.64128000	0.43438700
H	0.71206300	-3.88750200	-0.93845600	H	0.53219000	2.51473700	0.90763500
C	2.19251100	-5.17504500	-0.03595700	C	1.90023700	3.87946600	0.00512100
H	1.73958500	-6.08906900	-0.40436900	H	1.25827500	4.74168600	0.15562000
C	3.34844800	-5.22909100	0.74402900	C	3.14354000	4.05304800	-0.65825000
H	3.80167300	-6.18501600	0.97991400	C	3.99366300	2.92218200	-0.84334300
C	3.92262400	-4.04769100	1.21554600	C	3.58398400	1.64364700	-0.32912600
H	4.82545000	-4.08146700	1.81443800	C	3.55012900	5.32317800	-1.15148000
C	3.35215300	-2.81202800	0.90324100	H	2.89400500	6.17336600	-0.99457600
H	3.83946000	-1.90628100	1.25071100	C	4.74242500	5.47035100	-1.81660900
C	2.71985100	-0.66752000	-1.83983300	H	5.04555900	6.44100300	-2.19061900
H	2.64820600	-1.43101400	-2.61780500	C	5.57935600	4.34520900	-2.02351900
H	2.37483500	0.28984300	-2.24419300	H	6.51206200	4.46547000	-2.56182800
C	4.10666800	-0.60088000	-1.27383500	C	5.21709200	3.10594600	-1.55129600
C	4.99629000	-1.68794000	-1.49183500	H	5.86325300	2.25327400	-1.72101700
H	4.67397100	-2.50812800	-2.12622800	Si	-3.00994700	-1.42138100	3.43401400
C	6.23354100	-1.71500500	-0.90289900	H	-2.51484500	-2.50709200	4.32886500
H	6.91139100	-2.54381700	-1.07859000	H	-1.23266100	-2.00123800	-0.00149800
C	6.64084000	-0.66905600	-0.03153200	H	-4.48179400	-1.23880200	3.54511900
C	5.76256400	0.43477000	0.19232800	C	-2.03564800	0.15607100	3.75800200
C	4.49232000	0.46755800	-0.47586900	C	-2.12084000	1.27535400	2.91910600
C	7.90159000	-0.70262000	0.62638700	C	-1.13927500	0.18277700	4.84035400
H	8.56186400	-1.54296800	0.43802100	C	-1.29373800	2.38204100	3.12584700
C	8.27527400	0.30484200	1.48129300	H	-2.80041900	1.29001100	2.07490000
H	9.23767500	0.27276800	1.97791500	C	-0.33414800	1.29913900	5.06630600
C	7.39805400	1.39312000	1.72005300	H	-1.05122700	-0.67945100	5.49555300
H	7.69709900	2.17938900	2.40308000	C	-0.39921300	2.39246200	4.19784600
C	6.17643900	1.45863500	1.09346800	H	-1.35327300	3.22404400	2.44455200
H	5.51266800	2.29437400	1.28048100	H	0.34901800	1.31175000	5.90785400
C	1.86238900	0.18127000	0.82077600	H	0.24445000	3.25019100	4.35730300

C	0.88363900	-4.38592800	3.26600600	S	-0.34708600	1.75489800	0.44590100
C	-0.21702500	-4.28727900	2.41514700	P	-0.77688700	-1.52773600	0.70635400
C	-0.70111800	-3.02649300	2.04531100	C	0.69577800	1.35120200	3.32127100
C	-0.05543000	-1.87665400	2.50989200	C	2.08307500	1.46942400	2.93598200
C	1.03521600	-1.97514900	3.36893800	C	2.86541500	0.30131500	2.88743600
C	1.50485100	-3.23371900	3.75063600	H	3.89713500	0.37835000	2.55987800
H	1.25766600	-5.36308600	3.54661100	C	2.35686400	-0.97281000	3.27699700
H	-0.69199600	-5.19083200	2.05066400	C	1.03038700	-1.02707200	3.74964000
H	-0.41436000	-0.91071100	2.17193600	H	0.63955600	-1.98376500	4.07827700
H	1.51582700	-1.07277000	3.73062800	C	0.19158800	0.12074200	3.82560900
H	2.36075000	-3.31779700	4.40997600	C	2.66404900	2.81501500	2.60346500
C	-1.91456400	-2.88817800	1.19102900	H	2.80132800	3.39845200	3.52060700
N	-2.92724900	-2.14507900	1.70311300	H	1.99724600	3.38677000	1.95279000
C	-2.24091900	-4.05001500	0.27712400	H	3.63243600	2.71478200	2.10705600
H	-2.67952500	-4.85840800	0.87503900	C	3.21558100	-2.20981700	3.29395900
H	-2.95824100	-3.76101800	-0.48658100	H	3.65851300	-2.35407800	4.28502600
H	-1.32691700	-4.41066100	-0.19437900	H	4.03434500	-2.14394600	2.57368000
C	-4.17117100	-1.97891400	0.97506200	H	2.61889000	-3.09797500	3.06073700
C	-5.11440000	-3.00785200	0.90421600	C	-1.18743300	0.03433400	4.42181100
C	-4.45462900	-0.72334400	0.43967700	H	-1.19826900	0.49492600	5.41543300
C	-6.33724300	-2.77615900	0.27245300	H	-1.50008300	-1.00694200	4.53771300
H	-4.90526000	-3.96896100	1.36088600	H	-1.92135600	0.56532200	3.81080100
C	-5.68332500	-0.49282900	-0.18297700	C	-0.71945600	2.82604300	1.89142200
H	-3.69679400	0.04949600	0.49613200	C	-0.20519400	2.52767300	3.16684800
C	-6.62503100	-1.52010000	-0.26914200	C	-0.50998300	3.33310700	4.26753200
H	-7.07198000	-3.57075200	0.22149200	H	-0.09911400	3.08336000	5.24121300
H	-5.88814000	0.48452800	-0.60806100	C	-1.32707500	4.45003200	4.10876200
H	-7.58053300	-1.34381600	-0.74826600	H	-1.57240100	5.07427000	4.95911400
TS _{SI4-II}				C	-1.81473400	4.76194200	2.84102600
				H	-2.43918600	5.63787100	2.69739600
				C	-1.51795300	3.97113400	1.72175300
				C	-2.01300600	4.41464600	0.38377300
				C	-1.33631500	5.46468000	-0.26775900
G _{gas} = -3958.422081 a. u.							
E _{gas} = -3959.51826435 a. u.							
Ru	0.86734100	-0.04135400	1.54563100				

C	-1.82536800	5.94421600	-1.48473400	C	-3.85094200	-3.40182000	1.67377700
H	-1.29574300	6.74827400	-1.98881300	H	-3.48328900	-3.45465900	2.69300200
C	-2.98991900	5.42448700	-2.05632000	C	-4.66598800	-4.38911000	1.18615700
C	-3.64390300	4.38267400	-1.39569600	H	-4.95220900	-5.22840100	1.81131100
H	-4.55633900	3.97166800	-1.81633200	C	-5.14038800	-4.33881800	-0.15172200
C	-3.16566000	3.85327700	-0.19294300	C	-4.78802100	-3.22662500	-0.97373200
C	-0.09751200	6.07676300	0.34291400	C	-3.97469800	-2.17694200	-0.42540200
H	0.44100500	6.67699200	-0.39530600	C	-5.95052400	-5.37708000	-0.68807200
H	0.57524600	5.30336600	0.73007400	H	-6.21631500	-6.21050400	-0.04596200
H	-0.34448000	6.72938000	1.18763600	C	-6.38243100	-5.32970500	-1.99065200
C	-3.54243300	5.99427400	-3.33966400	H	-6.99897000	-6.12470800	-2.39283000
H	-4.12405300	5.24733300	-3.88733100	C	-6.01457500	-4.23895600	-2.81795800
H	-2.74192100	6.34980700	-3.99386200	H	-6.34762600	-4.21483700	-3.84885200
H	-4.20505000	6.84319200	-3.13874900	C	-5.23996000	-3.21574000	-2.32541200
C	-3.87123800	2.68210400	0.44289700	H	-4.96241300	-2.38873800	-2.96763500
H	-3.93711100	2.78857500	1.53018000	C	-1.22229400	-1.63322700	-1.14044900
H	-3.31559900	1.75936700	0.22664500	H	-0.30534400	-1.46890700	-1.70767900
H	-4.88075100	2.56375800	0.03865100	H	-1.54554000	-2.66713000	-1.29578900
C	-0.42786200	-3.31466100	1.13203900	C	-2.32184900	-0.69252500	-1.56646600
C	0.05310500	-4.21232700	0.17574000	C	-2.01317700	0.45085000	-2.35137800
H	0.23169600	-3.88862700	-0.84443200	H	-0.97649900	0.67171400	-2.57292700
C	0.32369400	-5.53889300	0.52508600	C	-3.00200800	1.26774100	-2.83354000
H	0.69143100	-6.22540000	-0.22937000	H	-2.75691600	2.13494300	-3.43793600
C	0.11680900	-5.97787000	1.83160000	C	-4.36413400	1.01012700	-2.52493700
H	0.31955600	-7.00805900	2.09911600	C	-4.68991700	-0.09170900	-1.68048400
C	-0.36736300	-5.08687900	2.79334800	C	-3.64316000	-0.97200800	-1.24161500
H	-0.54765200	-5.42582400	3.80702800	C	-5.40624300	1.84383900	-3.01659600
C	-0.63804100	-3.76491200	2.44254400	H	-5.14456500	2.65387100	-3.69061700
H	-1.04280900	-3.08818700	3.18967700	C	-6.71165800	1.63518800	-2.64338400
C	-2.51919400	-1.27409300	1.41968000	H	-7.49932300	2.27749600	-3.01897500
H	-2.44875300	-1.34078800	2.50653300	C	-7.03114400	0.57618400	-1.75641800
H	-2.77770800	-0.24308900	1.15611200	H	-8.05932600	0.43023200	-1.44722200
C	-3.48260000	-2.28846200	0.86876000	C	-6.05019600	-0.26847900	-1.29315000

