

Supporting Information

Theoretical Elucidation of the Multi-Functional Synthetic Methodology for Switchable Ni(0)-Catalyzed C-H Allylations, Alkenylations and Dienylations with Allenes

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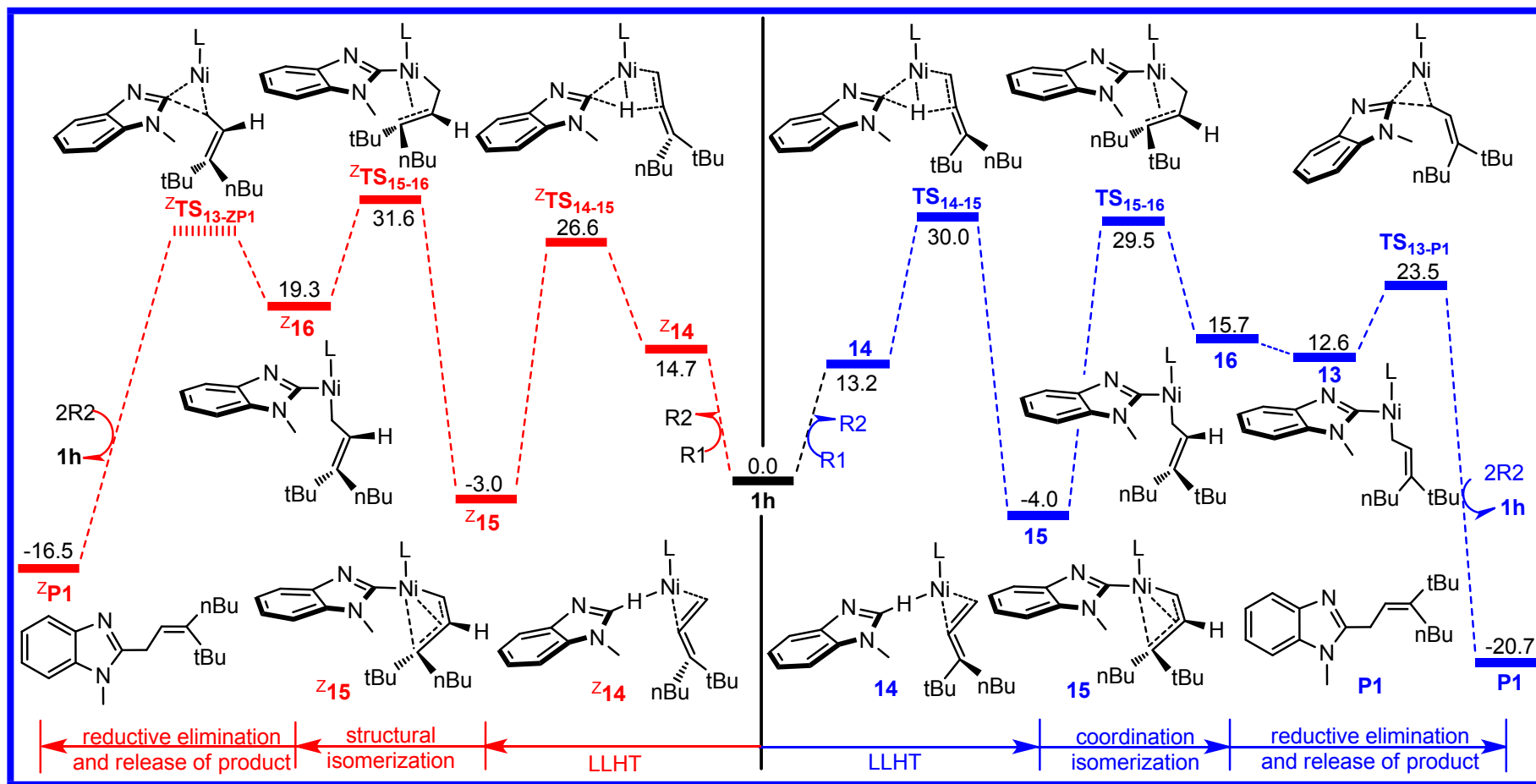


Fig. S1 Calculated free energy profiles in toluene along possible LLHT pathways in the absence of base. The relative free energies and bond distances are given in kcal mol⁻¹ and Å, respectively.