H	-6.30663600	-1.07912500	-0.62198900	C	3.88470400	1.96149300	-1.26026700
Si	5.32260700	-0.11685000	-0.08358900	C	2.95963200	2.86256200	-0.73728300
H	4.83988700	-1.09869700	0.91990900	C	4.91990500	2.39520800	-2.09422000
H	1.64862300	-0.24216300	0.08268500	C	3.08151700	4.21780700	-1.04933100
H	5.85499000	1.11144000	0.56600100	H	2.14045600	2.50630600	-0.11924900
C	6.55836700	-0.88073100	-1.26914300	C	5.03678800	3.75213900	-2.39228300
C	7.61666000	-0.11803500	-1.79076800	H	5.60914200	1.67325600	-2.52139100
C	6.45377800	-2.23588300	-1.62095000	C	4.11994400	4.66527300	-1.86732400
C	8.53857000	-0.69453000	-2.66470300	H	2.35679600	4.91993100	-0.65526700
H	7.73104200	0.92455100	-1.50654200	H	5.83487200	4.09229000	-3.04097600
C	7.37415000	-2.81000900	-2.49759900	H	4.21000700	5.71876200	-2.10264100
H	5.65796100	-2.84781100	-1.20567100				
C	8.41343600	-2.03875100	-3.02184300	TS _{I3-17}			
H	9.35457800	-0.10101600	-3.05946400	G _{gas} = -3747.457966 a. u.			
H	7.28455700	-3.85659300	-2.76471800	E _{gas} = -3748.46825113 a. u.			
H	9.13075400	-2.48625200	-3.69982200	Ru	0.95706500	-2.55224800	0.22148400
C	3.18364800	-3.90709700	-0.50136000	S	-0.78895200	-0.88352200	-0.33194000
C	2.90539500	-2.55207100	-0.30650600	P	2.64606800	-0.97412600	0.51227200
C	2.91687800	-1.66978800	-1.38911900	C	0.06989800	-3.58012200	-1.58505800
C	3.18141900	-2.16369100	-2.67841700	C	-0.47004600	-4.33549100	-0.47485800
C	3.43567600	-3.52036600	-2.87252300	C	0.42076700	-4.87856300	0.46586800
C	3.44395600	-4.39518300	-1.78269200	H	0.02423600	-5.38744500	1.33807400
H	3.16313700	-4.58114600	0.34719000	C	1.83591000	-4.74594900	0.32209400
H	2.64177900	-2.17811000	0.67621300	C	2.32272500	-4.12347300	-0.85307800
H	3.19852800	-1.48609500	-3.52584700	H	3.39703200	-4.04319800	-0.98468400
H	3.63360100	-3.89031900	-3.87131700	C	1.46559100	-3.57741200	-1.85407700
H	3.64602900	-5.44916500	-1.93356900	C	-1.95786500	-4.51703100	-0.35640100
C	2.73091900	-0.17686000	-1.28592600	H	-2.31656100	-5.15571800	-1.17143300
N	3.80953400	0.54715700	-0.94749500	H	-2.49095400	-3.56399200	-0.42847000
C	1.72233400	0.45433100	-2.21945900	H	-2.21904100	-4.99100700	0.59202500
H	1.11681400	1.21050500	-1.71306900	C	2.78452100	-5.31549200	1.34133000
H	2.25289600	0.94680900	-3.04289500	H	2.93979600	-6.38608500	1.17041700
H	1.06815000	-0.31355200	-2.62719200	H	2.39325800	-5.18509900	2.35319700

H	3.75661100	-4.81702100	1.28645200	H	0.36008600	2.42024700	-2.89113300
C	2.04182000	-2.93864000	-3.09010500	C	4.26349700	-1.81138200	0.90256500
H	1.90015000	-3.58206600	-3.96491600	C	4.54836800	-2.14127800	2.23281400
H	3.11616900	-2.77447400	-2.96993900	H	3.86025400	-1.86069400	3.02436700
H	1.56065700	-1.98121900	-3.30706600	C	5.71081600	-2.84678000	2.54879600
C	-1.29459800	-1.50433300	-2.00961400	H	5.92645100	-3.09391900	3.58162200
C	-0.84640000	-2.77173800	-2.44210600	C	6.59230200	-3.23310600	1.53734600
C	-1.18764500	-3.25321400	-3.70739000	H	7.49476700	-3.77987400	1.78295700
H	-0.83565900	-4.23359800	-4.01233500	C	6.31003100	-2.91056400	0.20867700
C	-1.94438400	-2.46896500	-4.57440800	H	6.99443200	-3.20370100	-0.57891400
H	-2.19426000	-2.83022600	-5.56450500	C	5.14933600	-2.20090600	-0.10729300
C	-2.34559800	-1.20314100	-4.16672400	H	4.94092200	-1.95477900	-1.14421700
H	-2.89356500	-0.56422600	-4.85069500	C	2.97150100	0.10471200	-1.00896500
C	-2.04420400	-0.69659800	-2.88859500	H	3.29275600	-0.55360000	-1.82088500
C	-2.52455700	0.69047500	-2.59329600	H	1.98026200	0.48469300	-1.26963400
C	-3.91103600	0.96355300	-2.65692900	C	3.95902600	1.20797500	-0.75715700
C	-4.36827100	2.27208800	-2.48475500	C	5.27529800	1.09197600	-1.28214800
H	-5.43823700	2.46398800	-2.51004800	H	5.52158100	0.22836100	-1.89048000
C	-3.48849000	3.33168600	-2.25745200	C	6.21828100	2.05739500	-1.04784800
C	-2.12200700	3.05303200	-2.21672700	H	7.21636900	1.96789200	-1.46362600
H	-1.41432700	3.86279200	-2.05740900	C	5.91068300	3.18698400	-0.24410500
C	-1.62288100	1.75812700	-2.39479000	C	4.59649900	3.32106100	0.29730500
C	-4.93268700	-0.12483400	-2.89942400	C	3.60696200	2.32180500	-0.00448500
H	-5.89741900	0.16886000	-2.47452200	C	6.89186400	4.17584300	0.04131400
H	-4.62380000	-1.08105000	-2.46630100	H	7.88236700	4.06004700	-0.38634600
H	-5.09306200	-0.30069100	-3.96869800	C	6.59635100	5.24774100	0.84659200
C	-3.99363300	4.73844500	-2.06080900	H	7.34948000	5.99615200	1.06195600
H	-4.00456100	5.29066200	-3.00675200	C	5.30191200	5.37020300	1.41043200
H	-3.35013800	5.28941900	-1.36721300	H	5.08045500	6.20789900	2.06118900
H	-5.01295200	4.74088100	-1.66426400	C	4.32950000	4.43542200	1.14537600
C	-0.12610300	1.58311500	-2.38124400	H	3.34831900	4.53817500	1.59204900
H	0.18566400	0.65123900	-2.86065500	C	2.55899800	0.35141900	1.86769300
H	0.23221800	1.56863400	-1.34635300	H	2.13963800	-0.12677600	2.75504200

H	3.59619300	0.63827000	2.06954500	C	-3.76258700	1.35174600	0.55970300
C	1.73764100	1.54420600	1.45941900	C	-4.90613100	0.53114800	0.53866200
C	0.47162700	1.74937100	2.07144900	C	-6.17101300	1.09094900	0.79636100
H	0.14092400	1.03926100	2.82091300	C	-6.28663300	2.44471600	1.09193600
C	-0.29692500	2.84213000	1.76668100	C	-5.14631400	3.25371400	1.10849900
H	-1.24020100	3.01135600	2.27772300	H	-3.01188800	3.34063700	0.78947200
C	0.14026100	3.78257800	0.79488100	H	-2.78811400	0.95383700	0.28548600
C	1.39882900	3.58010900	0.15113200	H	-7.05700100	0.46660700	0.79186500
C	2.22068900	2.46537900	0.53799400	H	-7.25902100	2.86995900	1.30685900
C	-0.63326700	4.93149900	0.46795600	H	-5.24065600	4.31258300	1.32162200
H	-1.56210800	5.10285500	1.00475100	C	-4.78398600	-0.89202900	0.25036400
C	-0.20860400	5.81900900	-0.49161700	C	-5.97428800	-1.72254300	-0.11370000
H	-0.79976900	6.69607600	-0.72901500	H	-5.64014300	-2.64748400	-0.58319600
C	1.01036500	5.58630200	-1.17774100	H	-6.49679700	-1.98077000	0.81783700
H	1.33027700	6.27750200	-1.94836600	H	-6.67197500	-1.19937700	-0.76588600
C	1.79518800	4.50177100	-0.86101000	O	-3.67503400	-1.50762500	0.36477300
H	2.73339500	4.34018400	-1.37875200				
Si	-2.19709900	-1.40533400	1.72927900	TS_{I7-I5}			
H	-1.06916500	-0.56773300	2.25337600	G_{gas} = -3747.463772 a. u.			
H	0.78095700	-2.22372600	1.76017500	E_{gas} = -3748.46466338 a. u			
H	-1.94357400	-2.86429400	1.76983400	Ru	-0.84878900	-2.40697100	0.14219500
C	-3.54882100	-0.94252300	2.99639900	S	0.57370400	-0.62553200	1.01069800
C	-4.65807800	-1.77247100	3.23499000	P	-2.60355300	-0.91373900	-0.29469300
C	-3.43176000	0.24415300	3.73087100	C	0.23173800	-3.61652500	1.69693000
C	-5.63109800	-1.41500200	4.16828600	C	0.53832000	-4.23890800	0.44679200
H	-4.75464300	-2.71271200	2.69556900	C	-0.54640100	-4.68912400	-0.35954500
C	-4.41052500	0.61529800	4.65644900	H	-0.33239600	-5.10122900	-1.33972800
H	-2.57369100	0.89279800	3.56887500	C	-1.88853400	-4.58418800	0.06616000
C	-5.51140600	-0.21336800	4.87328700	C	-2.14047500	-4.05518200	1.37166500
H	-6.47325600	-2.07174300	4.35634300	H	-3.17111200	-3.98573800	1.70685100
H	-4.31271500	1.54332700	5.20793800	C	-1.11194600	-3.61164700	2.21933800
H	-6.26874000	0.06824000	5.59569400	C	1.95484200	-4.37816600	-0.03246900
C	-3.88966000	2.70776100	0.83489600	H	2.43376700	-5.25580200	0.41708100

H	2. 54998100	-3. 50270100	0. 23787600	H	3. 28803600	5. 31138100	2. 20781800
H	1. 98431800	-4. 48836300	-1. 11919900	H	4. 60252500	4. 80111800	1. 12835800
C	-3. 01879100	-5. 09066400	-0. 78853000	C	0. 77463700	1. 29959300	3. 74028700
H	-2. 79899500	-4. 95367100	-1. 85003900	H	0. 67612900	0. 27364400	4. 10094500
H	-3. 95131000	-4. 56588100	-0. 56626700	H	-0. 03802000	1. 48805800	3. 03005100
H	-3. 18128600	-6. 15910000	-0. 60908600	H	0. 64106900	1. 97526200	4. 58985300
C	-1. 40124600	-3. 04983400	3. 58559400	C	-4. 18253400	-1. 77087700	-0. 77493200
H	-0. 95099100	-3. 67061200	4. 36673800	C	-4. 40202900	-2. 08967200	-2. 11976900
H	-2. 47805900	-3. 00548000	3. 76361100	H	-3. 68597700	-1. 78393000	-2. 87656800
H	-0. 98888700	-2. 04166900	3. 69344000	C	-5. 53590200	-2. 81206800	-2. 49494900
C	1. 58341000	-1. 57195700	2. 23563600	H	-5. 70077700	-3. 05212900	-3. 53876300
C	1. 31208600	-2. 93204900	2. 46833700	C	-6. 45694400	-3. 22142400	-1. 52882800
C	2. 05418600	-3. 64143200	3. 41634600	H	-7. 33854600	-3. 77934400	-1. 82083300
H	1. 83286600	-4. 69004800	3. 58734900	C	-6. 24155600	-2. 90704600	-0. 18554700
C	3. 06831900	-3. 00457100	4. 12991400	H	-6. 95699400	-3. 21807300	0. 56687900
H	3. 63943000	-3. 55153400	4. 87019000	C	-5. 10625000	-2. 18581900	0. 19081500
C	3. 34332400	-1. 66164800	3. 88523200	H	-4. 94783800	-1. 95166900	1. 23881500
H	4. 13185300	-1. 15783900	4. 43438000	C	-3. 06439700	0. 19053800	1. 18007300
C	2. 61622300	-0. 92402500	2. 93788200	H	-3. 48176400	-0. 45228200	1. 95999500
C	2. 97905600	0. 50597100	2. 69530000	H	-2. 10213400	0. 56570800	1. 54357900
C	4. 22974600	0. 81724300	2. 11434700	C	-4. 00326600	1. 30119700	0. 79828300
C	4. 56798000	2. 15552900	1. 89345200	C	-5. 37920200	1. 20815300	1. 14177100
H	5. 52489400	2. 38805700	1. 43218900	H	-5. 72027300	0. 35153100	1. 71324900
C	3. 72108000	3. 19891300	2. 27688400	C	-6. 26620400	2. 18659800	0. 77378500
C	2. 50060300	2. 87335000	2. 86861600	H	-7. 31313800	2. 11427500	1. 04914200
H	1. 82879900	3. 67021200	3. 17531700	C	-5. 83440000	3. 30735400	0. 01594400
C	2. 11055400	1. 54775200	3. 08142400	C	-4. 45755500	3. 41573000	-0. 34478800
C	5. 24624200	-0. 24385100	1. 74618800	C	-3. 53974300	2. 40054300	0. 08388300
H	5. 78022200	0. 04316800	0. 83383900	C	-6. 74719000	4. 31516400	-0. 40086200
H	4. 79326400	-1. 22727300	1. 59552700	H	-7. 78908600	4. 22145800	-0. 11256500
H	5. 99423900	-0. 35926400	2. 53883000	C	-6. 32188000	5. 37991900	-1. 15632400
C	4. 14237300	4. 63675400	2. 10739600	H	-7. 02348200	6. 14307500	-1. 47117800
H	4. 87830100	4. 91931100	2. 86792900	C	-4. 95907400	5. 47941800	-1. 53518100

H	-4.63417600	6.31583800	-2.14277700	H	7.06794400	2.06663000	-1.56079600
C	-4.05150500	4.52493900	-1.14235600	H	4.45688100	5.47597200	-1.34585400
H	-3.01313200	4.60669400	-1.44107300	H	6.61523400	4.38159900	-0.79176700
C	-2.38113300	0.40107500	-1.63741800	C	3.16561400	-2.10832200	-2.47185100
H	-1.90287000	-0.08165500	-2.49153900	C	2.45186000	-2.74585500	-3.49988900
H	-3.37751200	0.74955100	-1.92318700	C	4.23938300	-2.77311300	-1.85599000
C	-1.53302500	1.51827100	-1.09396000	C	2.79291100	-4.03934400	-3.88616700
C	-0.14483200	1.54007400	-1.38970400	H	1.63509900	-2.21673300	-3.97546700
H	0.26532300	0.75308600	-2.01811600	C	4.59003400	-4.05869500	-2.26125000
C	0.66143500	2.52758600	-0.88395900	H	4.82008900	-2.27395200	-1.08744100
H	1.72568800	2.55051400	-1.09894200	C	3.86448700	-4.69528800	-3.27136600
C	0.12964400	3.54459000	-0.04941700	H	2.23539100	-4.53211200	-4.67356100
C	-1.25652700	3.51378400	0.28932700	H	5.43144300	-4.55965000	-1.79810500
C	-2.08811100	2.48320000	-0.26256800	H	4.13930500	-5.69515100	-3.58617900
C	0.95204200	4.58999700	0.45371600	H	3.11871200	1.12851500	-5.19911300
H	2.00362900	4.59573700	0.17837500	H	1.34947500	2.28610700	-3.91043900
C	0.43087000	5.55672400	1.27860100	C	2.98145800	-0.22459900	-0.80467000
H	1.05833700	6.35844000	1.65212800	H	1.83537200	-0.42534100	-0.16201700
C	-0.93609000	5.50471800	1.65423200	H	3.61494500	-0.79695800	-0.13311000
H	-1.33505000	6.25934800	2.32171900	H	3.05041300	0.85465000	-0.67511500
C	-1.75720100	4.51079800	1.17670300	O	2.27491800	-0.00422400	-3.07484500
H	-2.80049600	4.48152700	1.46698100				
H	-0.36154400	-1.94185200	-1.28143000	TS_{RI7-II}			
C	2.82718300	-0.72989400	-2.09564400	G_{gas} = -3747.462321 a. u.			
Si	2.63574300	1.54824500	-3.85647100	E_{gas} = -3748.4678871 a. u.			
C	3.93336400	2.45926500	-2.84948900	Ru	0.15680900	-1.86218600	-0.92311300
C	5.16320100	1.85396800	-2.54003700	S	-1.89912000	-0.79991800	-0.22128700
C	3.68633900	3.76759500	-2.40465000	P	1.15334700	0.24955700	-1.03748600
C	6.12126100	2.54001200	-1.79420600	C	-1.24940100	-3.21771900	-2.03936900
H	5.37965900	0.84477200	-2.88252300	C	-0.55567500	-4.08132100	-1.13375200
C	4.65164200	4.46022200	-1.67136800	C	0.86829600	-4.10021200	-1.17500500
H	2.73895700	4.25064300	-2.62970400	H	1.40573900	-4.69393400	-0.43991400
C	5.86570400	3.84439000	-1.36226500	C	1.60265500	-3.35762200	-2.12844100

C	0.86714900	-2.57220000	-3.06576700	H	-5.19384500	-2.27008700	3.05297800
H	1.42240200	-1.98843500	-3.79351900	H	-3.95874200	-2.54259200	1.80334100
C	-0.54521100	-2.51587300	-3.07706800	H	-5.63284700	-2.99882600	1.49952400
C	-1.31373300	-4.93021600	-0.15095100	C	-6.66564300	2.48244200	2.59820300
H	-1.74418700	-5.80376400	-0.65297200	H	-6.25384300	2.47546000	3.61258500
H	-2.14255100	-4.37419400	0.29565900	H	-7.74382800	2.30967800	2.68459000
H	-0.64869300	-5.29040300	0.63812600	H	-6.52483700	3.48091400	2.17521200
C	3.10455700	-3.41566300	-2.18274500	C	-4.78337500	1.04175100	-1.86094800
H	3.43486600	-4.23250800	-2.83364700	H	-5.30089000	0.39074300	-2.57307300
H	3.51960700	-3.58728000	-1.18642200	H	-3.70547400	0.90319500	-2.01056400
H	3.52322900	-2.48339600	-2.57159700	H	-5.02931500	2.07869700	-2.09953000
C	-1.29299900	-1.66952200	-4.07114600	C	2.88696900	0.16238300	-1.70827200
H	-1.92521000	-2.29075300	-4.71330000	C	3.95674600	-0.05422100	-0.83101000
H	-0.59795800	-1.11649300	-4.70787400	H	3.79230200	-0.07479700	0.24475700
H	-1.94754400	-0.95536700	-3.56108000	C	5.24796600	-0.23472100	-1.33117600
C	-3.11760000	-1.90929100	-1.03214200	H	6.06978400	-0.39968600	-0.64387400
C	-2.70961900	-2.97550800	-1.85299000	C	5.48204200	-0.19237600	-2.70696600
C	-3.65584600	-3.79795300	-2.47015100	H	6.48528700	-0.32883400	-3.09276000
H	-3.32102500	-4.61538200	-3.10154800	C	4.42042600	0.03563500	-3.58464700
C	-5.01615300	-3.56526200	-2.27394100	H	4.59801500	0.08211300	-4.65280300
H	-5.75259700	-4.19788800	-2.75419300	C	3.12738300	0.20859300	-3.08623600
C	-5.42055300	-2.51378800	-1.45193300	H	2.30884500	0.38214100	-3.77803600
H	-6.47621100	-2.32541400	-1.28489000	C	0.25323400	1.51138200	-2.12563900
C	-4.48809000	-1.67814100	-0.82286100	H	0.27340100	1.14342000	-3.15525700
C	-4.96876900	-0.58161200	0.07080800	H	-0.78402000	1.46750300	-1.77644700
C	-5.25824800	-0.86554700	1.41794900	C	0.85098700	2.88436000	-1.99795900
C	-5.78007200	0.14470200	2.22941500	C	1.68599700	3.38725000	-3.03290400
H	-6.01915400	-0.07905100	3.26606100	H	1.83170900	2.78888900	-3.92600900
C	-6.02175800	1.42878100	1.73045000	C	2.28750300	4.61389900	-2.92223400
C	-5.68492800	1.70084400	0.40237800	H	2.91281400	4.99685100	-3.72196000
H	-5.83352400	2.70310900	0.01062600	C	2.10988600	5.40303200	-1.75467000
C	-5.15831200	0.71486700	-0.43694500	C	1.27523600	4.91501400	-0.70449200
C	-5.00012200	-2.24384800	1.97804400	C	0.62369500	3.64544600	-0.85734300

C	2. 75291100	6. 66305700	-1. 60820200	C	4. 95112200	-0. 64068700	2. 85157300
H	3. 37639900	7. 02367800	-2. 41990300	C	4. 81561300	2. 06568400	2. 15795000
C	2. 59076800	7. 40673600	-0. 46516900	H	2. 86761900	2. 05524500	3. 06212700
H	3. 08254700	8. 36664400	-0. 36171500	C	6. 02818700	-0. 03196700	2. 20700600
C	1. 77790700	6. 91668400	0. 58825100	H	5. 01716500	-1. 68870000	3. 13211700
H	1. 66034700	7. 50631300	1. 48991900	C	5. 95559500	1. 31821400	1. 85317000
C	1. 13791700	5. 70540300	0. 47376400	H	4. 76348500	3. 11429700	1. 89017700
H	0. 51621800	5. 34019200	1. 28257600	H	6. 92393500	-0. 60334200	1. 99163500
C	1. 35918600	1. 23998200	0. 56001800	H	6. 79066900	1. 79042100	1. 34872000
H	1. 62465100	0. 51802600	1. 33468400	C	2. 04545100	-5. 74958300	2. 39133000
H	2. 19775300	1. 92600000	0. 40170300	C	1. 12034800	-4. 72394000	2. 59348600
C	0. 09284600	1. 97216300	0. 91310100	C	1. 47055200	-3. 39767000	2. 29735400
C	-0. 74279500	1. 45863900	1. 94030700	C	2. 74806300	-3. 11267200	1. 78127200
H	-0. 43351200	0. 55534300	2. 45678300	C	3. 66344200	-4. 13858600	1. 57844000
C	-1. 92141600	2. 08197200	2. 26108700	C	3. 31401900	-5. 46005500	1. 88607900
H	-2. 57064500	1. 68054400	3. 03267900	H	1. 77779500	-6. 77009100	2. 63599500
C	-2. 33275100	3. 24902200	1. 56621200	H	0. 14568600	-4. 95146800	3. 01005200
C	-1. 51315600	3. 76802500	0. 51943100	H	2. 98667600	-2. 09584400	1. 48125100
C	-0. 27115700	3. 11849900	0. 21819900	H	4. 64168000	-3. 91482600	1. 16814600
C	-3. 54734700	3. 91115100	1. 89383900	H	4. 02838900	-6. 25923700	1. 72858900
H	-4. 14762200	3. 51166600	2. 70436500	C	0. 53106500	-2. 30288200	2. 56838100
C	-3. 95369100	5. 02282100	1. 19789100	C	-0. 93325300	-2. 45805400	2. 60063500
H	-4. 87966100	5. 52421700	1. 45649400	H	-1. 30509900	-2. 26690000	3. 61290800
C	-3. 16096700	5. 51804500	0. 13088700	H	-1. 40284200	-1. 70621800	1. 93019200
H	-3. 49568100	6. 38588500	-0. 42518900	H	-1. 24987000	-3. 43656400	2. 24388700
C	-1. 97301500	4. 91029700	-0. 19894600	O	0. 99397500	-1. 18563300	3. 08337300
H	-1. 37251900	5. 29770500	-1. 01346500				
Si	2. 39168500	-0. 68858900	4. 10827400	TS _{SI7-I1}			
H	2. 80652000	-1. 96292200	4. 75744300	G _{gas} = -3747. 460931 a. u.			
H	0. 59680400	-1. 72613400	0. 62184300	E _{gas} = -3748. 46135637 a. u.			
H	1. 70476200	0. 27573900	4. 99968600	Ru	-1. 38308700	-0. 38150600	-0. 87416100
C	3. 79448200	0. 09875000	3. 15586200	S	-0. 07705300	1. 61215500	-0. 43881900
C	3. 74501600	1. 46210800	2. 81776900	P	0. 56903400	-1. 63811800	-0. 53223400