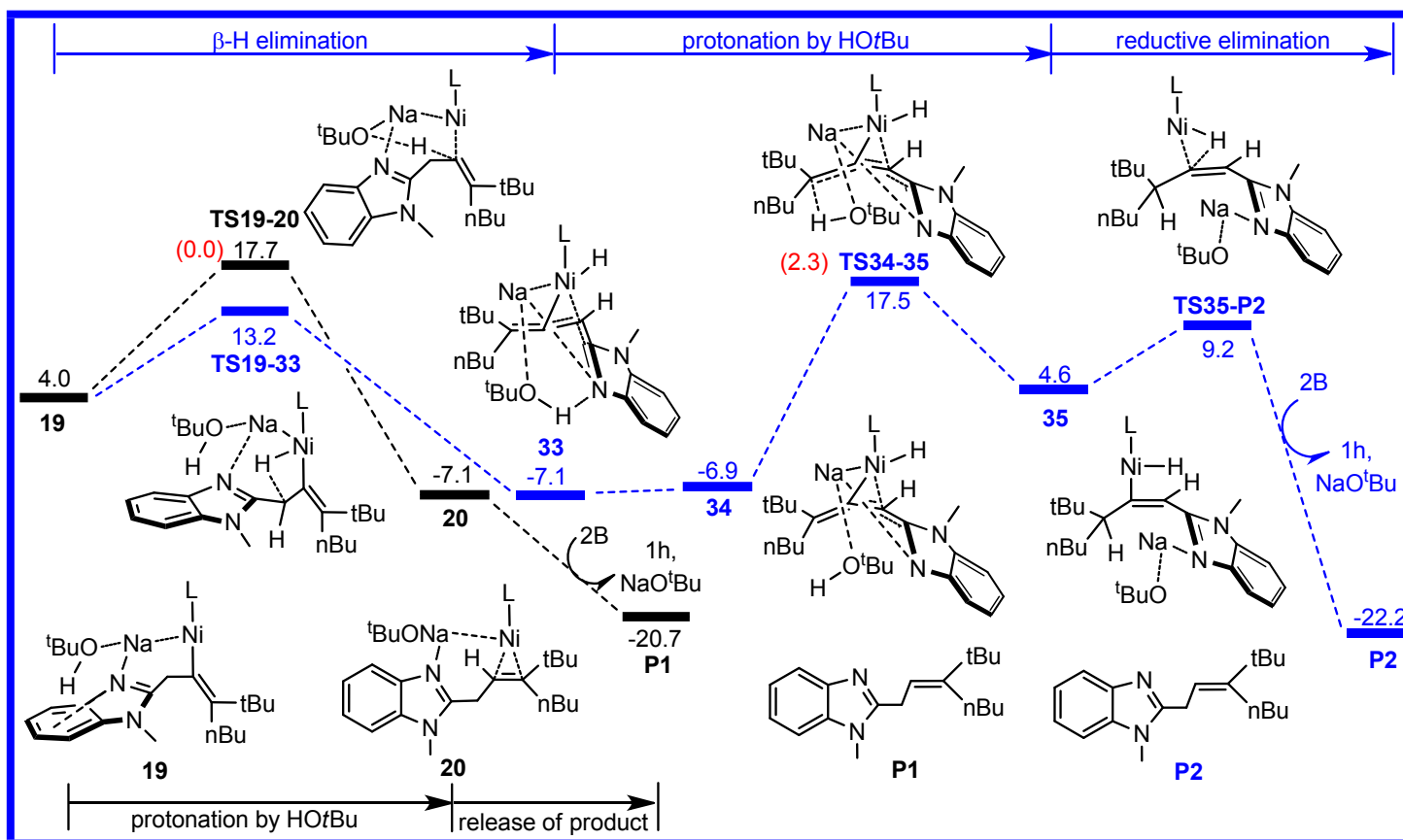


Fig. S2 Calculated free energy profiles in toluene along the possible pathways starting from intermediate **19** in Fig. 2. The optimized relative free energies in toluene solution are provided in the parentheses. The relative free energies are given in kcal mol⁻¹. L = IPr

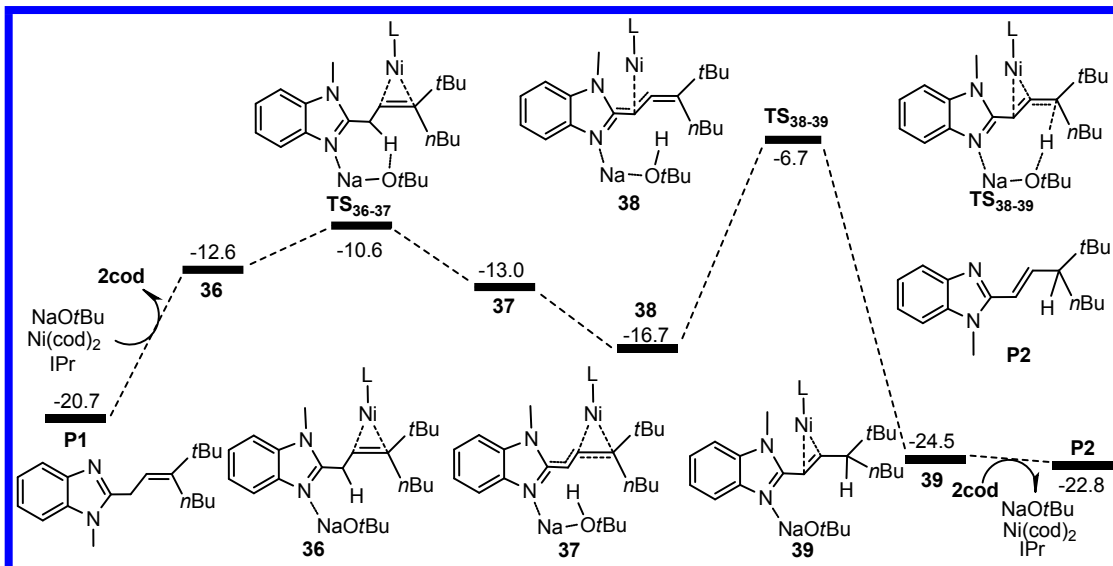


Fig. S3 Calculated free energy profile in toluene along the possible pathway for forming **P2** from **P1** with Ni(cod)₂ involvement in the presence of NaOtBu. The relative free energies are given in kcal mol⁻¹. L = IPr