C	-2.40504200	0.97977400	-2.36582600	C	2.39894900	5.67755800	1.26516200
C	-3.46178500	0.52383500	-1.52376900	C	2.76179200	5.15908400	0.02045400
C	-3.67135900	-0.88085200	-1.40718400	H	3.80705500	5.15965900	-0.27427100
H	-4.46013400	-1.22817300	-0.74787500	C	1.81244100	4.63210900	-0.86158800
C	-2.91010400	-1.82142900	-2.12690200	C	-1.38283300	5.14939900	1.17161600
C	-1.90015400	-1.32230400	-3.00740600	H	-1.49389600	5.43153300	2.22156200
H	-1.30403300	-2.03642400	-3.56788600	H	-1.82532900	4.15693900	1.02435000
C	-1.66272900	0.05545100	-3.18591900	H	-1.97034700	5.85017400	0.56861400
C	-4.35008600	1.47921300	-0.77510900	C	3.43384400	6.24711300	2.20562600
H	-5.20177100	1.77363200	-1.39924700	H	4.40415900	6.34478200	1.71171800
H	-3.81244800	2.39163400	-0.50627400	H	3.56703800	5.61024200	3.08843700
H	-4.74366500	1.00906000	0.13074900	H	3.13932500	7.23799400	2.56383800
C	-3.18473200	-3.29680900	-2.02309700	C	2.24252000	4.03674900	-2.17868900
H	-2.25789400	-3.87413700	-1.97403800	H	1.74546900	4.52424700	-3.02361200
H	-3.75132900	-3.64326800	-2.89423300	H	1.98471000	2.97109500	-2.21305800
H	-3.77249500	-3.52125000	-1.12918700	H	3.32274200	4.12826100	-2.31215300
C	-0.59902900	0.56061800	-4.12192800	C	0.28664700	-3.46904000	-0.73155700
H	-1.03105900	1.22285700	-4.87833500	C	-0.07216500	-4.23722300	0.38160700
H	-0.10501000	-0.26938100	-4.63266200	H	-0.11470400	-3.77509300	1.36323900
H	0.15600300	1.13743500	-3.57617600	C	-0.36197900	-5.59531100	0.23960900
C	-0.96794800	2.81802900	-1.49431800	H	-0.63100300	-6.18483500	1.10881600
C	-2.00572200	2.41655300	-2.35219800	C	-0.29023000	-6.19897600	-1.01721500
C	-2.65581200	3.35002600	-3.16458000	H	-0.50660100	-7.25488700	-1.12659700
H	-3.45533700	3.02018100	-3.82096900	C	0.07076100	-5.43943300	-2.13115400
C	-2.27691900	4.69066100	-3.12760800	H	0.13660600	-5.90453600	-3.10793400
H	-2.77456800	5.41597500	-3.75962700	C	0.35284500	-4.07879000	-1.98913800
C	-1.25689200	5.09179000	-2.26453500	H	0.62942100	-3.49971000	-2.86409400
H	-0.96091000	6.13485700	-2.21610500	C	1.95271500	-1.24084200	-1.76854300
C	-0.59493100	4.17283100	-1.44041800	H	1.57481800	-1.45475600	-2.77257800
C	0.45723500	4.65254400	-0.49409200	H	2.07912900	-0.15584700	-1.68418900
C	0.07119000	5.15273200	0.76422600	C	3.21427100	-2.00079200	-1.46314000
C	1.04755000	5.65301400	1.62781200	C	3.57034700	-3.12495600	-2.25778800
H	0.74725700	6.04937200	2.59467200	H	2.95709400	-3.37623800	-3.11634300

C	4. 68101400	-3. 87354700	-1. 96775700	H	-4. 68679900	-2. 20667300	3. 58299700
H	4. 95245500	-4. 72193000	-2. 58725300	H	-1. 50400700	-0. 49912200	0. 72423900
C	5. 49314700	-3. 55740600	-0. 84638600	H	-4. 10235500	-2. 87497900	1. 27245100
C	5. 15833500	-2. 42703500	-0. 04187300	C	-6. 29752700	-1. 16788300	1. 45257700
C	4. 01490800	-1. 63232500	-0. 38872900	C	-6. 92992600	-1. 83483000	0. 39192500
C	6. 62878700	-4. 34401500	-0. 50884700	C	-6. 87216700	0. 00556100	1. 96787400
H	6. 87371800	-5. 19572500	-1. 13508300	C	-8. 11888000	-1. 33827700	-0. 14459300
C	7. 39685500	-4. 03523700	0. 58665300	H	-6. 49716800	-2. 74277500	-0. 02083900
H	8. 26097100	-4. 63883400	0. 83747900	C	-8. 05634200	0. 50334100	1. 42706500
C	7. 05750800	-2. 92327200	1. 39832500	H	-6. 39338500	0. 53755200	2. 78468600
H	7. 66403700	-2. 69127700	2. 26590000	C	-8. 67897000	-0. 16924300	0. 37203600
C	5. 96959300	-2. 14015700	1. 09421200	H	-8. 60343900	-1. 85917800	-0. 96155900
H	5. 71722300	-1. 29194500	1. 71944800	H	-8. 49484000	1. 40986000	1. 82657800
C	1. 53108400	-1. 52286500	1. 10434900	H	-9. 60091000	0. 21794900	-0. 04535200
H	0. 79579000	-1. 43454500	1. 90745300	C	-0. 65878500	-2. 88404100	3. 94954300
H	2. 06817000	-2. 47089000	1. 21123600	C	-1. 53757000	-2. 14519000	3. 16628800
C	2. 48133400	-0. 35302800	1. 10860200	C	-1. 51772400	-0. 73856400	3. 20924000
C	2. 13843000	0. 82270300	1. 82636100	C	-0. 58076300	-0. 09178100	4. 03425700
H	1. 18533700	0. 85204500	2. 34203400	C	0. 30190200	-0. 83660400	4. 81366200
C	2. 96730900	1. 91392000	1. 83926500	C	0. 26120600	-2. 23103100	4. 77796500
H	2. 68541300	2. 82087800	2. 36572600	H	-0. 67560000	-3. 96665800	3. 90550600
C	4. 19354000	1. 89181300	1. 12425200	H	-2. 18379000	-2. 66123900	2. 46534100
C	4. 54383600	0. 73082800	0. 37215900	H	-0. 54086600	0. 98989000	4. 07314800
C	3. 67167100	-0. 40850200	0. 39599100	H	1. 02104300	-0. 32834500	5. 44351900
C	5. 07394600	3. 00856600	1. 13343600	H	0. 94908800	-2. 80890400	5. 38316000
H	4. 80120000	3. 87246000	1. 73083300	C	-2. 45284000	0. 06420100	2. 41349300
C	6. 23557300	2. 99657700	0. 40135100	C	-2. 26876300	1. 52280100	2. 23094300
H	6. 90138000	3. 85170400	0. 41437400	H	-1. 32012700	1. 73945300	1. 71279500
C	6. 56604400	1. 86063600	-0. 38061000	H	-3. 08673200	1. 91565700	1. 62985500
H	7. 47534300	1. 86406000	-0. 97006900	H	-2. 26587600	2. 02848900	3. 20402600
C	5. 74610400	0. 75773300	-0. 39400800	O	-3. 62542900	-0. 40111000	2. 08071800
H	6. 00968900	-0. 10534900	-0. 99311900				
Si	-4. 69670000	-1. 82268800	2. 14466500				

I8

$G_{\text{gas}} = -2234.538043 \text{ a. u.}$

$E_{\text{gas}} = -2235.271499 \text{ a. u.}$

				H	3.79459800	-0.52859200	2.76778600
				H	2.34864200	0.42062700	2.39999200
Ru	-1.08992600	-0.94273000	-0.17323000	H	3.67751400	1.15240500	3.31260300
S	0.99636600	0.05239400	-0.23338900	H	6.93988600	3.97745900	0.13261900
P	-2.21690600	1.38383100	-0.06083600	H	5.42063900	4.73481500	0.61569600
C	2.07740300	-1.41745800	0.02267300	H	5.78761200	4.49397500	-1.10016800
C	3.46243200	-1.23278200	0.11862400	H	5.16633100	-1.18862500	-2.26154500
C	4.27195600	-2.36748800	0.28439100	H	5.00847100	0.27331300	-3.24416400
C	3.72311300	-3.64608200	0.35795200	H	3.56484900	-0.55616500	-2.63976000
C	2.33943200	-3.81562700	0.27636700	H	-2.56295300	-2.84531700	-2.19899300
C	1.51673600	-2.70121600	0.11318000	H	-2.72620000	-2.41442900	2.07838500
C	4.06774400	0.13029600	0.05716800	H	1.04997700	-2.40480600	-2.46025800
C	4.06927100	0.94590600	1.20379300	H	-0.46889700	-2.68154900	-3.33712200
C	4.64737900	2.21538500	1.12827500	H	0.42734200	-4.04693800	-2.64807400
C	5.21977000	2.69120800	-0.05493800	H	-0.73060200	-2.03614100	3.32376200
C	5.19326000	1.86827900	-1.18451400	H	0.84755000	-1.87455600	2.52082500
C	4.62615800	0.59208600	-1.14825600	H	0.24053500	-3.47310700	2.95464900
C	3.44208100	0.47059100	2.49266200	C	-4.15823000	1.12260300	-0.02664000
C	5.87311200	4.04962100	-0.10540400	C	-4.51232700	0.41011900	1.29212300
C	4.59218700	-0.26533500	-2.39066600	C	-5.00294800	2.40324400	-0.13932300
C	0.03271400	-2.81894500	0.05653700	C	-4.55170000	0.19191600	-1.19399500
C	-0.63528700	-2.88257400	-1.20537100	H	-3.89695900	-0.48075000	1.44602700
C	-2.06510300	-2.81224200	-1.23623600	H	-4.40136500	1.05775300	2.16275800
C	-2.84197300	-2.74940500	-0.05803700	H	-5.56316500	0.09933000	1.24817900
C	-2.15764700	-2.56404400	1.16690900	H	-4.89634900	2.87909700	-1.11598800
C	-0.73267600	-2.61965800	1.25595200	H	-6.05804600	2.12173800	-0.03182400
C	0.13702600	-3.00285200	-2.48788900	H	-4.77718900	3.13799500	0.63386600
C	-0.05679800	-2.48345400	2.59046200	H	-5.54051600	-0.23283400	-0.98265200
H	5.34496500	-2.22733300	0.36022500	H	-4.62426600	0.72538400	-2.14052700
H	4.36690500	-4.50748100	0.48624200	H	-3.84360300	-0.62992300	-1.32174400
H	1.89959400	-4.80510200	0.34453600	C	-1.81811300	2.61828100	-1.52501300
H	4.65562500	2.84500300	2.01359500	C	-2.56915700	2.15317200	-2.78608200
H	5.62341600	2.22794100	-2.11487900	C	-2.21714600	4.07176800	-1.21345600

C	-0.31750600	2.56636100	-1.86181700	P	-2.84289400	-1.53029900	-1.08759300
H	-2.43314900	1.08223700	-2.97270000	C	-2.88535800	2.46140100	1.09023300
H	-3.63607000	2.37816200	-2.74483600	C	-2.49533900	1.87498600	2.34200400
H	-2.15548200	2.69559500	-3.64384600	C	-3.35635100	0.94559600	2.94564500
H	-1.58762900	4.52008700	-0.44329800	H	-3.05382100	0.47969800	3.87819200
H	-2.07816200	4.66105200	-2.12798600	C	-4.62164700	0.63108800	2.39913200
H	-3.26006700	4.17458900	-0.91137300	C	-5.00319600	1.27101600	1.20881800
H	-0.12177900	3.32522100	-2.62880900	H	-5.98853900	1.06720700	0.79744500
H	0.33368300	2.77632500	-1.01356600	C	-4.17473400	2.21084600	0.55282900
H	-0.03727100	1.59387500	-2.27272800	C	-1.19520000	2.25750400	2.99764000
C	-1.66829400	2.21645200	1.63347100	H	-1.12504600	3.34394500	3.10900000
C	-0.28976000	2.88956900	1.48847600	H	-0.34415400	1.92900800	2.39046900
C	-2.66246900	3.27247500	2.14573900	H	-1.11892900	1.79898500	3.98646700
C	-1.50468600	1.09725600	2.68260100	C	-5.56973900	-0.27795600	3.13715800
H	0.47349600	2.20528300	1.11227500	H	-6.30817300	-0.71710700	2.46206200
H	-0.31618600	3.77762200	0.85621900	H	-6.11244500	0.28322700	3.90549300
H	0.02311600	3.21238300	2.48897600	H	-5.03529200	-1.09126300	3.63567200
H	-3.62546800	2.84854700	2.43421000	C	-4.68621000	2.94955500	-0.65848500
H	-2.23109500	3.73459900	3.04170100	H	-5.17018600	3.88521500	-0.35564700
H	-2.83417000	4.06745300	1.41690700	H	-5.42702600	2.35402000	-1.19839400
H	-1.26919200	1.56198200	3.64749300	H	-3.87937500	3.20897200	-1.34609900
H	-2.40266100	0.48997000	2.81389700	C	-0.76792500	2.79735400	-0.20102300
H	-0.67105000	0.44009200	2.41373300	C	-1.91731000	3.35360500	0.38827900
C	-4.33367400	-2.91825400	-0.09792100	C	-2.12572800	4.73715100	0.34992400
H	-4.73533600	-2.73486700	-1.09554500	H	-3.01748100	5.15145000	0.81040500
H	-4.57452900	-3.95197900	0.17389300	C	-1.19450000	5.57387800	-0.26063900
H	-4.84454200	-2.26211100	0.60947100	H	-1.36042900	6.64372100	-0.29381300
				C	-0.03862000	5.02328400	-0.81489800
I9				H	0.70463700	5.66557600	-1.27686400
G _{gas} = -3352.64306 a. u.				C	0.19392500	3.64357300	-0.78686800
E _{gas} = -3353.711028 a. u.				C	1.48017800	3.09930400	-1.31939700
Ru	-2.58270200	0.10755800	0.64200300	C	2.64901800	3.23394600	-0.54450500
S	-0.48883300	0.99643200	-0.20055300	C	3.86367400	2.76947300	-1.05836700

H	4. 76704700	2. 90738200	-0. 47040000	C	1. 30441200	-3. 99841800	2. 17695100
C	3. 94202600	2. 13842000	-2. 30237100	C	2. 40434600	-3. 14788500	1. 98640400
C	2. 76655400	1. 99184300	-3. 04582900	C	2. 87635300	-2. 36505300	3. 05180900
H	2. 80954400	1. 51631200	-4. 02270800	C	2. 23794800	-2. 41643600	4. 28815300
C	1. 53936200	2. 48126600	-2. 58259500	C	1. 12150000	-3. 23685700	4. 46392600
C	2. 60540300	3. 87043500	0. 82475800	H	-0. 20989600	-4. 66233400	3. 54639500
H	3. 54515100	3. 70053000	1. 35850400	H	0. 93506100	-4. 60762300	1. 35889500
H	1. 78907400	3. 45330100	1. 42552200	H	3. 74728400	-1. 73323700	2. 91381600
H	2. 43576100	4. 95063400	0. 76214200	H	2. 61315400	-1. 81826200	5. 10961900
C	5. 26989300	1. 63852100	-2. 81510300	H	0. 62087600	-3. 27055400	5. 42411700
H	5. 18680000	1. 26659000	-3. 83935500	C	3. 08519000	-3. 08413000	0. 68110400
H	5. 65174100	0. 81686200	-2. 19552600	N	3. 34251400	-1. 92332700	0. 12801900
H	6. 02004900	2. 43531800	-2. 80404800	C	3. 50326700	-4. 37150300	0. 03519300
C	0. 30358200	2. 38496900	-3. 44223100	H	3. 51937100	-4. 29642500	-1. 05300100
H	-0. 00513000	3. 37664200	-3. 79119300	H	4. 51292300	-4. 63928700	0. 36863800
H	-0. 53231800	1. 96250600	-2. 87605000	H	2. 84040500	-5. 17766800	0. 35041700
H	0. 48432100	1. 75841100	-4. 31993500	C	4. 18366600	-1. 86369500	-1. 05579700
Si	2. 45065700	-0. 26242900	0. 58361100	C	3. 61359300	-1. 62691800	-2. 30820100
H	1. 26531500	-0. 76470900	1. 30901600	C	5. 55746300	-2. 06990400	-0. 91383000
H	-1. 73696700	-1. 04621300	1. 26280100	C	4. 43343200	-1. 63489700	-3. 43681200
H	2. 32438100	0. 25084800	-0. 79747400	H	2. 54845600	-1. 44181100	-2. 39566600
C	3. 59678900	0. 66779600	1. 74454800	C	6. 36863800	-2. 06599600	-2. 04942500
C	4. 93965600	0. 91406700	1. 41938900	H	5. 97910200	-2. 22879600	0. 07354900
C	3. 09596100	1. 12517900	2. 97360500	C	5. 80602700	-1. 85958200	-3. 31063500
C	5. 76395600	1. 61128600	2. 30362300	H	3. 99781300	-1. 46008800	-4. 41324300
H	5. 34020500	0. 57888300	0. 46563300	H	7. 43498900	-2. 22603900	-1. 94767400
C	3. 91735400	1. 83178100	3. 85400700	H	6. 43697400	-1. 86225500	-4. 19106700
H	2. 05974300	0. 93310500	3. 24046200	C	-3. 86207800	-3. 02660600	-0. 32888200
C	5. 25061100	2. 07476900	3. 51830900	C	-4. 88703500	-2. 42726000	0. 65212400
H	6. 79977100	1. 79943900	2. 04580100	C	-4. 59639000	-3. 91614200	-1. 34489200
H	3. 51949900	2. 19370500	4. 79485800	C	-2. 93061000	-3. 89937600	0. 53627500
H	5. 88942700	2. 62356300	4. 20040400	H	-4. 36466600	-1. 92352600	1. 47049700
C	0. 65487900	-4. 02506500	3. 40833600	H	-5. 57188400	-1. 71624600	0. 18627200

H	-5.48400600	-3.24405200	1.07784400
H	-3.93265000	-4.33995400	-2.09985600
H	-5.05755000	-4.75112600	-0.80207200
H	-5.40051700	-3.38131100	-1.85507700
H	-3.55610900	-4.59563300	1.10895000
H	-2.23349400	-4.49805500	-0.05212200
H	-2.36823400	-3.28463100	1.24679300
C	-1.22654200	-2.30779400	-1.88339700
C	-1.46864400	-3.64402200	-2.60786000
C	-0.58695200	-1.33361200	-2.89273100
C	-0.19258600	-2.51352500	-0.76113700
H	-1.76826700	-4.44647300	-1.93266500
H	-2.21862000	-3.56087900	-3.39665300
H	-0.52597500	-3.94904800	-3.08104900
H	-0.41204300	-0.34877400	-2.45208200
H	0.38214400	-1.75870800	-3.19043500
H	-1.17505500	-1.22535100	-3.80509600
H	0.71018100	-2.96474900	-1.20414200
H	0.06789000	-1.55210700	-0.31542300
H	-0.54766000	-3.16506500	0.03733300
C	-3.87968800	-0.77461100	-2.56746400
C	-3.24507400	0.58660200	-2.92019800
C	-3.97390300	-1.63739500	-3.83614800
C	-5.30710400	-0.49633000	-2.06400500
H	-3.06332600	1.18625900	-2.02309900
H	-2.29622000	0.48286700	-3.44669800
H	-3.93343500	1.13417700	-3.57648100
H	-4.40303400	-2.62304600	-3.64509700
H	-4.63013700	-1.12351900	-4.55025400
H	-3.00770200	-1.76869200	-4.32606700
H	-5.82917300	0.10560700	-2.81794800
H	-5.88704400	-1.40961400	-1.91499500
H	-5.29142300	0.06938900	-1.12878900