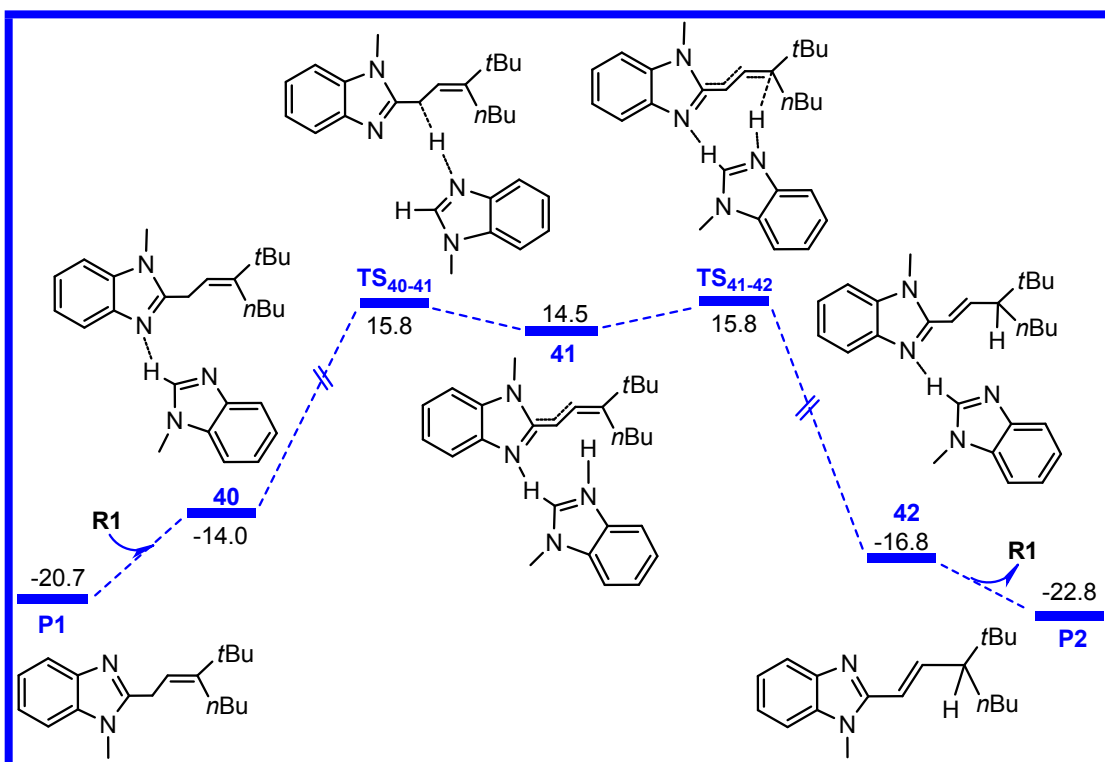


Fig. S4 Calculated free energy profile in toluene for forming **P2** from **P1** assisted by **R1**. The relative free energies are given in kcal mol⁻¹.

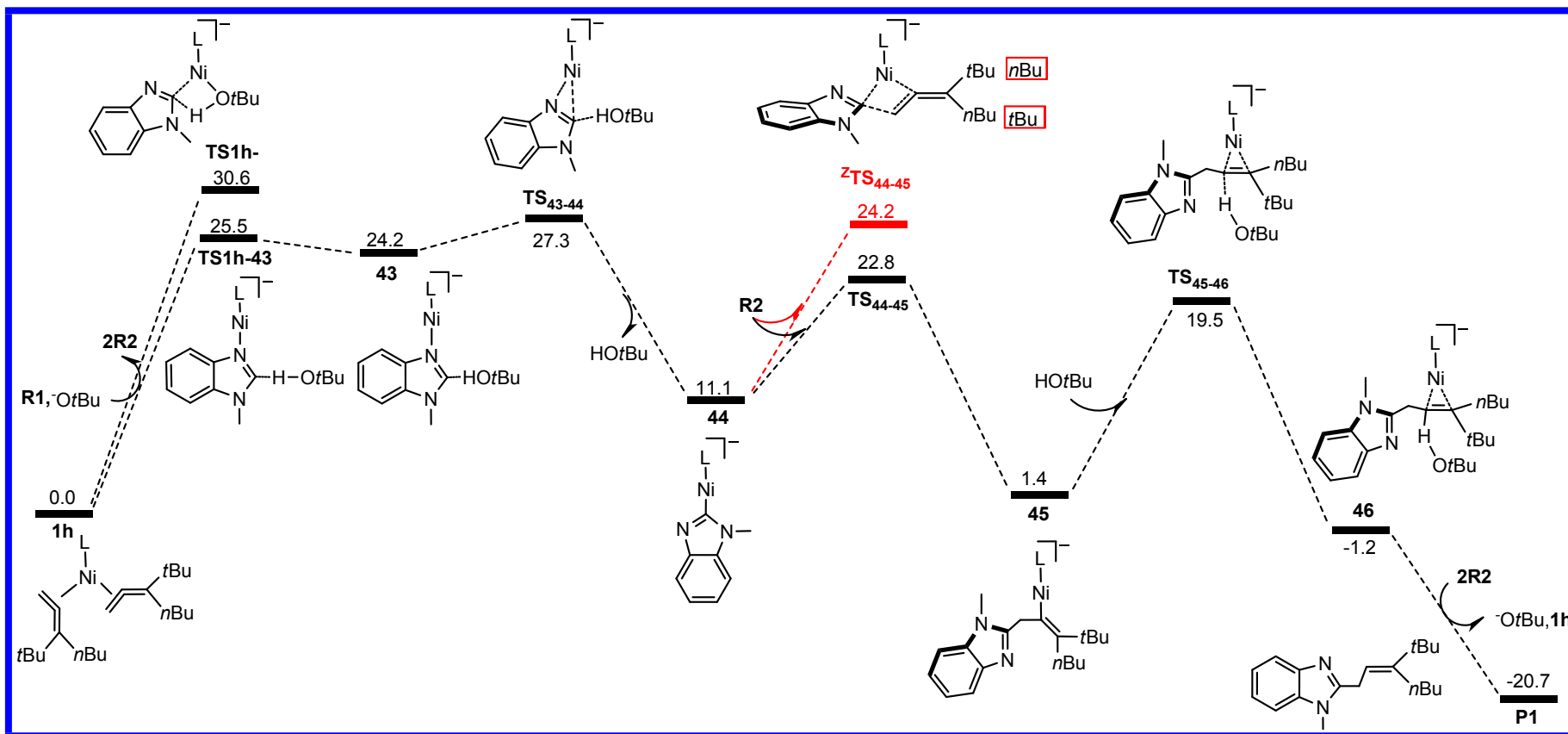


Fig. S5 Calculated free energy profiles in toluene along the possible pathways for forming **P1** assisted by the $\text{O}t\text{Bu}$. The relative free energies are given in kcal/mol. L = IPr

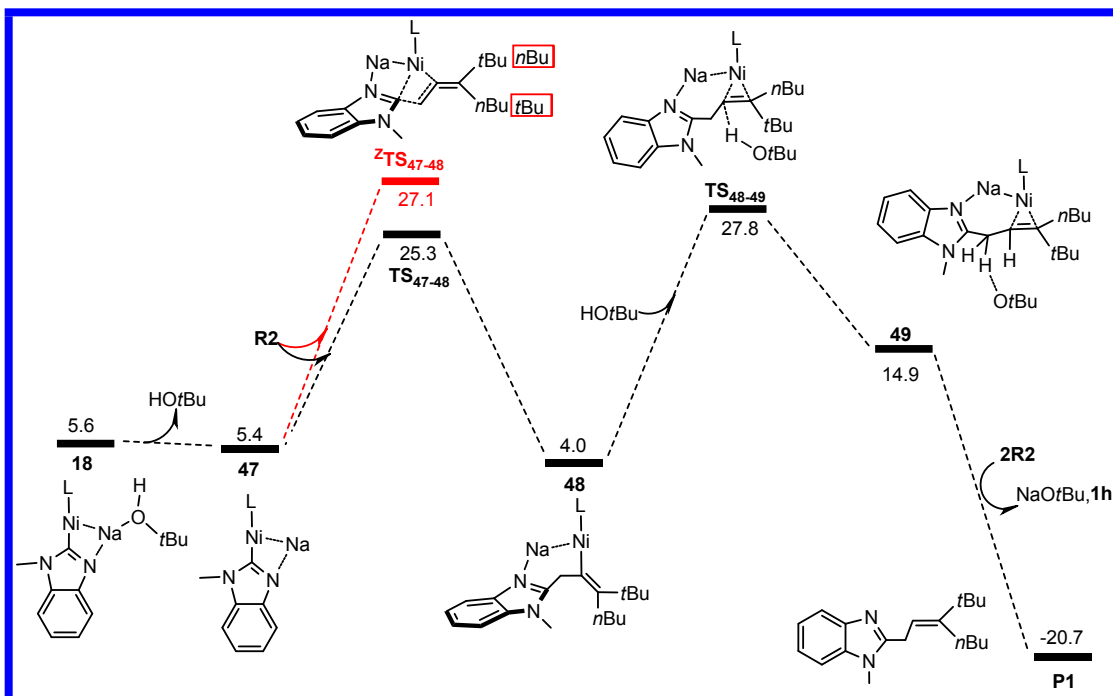


Fig. S6 Calculated free energy profile in toluene along the possible pathways starting from intermediate **18** in Fig. 2. The relative free energies are given in kcal mol⁻¹. L = IPr

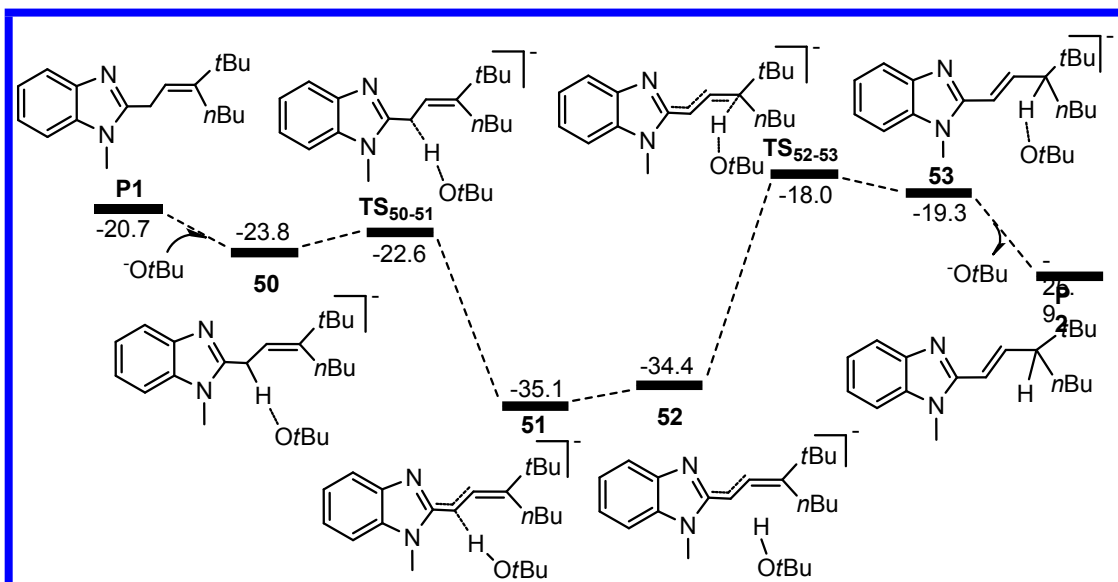


Fig. S7 Calculated free energy profile in toluene for forming **P2** from **P1** assisted by the ⁻OtBu. The relative free energies are given in kcal mol⁻¹.