I10

$G_{\text{gas}} = -3141.703006 \text{ a. u.}$

$E_{\text{gas}} = -3142.68325088 \text{ a. u.}$

Ru	1.44389700	-0.35623600	-0.72403900
S	-0.95529300	-0.47893800	-0.21806600
P	1.51090000	1.90803200	-0.09422500
C	0.80997800	-1.68913600	-2.43346000
C	1.57375600	-2.56862900	-1.58582600
C	2.89037100	-2.18712200	-1.25086000
H	3.45657700	-2.80295400	-0.55754800
C	3.48324200	-0.99893900	-1.76415300
C	2.73921400	-0.23214900	-2.70101200
H	3.19906600	0.65229500	-3.13237900
C	1.42443700	-0.58121300	-3.10024500
C	0.97322200	-3.83111700	-1.02481000
H	0.20455900	-4.22938300	-1.69171100
H	0.52628500	-3.64232400	-0.04246000
H	1.74912000	-4.59069200	-0.90054200
C	4.89632900	-0.62854700	-1.40612800
H	5.08271900	0.43405600	-1.57966900
H	5.60792900	-1.19815000	-2.01331200
H	5.09718900	-0.85064500	-0.35592300
C	0.68763800	0.22942100	-4.13539300
H	0.55076500	-0.34914500	-5.05490800
H	1.24995300	1.13102200	-4.38879200
H	-0.30603400	0.52585400	-3.78692600
C	-1.58401900	-1.28414500	-1.77119900
C	-0.65804500	-1.88493700	-2.64232700
C	-1.11714600	-2.53461800	-3.79235200
H	-0.39889100	-3.00134500	-4.45839800
C	-2.47795700	-2.55226400	-4.09189000
H	-2.83136700	-3.05682200	-4.98289400

C	-3.37635100	-1.87801600	-3.26866200	H	1.87021500	-4.67596700	1.97602500
H	-4.42830300	-1.83466500	-3.52947200	C	5.13272600	-3.87554700	1.45616500
C	-2.95280800	-1.22358600	-2.10110600	H	5.99619600	-1.92681100	1.77315400
C	-3.94302900	-0.43840100	-1.30046400	H	4.00292700	-5.70037100	1.26167600
C	-5.00678900	-1.06868300	-0.62286400	H	6.07152200	-4.33163600	1.16390300
C	-5.86017800	-0.29195300	0.17068200	C	-2.70210600	-0.84621200	4.71787500
H	-6.65856800	-0.78686500	0.71725200	C	-2.01818300	-1.48402200	3.68349400
C	-5.72502500	1.09296200	0.26723300	C	-2.04278000	-0.96332200	2.37954100
C	-4.72118800	1.71077800	-0.48676200	C	-2.82039100	0.17254400	2.12439500
H	-4.63375600	2.79375700	-0.47065800	C	-3.51217200	0.80393800	3.16004100
C	-3.83806600	0.97196900	-1.27709200	C	-3.44402000	0.30809700	4.46196500
C	-5.30921700	-2.54660000	-0.75459700	H	-2.66610200	-1.26031700	5.71848700
H	-5.58908000	-2.97355800	0.21279000	H	-1.48883700	-2.40772800	3.88678200
H	-4.47159800	-3.11992300	-1.15454500	H	-2.90497600	0.56701000	1.11998700
H	-6.15874400	-2.69398100	-1.43103500	H	-4.10721700	1.68344200	2.93671600
C	-6.66486800	1.89994100	1.12734400	H	-3.97633600	0.80297800	5.26548300
H	-6.29316200	2.91680800	1.27539700	C	-1.34389500	-1.77055300	1.28964100
H	-6.79497500	1.43525000	2.10914800	C	-2.24528100	-2.86327400	0.74801200
H	-7.65491700	1.97228100	0.66534200	H	-3.19849100	-2.43931500	0.44110400
C	-2.82664600	1.69591100	-2.13304100	H	-1.78138300	-3.38885900	-0.08924600
H	-2.92958900	1.41224600	-3.18651000	H	-2.41975600	-3.57284900	1.56253500
H	-1.80127200	1.46302700	-1.83066900	O	-0.14522400	-2.35302500	1.69608500
H	-2.96511500	2.77763700	-2.05807000	C	3.28072100	2.46123900	0.25638800
Si	1.09826600	-1.94362300	2.85948800	H	3.72684600	1.63768100	0.82942000
H	0.70876900	-2.63322300	4.12497000	H	3.76128000	2.44671800	-0.73111300
H	1.79674400	-0.38296300	0.80374200	C	0.86168400	2.96987300	-1.51787800
H	1.20405400	-0.47283000	3.08173600	H	-0.18809600	2.67308000	-1.61045600
C	2.70479300	-2.69928800	2.24086300	H	1.36962300	2.56546100	-2.40424900
C	3.87863400	-1.93485800	2.17410900	C	3.56602900	3.80206900	0.96742600
C	2.76475500	-4.06261400	1.91440700	H	2.86263800	4.56563600	0.61002800
C	5.08900000	-2.52080700	1.79606500	C	0.99618600	4.50671200	-1.51512200
H	3.84870300	-0.87612500	2.41905800	H	0.89688100	4.88513200	-0.48955800
C	3.96857100	-4.64614500	1.51187100	C	4.99258300	4.25514500	0.61383100

H	5.23528600	5.19833200	1.11115500	S	-0.89397300	-0.65491100	-0.68195700
H	5.71860200	3.50302800	0.94449300	P	2.39270500	-0.00492100	-1.86048000
H	5.11920300	4.39672900	-0.46417500	C	0.10606900	-3.16231400	0.99989400
C	-0.13208900	5.11713900	-2.36282400	C	0.84031400	-2.96372700	2.19210800
H	-1.11895700	4.89256200	-1.94628500	C	2.23176100	-3.19898100	2.19123400
H	-0.02813000	6.20435900	-2.42282200	H	2.78486200	-3.04121000	3.11386800
H	-0.09426900	4.71765500	-3.38322100	C	2.89723700	-3.69846300	1.07283300
C	2.35190600	4.94688700	-2.08586400	C	2.12963200	-3.99785800	-0.06886800
H	2.40665600	4.68563300	-3.14950800	H	2.60530400	-4.49408800	-0.91065800
H	2.47760900	6.03015400	-2.00074700	C	0.75355300	-3.76260500	-0.12117600
H	3.19361000	4.46937500	-1.57932500	C	0.14251600	-2.70939800	3.50449000
C	3.43475100	3.69556100	2.49343200	H	-0.28438900	-3.64801400	3.87648300
H	3.72982200	4.63791700	2.96419700	H	-0.67947500	-2.00418500	3.40522700
H	2.41618800	3.47222000	2.81544200	H	0.83902600	-2.34993800	4.26611500
H	4.09666700	2.90939900	2.87585800	C	4.37963000	-3.96876000	1.10626700
C	0.52040300	2.17244600	1.49166400	H	4.66984500	-4.44613500	2.04587100
H	-0.28261900	1.42700700	1.47102100	H	4.95457600	-3.03941200	1.01736000
H	1.21445800	1.84938900	2.27657700	H	4.68098900	-4.62311700	0.28487200
C	-0.09848500	3.53854400	1.82873900	C	-0.07154900	-4.32856800	-1.25027200
H	0.62626700	4.34010000	1.62786400	H	-0.65902300	-5.17419100	-0.87382400
C	-0.44717600	3.56186300	3.32598100	H	0.56540600	-4.68760200	-2.06102700
H	-0.93548000	4.50249200	3.59690100	H	-0.78308000	-3.60499700	-1.65271000
H	-1.13423500	2.73956200	3.56089300	C	-1.92402000	-1.96486200	0.08830600
H	0.44410200	3.44846200	3.95125600	C	-1.37429500	-2.97012400	0.90801100
C	-1.37007100	3.78416000	1.00434300	C	-2.21718900	-3.89997400	1.52861500
H	-1.80639900	4.75873600	1.24377000	H	-1.78021600	-4.67919600	2.14555800
H	-1.18080300	3.75386100	-0.07108200	C	-3.59485200	-3.85671400	1.32614600
H	-2.11345400	3.00988300	1.23520100	H	-4.24048400	-4.58681400	1.79902100
TS _{RI9-II}				C	-4.12901300	-2.89014900	0.47562600
				H	-5.19432900	-2.87489100	0.26793000
				C	-3.31536400	-1.93550300	-0.15281500
				C	-3.94513900	-0.97363300	-1.11489600
				C	-4.81085300	0.04785700	-0.66377500
G _{gas} = -3352.593394 a. u.							
E _{gas} = -3353.66692 a. u.							
Ru	1.31608900	-0.91656800	0.12801400				

C	-5.41316600	0.89503400	-1.59770200	C	3.88526100	3.95886700	2.63059800
H	-6.07217300	1.68261200	-1.24263700	C	3.14536100	2.78259200	2.75910600
C	-5.19216900	0.75858400	-2.97102700	C	1.92128600	2.63039200	2.08668600
C	-4.35789000	-0.27364800	-3.40141900	C	1.48635700	3.67453300	1.26144700
H	-4.19805000	-0.41938000	-4.46612000	C	2.21025800	4.85875100	1.15328300
C	-3.73974900	-1.14804200	-2.49993300	C	3.41482200	5.00790200	1.84049400
C	-5.11126500	0.26019100	0.80191800	H	4.82324800	4.05820000	3.16351800
H	-4.23501900	0.62015000	1.35114000	H	3.52733900	2.00232300	3.40355900
H	-5.44367700	-0.65943500	1.29146300	H	0.60731800	3.54822600	0.64554300
H	-5.89956600	1.00648800	0.92185300	H	1.84168500	5.65006800	0.50966900
C	-5.83557900	1.71016400	-3.94820800	H	3.98508800	5.92506600	1.75551200
H	-6.91612600	1.77037900	-3.78880800	C	1.07686500	1.40617500	2.33003100
H	-5.66242200	1.39670000	-4.98006900	N	-0.24966800	1.64083000	2.62251000
H	-5.43237600	2.72247000	-3.83019300	C	1.76218800	0.31899700	3.14494500
C	-2.89505000	-2.27725900	-3.03993500	H	1.90366600	0.66116800	4.17587700
H	-3.06676400	-3.20449300	-2.48451900	H	1.15431100	-0.57853100	3.16434500
H	-1.82714500	-2.03806300	-2.96663400	H	2.73380800	0.08279200	2.70810000
H	-3.12918700	-2.46130400	-4.09117000	C	-1.03416900	0.64625200	3.33750100
Si	-1.28821500	3.17693500	2.38522500	C	-0.89344000	0.51045700	4.72305700
H	-0.55206700	4.32621500	2.98337000	C	-2.03802900	-0.04645500	2.66521000
H	1.19500200	0.65710500	0.98715100	C	-1.74731700	-0.34101500	5.42420200
H	-2.47926900	2.82554300	3.20104800	H	-0.14424000	1.09270900	5.24836600
C	-1.74686300	3.56518600	0.59521500	C	-2.89875500	-0.89072600	3.37101200
C	-2.28536700	2.59182500	-0.25713300	H	-2.12997500	0.07562000	1.59316100
C	-1.53597000	4.86341700	0.09641600	C	-2.75299900	-1.04116500	4.75053600
C	-2.58134700	2.89574800	-1.58851500	H	-1.64174800	-0.44014400	6.49799700
H	-2.45094900	1.57707600	0.08659700	H	-3.67050600	-1.43081600	2.83376600
C	-1.85311500	5.17556000	-1.22570000	H	-3.42257200	-1.69101900	5.30096500
H	-1.11837400	5.63285900	0.74164300	C	4.25673900	-0.53648000	-1.57801200
C	-2.36753400	4.18780600	-2.07110400	C	4.53242500	-0.31754800	-0.07374200
H	-2.97179000	2.11651300	-2.23483700	C	4.43676200	-2.04217800	-1.83837900
H	-1.69657300	6.18200400	-1.59663800	C	5.29375000	0.20113200	-2.44139200
H	-2.60041900	4.42736200	-3.10260200	H	4.43130400	0.72072200	0.24342000