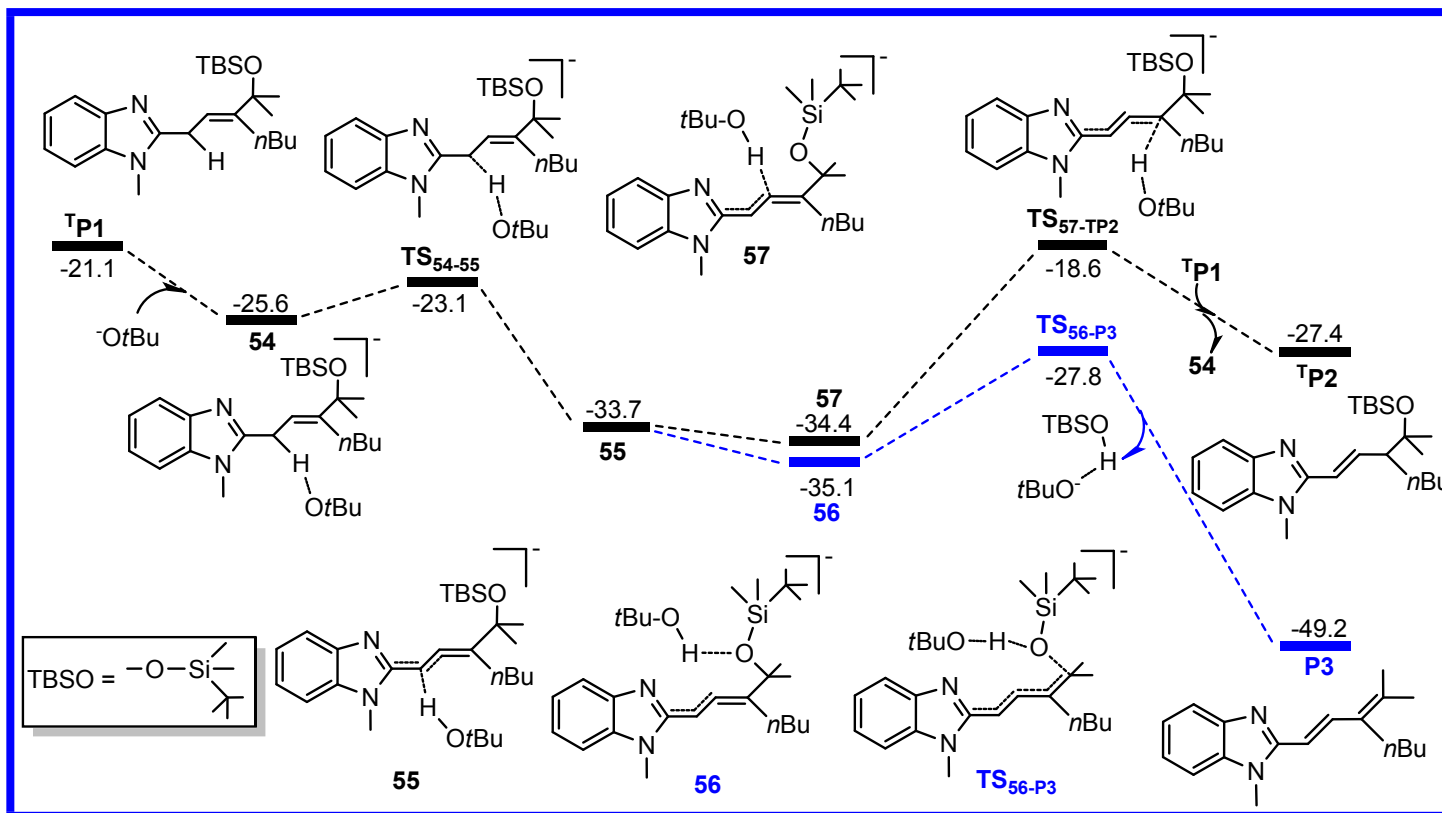


Fig. S8 Calculated free energy profiles in toluene along the possible pathways for forming **TP2** and **P3**, respectively, from **TP1** assisted by the ⁻O*t*Bu. The relative free energies are given in kcal mol⁻¹.

Table S1. Calculated Gibbs free energies in the gas-phase using B3LYP functional, single-point HF energies in SMD solvent using M06-L functional, and imaginary frequencies for all structures in the present work. The relative energies and the imaginary frequencies are given in Hartree and cm^{-1} , respectively.

Structure	Gibbs Free Energy (B3LYP gas-phase optimized calculation)	Solvation HF Energy (M06L single-point calculation)	Imaginary Frequency
R1	-419.056343	-419.1602652	
R2	-430.917515	-431.1365088	
R3	-993.274754	-993.6135699	
Ni(cod)₂	-794.718981	-795.0784129	
IPr	-1159.231473	-1159.9707368	
NaO<i>t</i>Bu	-395.277268	-395.3568238	
1a	-2061.132499	-2062.2112328	
1b	-2168.305857	-2169.3326075	
1c	-2180.190551	-2181.3579154	
1d	-1749.273313	-1750.1696492	
1e	-2072.981366	-2074.1991285	
1f	-1761.144469	-1762.1652356	
1g	-2020.702242	-2021.7316291	
1h	-2192.037523	-2193.3459105	
1i	-1749.278226	-1750.1684496	
10	-1749.273313	-1750.1696492	
TS₁₀₋₁₁	-1749.249987	-1750.1354702	-690.54
11	-1750.1354702	-1750.1472277	
12	-2180.142213	-2181.3080767	
TS₁₂₋₁₃	-2180.137563	-2181.3043791	-542.69
13	-2180.186095	-2181.3482816	
TS_{13-P1}	-2180.169434	-2181.3264876	-306.27
P1	-850.001642	-850.3536755	
14	-2180.188929	-2181.3376013	
TS₁₄₋₁₅	-2180.149777	-2181.3152718	-989.38

15	-2180.198550	-2181.37967	
TS₁₅₋₁₆	-2180.161558	-2181.3193375	-228.34
16	-2180.188213	-2181.339702	
^z14	-2180.188720	-2181.3330026	
^zTS₁₄₋₁₅	-2180.155171	-2181.3205875	-998.30
^z15	-2180.194592	-2181.3778079	
^zTS₁₅₋₁₆	-2180.156286	-2181.3163507	-221.50
^z16	-2180.182879	-2181.3326602	
^zP1	-849.995028	-850.3452907	
TS_{1h-17}	-2144.572063	-2145.5476498	-440.31
17	-2144.570684	-2145.5509018	
TS₁₇₋₁₈	-2144.554758	-2145.5409856	-73.25
18	-2144.583753	-2145.5708046	
TS₁₈₋₁₉	-2575.440233	-2576.7095025	-314.30
^zTS₁₈₋₁₉	-2575.440233	-2576.7067177	-318.82
19	-2575.440233	-2576.7378025	
TS₁₉₋₂₀	-2575.460367	-2576.7179092	-1328.38
20	-2575.497791	-2576.7596799	
21	-1245.299405	-1245.7390956	
TS₂₁₋₂₂	-1245.287879	-1245.729112	-1258.83
22	-1245.294498	-1245.7429265	
23	-1245.296923	-1245.7451753	
TS₂₃₋₂₄	-1245.281282	-1245.7250166	-1393.53
24	-1245.303616	-1245.7439498	
^T1h	-3316.753188	-3318.3042322	
TS_{1h-25}	-2144.572063	-2145.5476498	-440.31
25	-2144.570684	-2145.5509018	
TS₂₅₋₂₆	-2144.554758	-2145.5409856	-73.25
26	-2144.583753	-2145.5708046	
TS₂₆₋₂₇	-3137.801128	-3139.1924654	-314.52
27	-3137.850362	-3139.2200103	
TS_{27-TP1}	-3137.819833	-3139.2001427	-1326.43