H	3.85250200	-0.93534800	0.54053700	H	0.52076100	1.96501800	-0.86508000
H	5.55526000	-0.64528500	0.15196700				
H	4.36226700	-2.30384600	-2.89459800	TS _{SI9-I1}			
H	5.44194600	-2.32624400	-1.50188100	G _{gas} = -3352.598893 a. u.			
H	3.71557400	-2.63468100	-1.27535700	E _{gas} = -3353.66581105 a. u.			
H	6.28261200	-0.22030600	-2.22089200	Ru	-0.03714900	-1.01330800	-0.75133300
H	5.10677000	0.05624200	-3.50783400	S	1.85009600	0.19311200	0.06381400
H	5.34829300	1.27052500	-2.24596700	P	-0.47749800	-1.99316800	1.38366300
C	1.76414700	-0.80311600	-3.52858300	C	1.80810500	-1.68112000	-2.47801500
C	2.79818300	-0.74329900	-4.66600500	C	1.06568800	-0.65474100	-3.13895600
C	1.39760100	-2.26426500	-3.23492900	C	-0.23438500	-0.93210100	-3.57434700
C	0.46394200	-0.11701200	-3.99536500	H	-0.78712700	-0.14601600	-4.08208400
H	3.13112400	0.27141400	-4.88785500	C	-0.80613200	-2.21889200	-3.45624600
H	3.67609000	-1.36089800	-4.46900400	C	-0.02334800	-3.23178700	-2.90428400
H	2.32119800	-1.13937200	-5.57089200	H	-0.41452000	-4.24563000	-2.86527200
H	0.58514700	-2.29244200	-2.50813700	C	1.28875600	-2.99498300	-2.43093900
H	1.04269000	-2.73073900	-4.16267600	C	1.72104200	0.66030900	-3.45489800
H	2.23387700	-2.85708100	-2.85974900	H	2.60160100	0.49146600	-4.08450100
H	0.05385100	-0.71721200	-4.81728100	H	2.05731500	1.16784900	-2.54787600
H	-0.28795200	-0.08313600	-3.20229200	H	1.03154600	1.31900800	-3.98522900
H	0.62609800	0.88960700	-4.38126500	C	-2.20191200	-2.49836200	-3.95463200
C	2.33946100	1.92266900	-2.09148300	H	-2.24017200	-3.44318400	-4.50286100
C	3.25799700	2.57950200	-1.05192500	H	-2.54791300	-1.70719800	-4.62478700
C	2.78748200	2.41639200	-3.47745600	H	-2.91602300	-2.57556700	-3.12485500
C	0.88704200	2.35959400	-1.81841600	C	2.15998400	-4.16893700	-2.05310100
H	3.04552500	2.23186300	-0.04179600	H	2.81443000	-4.41893200	-2.89544000
H	4.31504200	2.42374400	-1.26441300	H	1.55974000	-5.05344100	-1.83403500
H	3.07879200	3.65901900	-1.07463400	H	2.80586500	-3.95637400	-1.20005400
H	2.12688400	2.09597100	-4.28251800	C	3.29293100	-0.49396200	-0.83154000
H	2.76943600	3.51310800	-3.45989400	C	3.16113100	-1.34566100	-1.94456500
H	3.80818300	2.10849100	-3.71811600	C	4.30618000	-1.83056200	-2.59043800
H	0.84089700	3.45667500	-1.78127000	H	4.19200000	-2.47119500	-3.45942800
H	0.19451900	2.02956200	-2.59399800	C	5.57607500	-1.48178100	-2.14007200

H	6.45719600	-1.85913700	-2.64444900	C	-6.89183400	-1.25191800	0.10307100
C	5.70230000	-0.63470900	-1.03904900	H	-5.96754400	0.02612400	-1.35152400
H	6.68487600	-0.35026100	-0.67672300	C	-7.12873300	-1.48367600	1.46152400
C	4.57726700	-0.13003800	-0.37850900	H	-6.81128000	-0.78034500	3.47267500
C	4.74982400	0.77983500	0.79465000	H	-7.31917200	-1.91204100	-0.64265000
C	4.66607100	2.17394100	0.61637000	H	-7.73256200	-2.32983700	1.76802000
C	4.82499000	3.01202800	1.72120300	C	-2.13588500	1.46288100	-1.09872100
H	4.76379900	4.08805900	1.58166100	N	-2.75656300	2.21324900	-0.14427000
C	5.06295100	2.50041500	3.00114600	C	-2.19649100	3.48516500	0.30843500
C	5.13837500	1.11519300	3.15750000	C	-2.30179700	4.60269200	-0.52624500
H	5.32001000	0.69971800	4.14527100	C	-1.65252200	3.60521700	1.58396400
C	4.99396400	0.24563400	2.07124400	C	-1.81783300	5.83533800	-0.09255700
C	4.39591100	2.75256500	-0.75079900	H	-2.72932900	4.49665000	-1.51812800
H	4.41850400	3.84510100	-0.72179300	C	-1.16584900	4.84215400	2.01107100
H	3.41067500	2.43460500	-1.11375300	H	-1.61385200	2.74332600	2.23473400
H	5.13606000	2.41411400	-1.48298500	C	-1.24227100	5.95550400	1.17401800
C	5.26311500	3.42543000	4.17619700	H	-1.88895000	6.69805400	-0.74362100
H	4.65480400	4.32859600	4.07851400	H	-0.73188300	4.93321400	2.99940100
H	6.30952800	3.74076300	4.25161800	H	-0.86391800	6.91351500	1.50918300
H	4.99875100	2.93480100	5.11635700	C	-2.34115700	-2.54576900	1.24314400
C	5.11527900	-1.24501400	2.27677400	C	-2.56830400	-2.98739900	-0.21911400
H	6.13408300	-1.59145400	2.06697900	C	-2.80314900	-3.65775800	2.19714700
H	4.44732100	-1.79341000	1.60781800	C	-3.23954300	-1.32139300	1.46269400
H	4.87941800	-1.51629700	3.30966500	H	-2.28626600	-2.18396100	-0.91730600
Si	-4.60522700	2.24914500	0.18989100	H	-2.01943800	-3.88876300	-0.49362600
H	-5.13117000	2.80304400	-1.09673300	H	-3.63968700	-3.18218000	-0.36270100
H	-1.11869400	0.30441200	-0.39534600	H	-2.63327000	-3.40003700	3.24470800
H	-4.67883000	3.21914700	1.30878500	H	-3.88377900	-3.79696800	2.06190500
C	-5.56781100	0.70774400	0.66494400	H	-2.32398100	-4.61689200	1.99538200
C	-5.83555200	0.47831200	2.02436700	H	-4.25522600	-1.58524300	1.14767600
C	-6.12339100	-0.15717100	-0.29198200	H	-3.29803900	-1.01296400	2.50764500
C	-6.60951700	-0.61335400	2.42124400	H	-2.90560300	-0.46306000	0.87134400
H	-5.44074800	1.15314500	2.77842100	C	-0.26394900	-0.89197900	2.98035400

C	-1.08578300	-1.40051100	4.17918200	H	1.71161900	4.05963000	-1.65718800
C	1.21351700	-0.80621400	3.41884200	H	-0.95935900	3.64535700	-5.00120400
C	-0.70314000	0.53481800	2.61599500	H	1.05513000	4.67688400	-3.97540200
H	-2.16272300	-1.33712000	4.01788800	C	-3.03159300	0.46460000	-1.79975200
H	-0.83662400	-2.42809500	4.45058900	H	-3.53360000	-0.18907600	-1.08420000
H	-0.84728800	-0.76595800	5.04151800	H	-3.79959000	1.00600400	-2.36901400
H	1.87158100	-0.50558200	2.60081200	H	-2.45265500	-0.14961100	-2.48728600
H	1.27709900	-0.03643600	4.19811400				
H	1.57537400	-1.73724500	3.85862600	TS_{RII0-II}			
H	-0.61498800	1.15721400	3.51638200	G_{gas} = -3141.655022 a. u.			
H	-0.05330300	0.95593000	1.84304500	E_{gas} = -3142.630049 a. u.			
H	-1.73606900	0.58397700	2.26408700	Ru	-0.05227200	-1.28725300	-0.39408800
C	0.58983200	-3.60189200	1.64051500	S	-1.65043000	0.31789200	0.41009300
C	2.05908400	-3.23225000	1.37009100	P	0.80686100	0.26693400	-2.06145700
C	0.47695000	-4.23187500	3.03906300	C	-2.01044300	-2.71467700	-0.14653200
C	0.16302500	-4.65400500	0.60360300	C	-1.16201100	-3.02879600	0.96389000
H	2.18278200	-2.72368300	0.40944100	C	0.08794300	-3.61841700	0.71166300
H	2.46710300	-2.57796800	2.13863800	H	0.74576700	-3.83771100	1.54847700
H	2.65579100	-4.15352600	1.35937200	C	0.48681700	-4.00065100	-0.59178800
H	-0.55058400	-4.48606200	3.30663800	C	-0.39598800	-3.74742100	-1.64888200
H	1.05826500	-5.16249300	3.03701000	H	-0.12493400	-4.07617000	-2.64864800
H	0.89303100	-3.59412100	3.81986500	C	-1.65374300	-3.12672000	-1.45544700
H	0.91296800	-5.45409400	0.59566400	C	-1.64194200	-2.77381400	2.36687800
H	-0.79919200	-5.11087300	0.84255900	H	-2.52206500	-3.38962400	2.58030100
H	0.11183900	-4.22920400	-0.40090000	H	-1.94433600	-1.72981800	2.49931800
C	-1.10365800	2.17684900	-1.92970200	H	-0.86515100	-3.02535500	3.09235900
C	0.05169600	2.73329500	-1.37004100	C	1.77537300	-4.74659800	-0.81667500
C	-1.45163800	2.49553400	-3.25234000	H	1.65791300	-5.80162200	-0.54659500
C	0.82545900	3.62783200	-2.10670700	H	2.58223100	-4.33679200	-0.20364300
H	0.33987600	2.47206200	-0.35916200	H	2.08192000	-4.70179600	-1.86453600
C	-0.67335500	3.39291800	-3.98695500	C	-2.62906300	-3.02435600	-2.60070300
H	-2.34744300	2.08168700	-3.70307800	H	-3.25694600	-3.92251400	-2.62919200
C	0.45886500	3.97037000	-3.41029900	H	-2.11252900	-2.95119000	-3.56030900

H	-3.29487300	-2.16714400	-2.49310500	H	4.75411400	0.84680700	3.50873000
C	-3.23039000	-0.59922000	0.37863600	C	4.57528900	2.64535100	1.29293500
C	-3.28080300	-1.97600400	0.10718200	C	3.79274000	3.69572400	1.79850800
C	-4.50864900	-2.64800800	0.09747500	C	5.40851900	2.87772900	0.18797900
H	-4.53045900	-3.71315400	-0.11305000	C	3.83647700	4.95424100	1.20104400
C	-5.68884200	-1.95605200	0.35813000	H	3.13524000	3.52970100	2.64683900
H	-6.63922300	-2.47552000	0.34961900	C	5.45376900	4.13905400	-0.40754800
C	-5.63645500	-0.58772000	0.62950200	H	6.01902700	2.07446700	-0.21530200
H	-6.54827200	-0.03492200	0.83153600	C	4.66514300	5.17429800	0.09752700
C	-4.42053100	0.10400100	0.64533600	H	3.22810800	5.76064000	1.59285400
C	-4.38896000	1.56949400	0.93264400	H	6.10031800	4.31311600	-1.25932200
C	-4.24925100	2.02355100	2.25512000	H	4.69861400	6.15360200	-0.36530900
C	-4.22242800	3.39891700	2.50214800	C	2.16782200	-3.65815100	4.01252100
H	-4.11918000	3.75024700	3.52529000	C	1.70448500	-2.38017400	3.69855400
C	-4.32434000	4.33051800	1.46563000	C	2.24833500	-1.68539800	2.60731700
C	-4.44196000	3.85713500	0.15545100	C	3.24784000	-2.28801300	1.82532400
H	-4.50996200	4.56806000	-0.66370800	C	3.70200800	-3.56511400	2.13997000
C	-4.47814300	2.48965400	-0.12698100	C	3.16473800	-4.25092400	3.23571400
C	-4.09639000	1.03755000	3.38751300	H	1.75609000	-4.18495600	4.86458700
H	-4.03504500	1.55332200	4.34850800	H	0.94019100	-1.91920700	4.31315300
H	-3.18255900	0.44381300	3.25556400	H	3.63265900	-1.77252000	0.95104700
H	-4.93508000	0.33555000	3.42758500	H	4.47061100	-4.02977600	1.53368300
C	-4.33135700	5.81154500	1.75392800	H	3.52453800	-5.24274100	3.48179700
H	-5.35573500	6.18285200	1.86746900	C	1.82113000	-0.29840000	2.34809300
H	-3.86632200	6.37595900	0.94126800	C	0.57919300	0.26242800	2.94226000
H	-3.79492400	6.03823800	2.67888400	H	0.79322100	0.49943300	3.99466900
C	-4.59362800	1.99985800	-1.54929500	H	0.29998900	1.18459400	2.43465300
H	-5.54878000	1.49171700	-1.72161000	H	-0.25652200	-0.43068100	2.87544300
H	-3.79998600	1.27774700	-1.77282500	O	2.72611600	0.58184400	2.01270200
H	-4.51786100	2.83005800	-2.25591800	C	0.83226400	2.18294500	-1.63924000
Si	4.47899300	0.94617000	2.04917400	C	1.17459100	2.33898400	-0.14946500
H	5.23217400	-0.06723500	1.26410200	C	1.84744400	2.98645000	-2.47361200
H	1.05198600	-0.59486100	0.60936900	C	-0.56129500	2.81398000	-1.84527300

H	0.38453100	1.90732400	0.46847000
H	2.12432100	1.88329200	0.12508600
H	1.24168500	3.41094200	0.07710600
H	1.69791200	2.87212800	-3.54892800
H	1.70700800	4.04733300	-2.23122600
H	2.88467300	2.74196800	-2.23486400
H	-0.53295800	3.81631500	-1.39991300
H	-0.81676900	2.93804700	-2.89873600
H	-1.34814300	2.25077800	-1.33920700
C	-0.17833800	0.08539800	-3.74155500
C	0.16863400	1.12210900	-4.82353700
C	0.08447100	-1.31345700	-4.32426300
C	-1.68055000	0.18854900	-3.40738400
H	-0.09350800	2.13848500	-4.52926100
H	1.22289900	1.10274900	-5.10582200
H	-0.41815900	0.88305600	-5.71962500
H	-0.08041500	-2.09274000	-3.57813600
H	-0.61487800	-1.48036900	-5.15259100
H	1.09487700	-1.41792700	-4.72517000
H	-2.25872400	-0.18853100	-4.26045100
H	-1.94182400	-0.39650500	-2.52051000
H	-1.98983800	1.21742100	-3.22612500
C	2.65475400	-0.29438900	-2.39968900
C	3.26324000	0.16130100	-3.73466100
C	3.53458800	0.21377200	-1.24526800
C	2.70420300	-1.83220500	-2.31446600
H	2.78303400	-0.31323600	-4.59253900
H	3.22073400	1.24307000	-3.86927800
H	4.32006800	-0.13515000	-3.75133600
H	3.06740300	-0.03007300	-0.28564800
H	4.51022000	-0.28949300	-1.30411300
H	3.71296700	1.28910300	-1.28100900
H	3.73292700	-2.16065100	-2.51311100

TS_{SI10-I1}

G_{gas} = -3141.685000 a. u.

E_{gas} = -3142.657683 a. u.

Ru	0.91697600	0.29227700	-0.87519400
S	-1.34351900	-0.48373900	-0.54805300
P	0.13815700	2.42235400	-0.23208900
C	0.83767700	-1.18132200	-2.61594300
C	2.01109200	-1.59250800	-1.92234300
C	3.02904600	-0.62548400	-1.68793900
H	3.90083800	-0.92771200	-1.11761500
C	2.95794400	0.68502700	-2.20009300
C	1.81240100	1.03014300	-2.97808300
H	1.75016800	2.03065100	-3.39823700
C	0.77054400	0.11785300	-3.23647200
C	2.20672900	-3.02173700	-1.48984800
H	2.46454400	-3.63773800	-2.35848200
H	1.29734800	-3.44527300	-1.05678400
H	3.02702700	-3.10785900	-0.76995400
C	4.09838000	1.65186800	-2.02442100
H	3.75417000	2.68822900	-2.04484000
H	4.82945200	1.52980300	-2.83088500
H	4.61535700	1.48508100	-1.07552400
C	-0.41580900	0.47924200	-4.08785700
H	-0.53217400	-0.24148500	-4.90281800
H	-0.29838200	1.47421500	-4.52345100
H	-1.33973700	0.45864800	-3.49827200
C	-1.40078900	-1.86180400	-1.75581600
C	-0.35549600	-2.07738400	-2.67056600
C	-0.43240300	-3.12637900	-3.59256600
H	0.38015500	-3.27756600	-4.29679000

C	-1.54367100	-3.96744600	-3.60548700	H	5.86408900	-0.96510600	0.12388200
H	-1.60663000	-4.77580700	-4.32355100	C	4.89011000	-4.32254300	1.80620100
C	-2.56834700	-3.76871800	-2.67870600	H	3.58158200	-3.16339500	3.05465600
H	-3.42812800	-4.43080100	-2.66450500	C	5.82460000	-4.29973700	0.76762000
C	-2.51107300	-2.72652000	-1.74678600	H	6.90964000	-3.06948000	-0.62920400
C	-3.57458000	-2.56466500	-0.71063800	H	4.62792200	-5.26127500	2.27948500
C	-3.48967300	-3.30859000	0.48008600	H	6.28376000	-5.22239100	0.43323000
C	-4.46254300	-3.12671000	1.46881500	C	-1.12943100	0.78029600	4.77378000
H	-4.39966800	-3.70611700	2.38684200	C	-0.00819300	0.39423900	4.05674600
C	-5.51934300	-2.22755800	1.29620900	C	-0.12808900	-0.54589300	3.01056800
C	-5.58128700	-1.49535500	0.10642400	C	-1.39165400	-1.08723400	2.69874300
H	-6.39341200	-0.78876200	-0.04107400	C	-2.51807000	-0.66987500	3.40597200
C	-4.62477900	-1.64865700	-0.90041600	C	-2.38743600	0.25436200	4.44267300
C	-2.36370100	-4.29295000	0.69549900	H	-1.03630800	1.49057600	5.58642800
H	-2.32958100	-4.62381100	1.73680300	H	0.97123600	0.78834700	4.29811900
H	-1.39425300	-3.85249000	0.43409700	H	-1.51187600	-1.80722600	1.90058900
H	-2.48286100	-5.17980500	0.06361400	H	-3.48753500	-1.07533100	3.14041800
C	-6.58201200	-2.06859100	2.35601600	H	-3.26294400	0.56585900	5.00155000
H	-6.92601300	-1.03280200	2.42161200	C	1.06255700	-0.99124400	2.30854600
H	-6.21170200	-2.37099900	3.33946300	C	1.05107900	-2.25855400	1.51985300
H	-7.45528400	-2.68970000	2.12957200	H	0.23483300	-2.24218100	0.79366400
C	-4.69844400	-0.82449200	-2.16163700	H	1.99452400	-2.39392200	0.99689300
H	-4.66859000	-1.45663900	-3.05439200	H	0.89719700	-3.09778600	2.21199600
H	-3.84600100	-0.13620100	-2.21750000	O	2.20861800	-0.52182400	2.77051800
H	-5.61716900	-0.23470200	-2.18941200	C	1.58322100	3.63124700	-0.08634700
Si	3.86903600	-0.29501800	2.20616600	H	2.35951000	3.08783700	0.46937600
H	4.47932200	0.27206000	3.43423500	H	1.94432000	3.71551200	-1.11962500
H	1.05486100	0.09374000	0.75504500	C	-0.97429300	3.01636200	-1.64220300
H	3.78546100	0.69901400	1.09498300	H	-1.83908700	2.34430400	-1.57512500
C	4.63046800	-1.91360900	1.63219800	H	-0.43780000	2.71934100	-2.55126600
C	5.57876200	-1.90227900	0.59670800	C	1.40057200	5.03398200	0.52728300
C	4.30077700	-3.13524400	2.24066800	H	0.43540700	5.45058400	0.21062400
C	6.17546800	-3.08932600	0.16737400	C	-1.40685500	4.48906100	-1.78950600

H	-1.59241700	4.92934200	-0.80198100
C	2.51669500	5.95709700	0.01156500
H	2.43488000	6.95258800	0.45711400
H	3.49771600	5.54717000	0.28004000
H	2.48194900	6.06855900	-1.07677200
C	-2.71517100	4.54818700	-2.59542700
H	-3.53039000	4.02811900	-2.08391500
H	-3.02253700	5.58467100	-2.76227600
H	-2.57388600	4.07575700	-3.57492700
C	-0.33290300	5.31540900	-2.51157600
H	-0.20748900	4.94385700	-3.53619000
H	-0.62644200	6.36751300	-2.57209200
H	0.63809100	5.26602300	-2.01380400
C	1.44329100	4.99315200	2.06021100
H	1.29262700	5.99374800	2.47596500
H	0.67863200	4.33746800	2.48001500
H	2.42332000	4.63375800	2.39659300
C	-0.83506600	2.44258500	1.38224800
H	-1.40283800	1.50233300	1.39385800
H	-0.06558400	2.34708200	2.15742800
C	-1.78176800	3.62521400	1.67330000
H	-1.33365700	4.55539900	1.29899400
C	-1.99189500	3.78261000	3.18732500
H	-2.62133500	4.65259400	3.39748200
H	-2.49308800	2.89542800	3.58722900
H	-1.04574200	3.90690900	3.72451400
C	-3.14596300	3.41456800	1.00149100
H	-3.79985800	4.27565700	1.17035800
H	-3.06180700	3.25754000	-0.07493700
H	-3.63025300	2.52766400	1.42700400