TP1	-1412.359739	-1412.8344986	
28	-1807.659350	-1808.2210585	
TS₂₈₋₂₉	-1807.644791	-1808.209467	-1238.67
29	-1807.651999	-1808.2231246	
30	-1807.661950	-1808.2312804	
TS_{30-TP2}	-1807.641927	-1808.2059069	-1397.34
31	-1807.655467	-1808.2307038	
TS_{31-P3'}	-1807.645249	-1808.2200586	-261.50
TP2	-809.529738	-809.8335205	
P3	-1412.364123	-1412.8358576	
TS₁₉₋₃₃	-2575.466870	-2576.7185291	-920.50
33	-2575.496727	-2576.7564659	
34	-2575.494658	-2576.7555754	
TS₃₄₋₃₅	-2575.454084	-2576.7172515	-711.34
35	-2575.485820	-2576.7384357	
TS_{35-P2}	-2575.471494	-2576.7294367	-760.52
36	-2575.501446	-2576.7527193	
TS₃₆₋₃₇	-2575.484611	-2576.7512412	-1278.87
37	-2575.490194	-2576.7549923	
38	-2575.504591	-2576.7558383	
TS₃₈₋₃₉	-2575.481111	-2576.7429166	-1230.13
39	-2575.516684	-2576.7714547	
40	-1269.050843	-1269.5221002	
TS₄₀₋₄₁	-1268.988272	-1269.4764523	-77.21
41	-1268.991611	-1269.4794664	
TS₄₁₋₄₂	-1268.992264	-1269.4744339	-669.62
42	-1269.053623	-1269.5252297	
TS_{1h-}	-1982.229381	-1983.2665231	-1206.92
TS_{1h-43}	-1982.247816	-1983.2745565	-1074.72
43	-1982.247706	-1983.280424	
TS₄₃₋₄₄	-1982.239016	-1983.2756296	-68.78
44	-1748.702521	-1749.6200966	

TS₄₄₋₄₅	-2179.572201	-2180.7692617	-292.19
^zTS₄₄₋₄₅	-2179.567063	-2180.7661592	-279.77
45	-2179.616106	-2180.7999256	
TS₄₅₋₄₆	-2413.147950	-2414.452774	-533.23
46	-2413.181775	-2414.4896336	
47	-1911.022220	-1911.8905602	
TS₄₇₋₄₈	-2341.874029	-2343.026232	-314.41
^zTS₄₇₋₄₈	-2341.873872	-2343.024277	-320.86
48	-2341.927280	-2343.0582915	
TS₄₈₋₄₉	-2575.435148	-2576.7006926	-1022.07
49	-2575.457979	-2576.723611	
50	-1082.980298	-1083.4780921	
TS₅₀₋₅₁	-1082.977956	-1083.472082	-1063.89
51	-1082.991733	-1083.4943482	
52	-1082.989732	-1083.4932465	
TS₅₂₋₅₃	-1082.967128	-1083.4626036	-1038.71
53	-1082.970863	-1083.4665548	
P2	-850.004658	-850.357763	
54	-1645.340294	-1645.9587777	
TS₅₄₋₅₅	-1645.337851	-1645.9501568	-1142.44
55	-1645.352040	-1645.9712787	
56	-1645.346433	-1645.9711231	
57	-1645.349849	-1645.9712787	
TS_{56-P3}	-1645.339035	-1645.9599708	-274.07
TS_{57-TP2}	-1645.327574	-1645.9415882	-1085.59
^TP2	-809.529738	-809.8335205	
P3	-1412.364123	-1412.8358576	

Cartesian coordinates for the stationary points given in Table 1.

Ni(cod)₂

C	1.36904400	-1.52773300	-0.61304700
H	0.76216400	-2.36092200	-0.96465500
C	1.51009300	-0.45076600	-1.47299100
C	2.23849000	-1.84126200	0.58850700
H	1.67924700	-2.53230300	1.23262500
H	3.14844400	-2.38567100	0.28532700
C	2.62240900	-0.59230200	1.41621100
H	2.86898900	-0.90625800	2.43788900
H	3.53782300	-0.14135200	1.01903600
C	1.51189300	0.45092200	1.47330900
H	0.98228400	0.51247800	2.42101400
C	1.36995300	1.52769000	0.61402300
H	0.76145800	2.35980600	0.96523300
C	2.23801700	1.84132000	-0.58845100
H	3.14837300	2.38546700	-0.28604300
H	1.67816700	2.53270200	-1.23164200
C	2.62075300	0.59257800	-1.41707800
H	3.53682100	0.14158700	-1.02141500
H	2.86587400	0.90700600	-2.43895700
H	0.98158100	-0.51403300	-2.42122900
C	-1.51062500	-0.45050400	1.47343500
H	-0.98098000	-0.51296100	2.42107600
C	-1.37010900	-1.52755900	0.61393300
C	-2.62068900	0.59333000	1.41731200
H	-3.53674900	0.14283900	1.02109700
H	-2.86611900	0.90758700	2.43917300
C	-2.23690900	1.84197900	0.58906000
H	-3.14682800	2.38683200	0.28659900
H	-1.67671800	2.53283700	1.23254700
C	-1.36875200	1.52781300	-0.61323000
H	-0.76092000	2.36017800	-0.96508600
C	-1.51116500	0.45094700	-1.47280900
H	-0.98273400	0.51325600	-2.42114400
C	-2.62238500	-0.59170700	-1.41589900
H	-2.86864800	-0.90587000	-2.43758600
H	-3.53778300	-0.14014900	-1.01934000
C	-2.23959300	-1.84069600	-0.58769100
H	-1.68077900	-2.53240500	-1.23144100
H	-3.15000000	-2.38428400	-0.28442000
H	-0.76273600	-2.36055600	0.96507100
Ni	-0.00009900	-0.00107600	-0.00111700

1a

C	0.60890200	-1.02079900	0.23653100
C	1.78555200	-2.86961600	1.05074600
C	0.63635200	-3.34280800	0.51558100
N	-0.07784100	-2.23228800	0.03217400
N	1.77718200	-1.47232900	0.87436300
C	-1.35050800	-2.38257000	-0.63356500
C	-2.51173100	-2.59653800	0.14663100
C	-1.38981700	-2.39816600	-2.04807900
C	-3.72420400	-2.82336700	-0.52389000
C	-2.62894100	-2.62579000	-2.66891700
C	-3.78566300	-2.83663700	-1.91731500
H	-4.62887000	-2.99007400	0.05081300
H	-2.68418900	-2.64937400	-3.75209500
H	-4.73308000	-3.01489400	-2.41686800
C	2.92420000	-0.67201300	1.22935000
C	4.08874500	-0.76821000	0.43118100
C	2.88691100	0.12540100	2.39663800
C	5.22368900	-0.04277100	0.83021300
C	4.04376600	0.83931600	2.74479700
C	5.20311200	0.75741200	1.97139800
H	6.12865100	-0.10181200	0.23431900
H	4.04312200	1.45952300	3.63409600
H	6.08856700	1.31509000	2.26062000
C	-0.12904900	-2.24609000	-2.90008000
H	0.66548200	-1.86340800	-2.25363100
C	0.32351900	-3.62053900	-3.45216200
H	0.51528700	-4.33223600	-2.64095900

H	-0.44308500	-4.05344800	-4.10686700
H	1.24555900	-3.51195200	-4.03616800
C	-0.30517300	-1.22598400	-4.04539900
H	-1.05722000	-1.55208600	-4.77415300
H	-0.60101400	-0.24765800	-3.65370400
H	0.64201300	-1.10205500	-4.58345100
C	4.16099800	-1.64346300	-0.82351300
H	3.15706000	-2.02847500	-1.02568000
C	4.60077300	-0.84923300	-2.07453600
H	4.60968400	-1.50881900	-2.95072300
H	3.91515600	-0.02155800	-2.27595800
H	5.61026300	-0.43706000	-1.96001600
C	5.09580600	-2.85748300	-0.60038000
H	6.12453200	-2.53060600	-0.40552900
H	4.77176700	-3.46516100	0.25200800
H	5.10849200	-3.49866000	-1.48995700
C	1.65569600	0.15494200	3.30242300
H	0.79257500	-0.11577700	2.68561800
C	1.37779800	1.55080700	3.89866700
H	2.15895400	1.86162700	4.60211600
H	1.30738300	2.31066100	3.11244200
H	0.43431900	1.53681100	4.45990400
C	1.78494900	-0.90088300	4.42877000
H	1.91208100	-1.90714000	4.01524300
H	2.65042300	-0.68358200	5.06698600
H	0.88782500	-0.90377100	5.06066800
C	-2.46932100	-2.63075000	1.67549100
H	-1.51899500	-2.18664600	1.98962900
C	-3.60328200	-1.80593900	2.32378000
H	-3.62395000	-0.78491000	1.93405800
H	-4.58652000	-2.25673100	2.14346600
H	-3.45839600	-1.76331800	3.41035000
C	-2.51197900	-4.08774300	2.20055900
H	-3.44504200	-4.57983400	1.89970600
H	-1.67855100	-4.68205000	1.81224100
H	-2.45777300	-4.10272500	3.29604600
Ni	-0.01399900	0.67948500	-0.33560900
C	-3.87322000	1.95568500	0.95204300
C	-3.03381900	1.29984100	0.02227100
C	-3.51477800	0.97751000	-1.25104700
C	-4.82651000	1.32644300	-1.55659600
C	-5.65279300	1.98163500	-0.62056900
C	-5.19250500	2.30763200	0.65225300
C	-1.87395100	1.57928300	1.81220100
H	-2.87587700	0.46804900	-1.96316200
H	-5.22630200	1.08895600	-2.53833000
H	-6.67143200	2.23829300	-0.89811600
H	-5.83069900	2.81246100	1.37165600
H	-1.07388400	1.58593500	2.53838700
N	-1.78141000	1.08041300	0.59741900
N	-3.10337600	2.12276300	2.09261800
C	-3.50898100	2.76298600	3.32781200
H	-3.77639100	3.81101600	3.15234600
H	-4.36871100	2.24663800	3.76930000
H	-2.67766200	2.72781800	4.03543600
C	1.21443000	1.61331100	-1.56394200
H	1.40187700	0.99007900	-2.44527500
C	-0.06075000	2.25785500	-1.51752000
C	2.47929700	2.28612800	-1.05811000
H	2.26064200	2.89393400	-0.17497000
H	3.20889100	1.54166400	-0.72151600
C	3.18412200	3.14609100	-2.14467900
H	4.03488500	3.67689900	-1.68345500
H	3.64202000	2.45701400	-2.86983200
C	2.34518800	4.12934800	-2.93664000
H	2.67564300	4.27792100	-3.96625500
C	1.27389600	4.82509600	-2.53584500
H	0.78872100	5.47112500	-3.26905900
C	0.65561600	4.78913700	-1.16259800
H	0.13829500	5.74027100	-0.97360900
H	1.44994800	4.73262800	-0.41158400
C	-0.36553100	3.63149700	-0.91350000
H	-1.33983300	3.94913600	-1.30843000
H	-0.50205800	3.57606900	0.17778100
H	-0.73230000	2.01663900	-2.34815800
H	0.26107000	-4.34699700	0.42464100
H	2.60585600	-3.37869900	1.52594300

1b

C	-1.56274300	0.00111800	0.00019100
C	-3.82120000	-0.63248000	-0.23260600
C	-3.82006600	0.63826700	0.23433100
N	-2.47403600	1.03179900	0.37489000
N	-2.47586700	-1.02816200	-0.37386000
C	-2.06943500	2.31404300	0.87690600
C	-1.95694100	2.50272100	2.27389300
C	-1.82105600	3.37009000	-0.03520300
C	-1.57885100	3.77095200	2.74626100
C	-1.44509100	4.61874600	0.48473800
C	-1.32112200	4.81894800	1.86238400
H	-1.49290400	3.93848800	3.81575400
H	-1.25049300	5.44379800	-0.19179100
H	-1.03277100	5.79409900	2.24448700
C	-2.07355100	-2.31100900	-0.87619500
C	-1.96221800	-2.49975100	-2.27326300
C	-1.82623400	-3.36751600	0.03568100
C	-1.58643200	-3.76854300	-2.74596500
C	-1.45256800	-4.61671800	-0.48459700
C	-1.32979800	-4.81701100	-1.86233700
H	-1.50137400	-3.93611300	-3.81552200
H	-1.25879900	-5.44210800	0.19175400
H	-1.04321500	-5.79258200	-2.24469900
C	-2.00955500	3.16812600	-1.53951400
H	-1.84129000	2.10435700	-1.74060400
C	-3.45956800	3.51652100	-1.96220500
H	-4.19188200	2.90467300	-1.42630000
H	-3.67975200	4.57221400	-1.75782900
H	-3.59540700	3.34298800	-3.03710200
C	-1.00620200	3.96379500	-2.39991600
H	-1.18239700	5.04545100	-2.34189500
H	0.02693500	3.76673600	-2.09821200
H	-1.11410700	3.67498800	-3.45231100
C	-2.27435100	-1.37820800	-3.26405500
H	-2.45591200	-0.46857000	-2.68442200
C	-1.08892900	-1.08520600	-4.20966100
H	-1.34360900	-0.26347600	-4.89041000
H	-0.20592300	-0.78831100	-3.63550600
H	-0.83204500	-1.95817200	-4.82309300
C	-3.55770700	-1.69036600	-4.07091700
H	-3.43586800	-2.59692700	-4.67706000
H	-4.41558800	-1.84384000	-3.40651000
H	-3.79530800	-0.86084300	-4.74823500
C	-2.01322200	-3.16528600	1.54015500
H	-1.84213000	-2.10195800	1.74122600
C	-1.01132700	-3.96364700	2.39976600
H	-1.19076000	-5.04479800	2.34214200
H	0.02210400	-3.76968800	2.09705700
H	-1.11738200	-3.67430600	3.45220000
C	-3.46378100	-3.51005000	1.96393500
H	-4.19497600	-2.89620400	1.42880600
H	-3.68684800	-4.56513700	1.75954100
H	-3.59827900	-3.33640400	3.03898600
C	-2.27037400	1.38175800	3.26494000
H	-2.45370100	0.47237900	2.68545700
C	-1.08499400	1.08688900	4.20999500
H	-0.20275900	0.78845400	3.63545200
H	-0.82634000	1.95947900	4.82321700
H	-1.34071600	0.26565600	4.89095200
C	-3.55282300	1.69610200	4.07239600
H	-3.42922200	2.60260600	4.67826600
H	-4.41079800	1.85078600	3.40839200
H	-3.79139300	0.86710200	4.75001400
Ni	0.23921400	-0.00016800	-0.00061700
C	3.48642400	1.55517400	-2.28685500
C	2.42633900	1.67350300	-1.35678500
C	2.26341700	2.85586700	-0.62551700
C	3.17744300	3.88536000	-0.83964400
C	4.23289000	3.75130500	-1.76439500
C	4.40516800	2.58557100	-2.50716700
C	2.26193700	-0.28431500	-2.23142900
H	1.43354900	2.95789700	0.06701600
H	3.07149900	4.81611500	-0.28924500
H	4.92432800	4.57749000	-1.90618000
H	5.21577300	2.48900200	-3.22383000
H	1.93875300	-1.28515100	-2.48065000
N	1.67633400	0.49623900	-1.34525400
N	3.35815600	0.29122400	-2.83499000

C	4.20060700	-0.30414500	-3.85179200
H	4.17042900	0.28264700	-4.77713900
H	5.23912900	-0.36965100	-3.50778200
H	3.83943200	-1.31262500	-4.06527500
C	3.48428500	-1.56045000	2.28614100
C	2.42423800	-1.67717100	1.35582900
C	2.25953500	-2.85937800	0.62470200
C	3.17179400	-3.89034900	0.83923200
C	4.22723500	-3.75789500	1.76422900
C	4.40126900	-2.59232900	2.50685200
C	2.26289100	0.28106900	2.23005200
H	1.42968000	-2.96013200	-0.06803500
H	3.06446400	-4.82101200	0.28894700
H	4.91726800	-4.58520300	1.90631000
H	5.21187600	-2.49696900	3.22367500
H	1.94133300	1.28251100	2.47895100
N	1.67619300	-0.49869100	1.34392500
N	3.35794600	-0.29620500	2.83405700
C	4.20152200	0.29816300	3.85051600
H	4.17162500	-0.28911600	4.77555400
H	5.23985300	0.36323500	3.50582900
H	3.84106700	1.30672700	4.06481800
H	-4.63652400	1.29449500	0.48414800
H	-4.63882900	-1.28738200	-0.48207100

1c

C	1.48946000	-0.67368400	0.21908600
C	3.58454200	-1.31463400	1.00867500
C	3.02752100	-2.40945800	0.43904300
N	1.75849600	-2.02256300	-0.02909200
N	2.66039900	-0.26349700	0.86709900
C	0.89173100	-2.95168600	-0.71780600
C	0.15466300	-3.88979800	0.04305000
C	0.86743100	-2.95206000	-2.13178500
C	-0.61634400	-4.83740100	-0.64823200
C	0.07564600	-3.91864500	-2.77358900
C	-0.65845400	-4.85291200	-2.04263400
H	-1.18995500	-5.56898200	-0.08949100
H	0.04385200	-3.94333200	-3.85768900
H	-1.26088800	-5.59416700	-2.55871600
C	2.97389200	1.08094000	1.30057600
C	3.85589900	1.86099800	0.51538400
C	2.45128800	1.55327200	2.52673500
C	4.20184600	3.13732000	0.98827500
C	2.82437600	2.83820500	2.95026200
C	3.69042800	3.62501900	2.19000300
H	4.87506800	3.75606400	0.40510300
H	2.43805500	3.22717200	3.88548500
H	3.96685400	4.61634600	2.53557600
C	1.70829900	-1.98620200	-2.96680600
H	2.10477200	-1.21928700	-2.29575300
C	2.90829900	-2.72241900	-3.61107500
H	3.53667400	-3.20171600	-2.85151200
H	2.56767800	-3.49977000	-4.30629500
H	3.53087200	-2.01590600	-4.17313600
C	0.87225800	-1.25134600	-4.03774200
H	0.45795600	-1.94301500	-4.78148200
H	0.04720200	-0.69879900	-3.57684300
H	1.50147200	-0.53022700	-4.57247300
C	4.46628600	1.34927900	-0.79207100
H	3.89914700	0.46560500	-1.10192100
C	4.37486800	2.37762100	-1.94220300
H	4.74035000	1.92556400	-2.87206800
H	3.34435600	2.70458100	-2.10289000
H	4.99133100	3.26287700	-1.74568900
C	5.94172000	0.92388100	-0.58328800
H	6.55260300	1.78265500	-0.27888400
H	6.03842100	0.15350500	0.18911700
H	6.35942300	0.52464600	-1.51538200
C	1.55997600	0.67899100	3.40947500
H	1.07706200	-0.05855000	2.75985000
C	0.44085300	1.47645200	4.11275500
H	0.83762200	2.16528600	4.86733800
H	-0.13966400	2.06513800	3.39346500
H	-0.23563300	0.78808200	4.63562400
C	2.40871000	-0.09198600	4.45152200
H	3.16119500	-0.72134200	3.96451100
H	2.92957600	0.60556900	5.11906800

H	1.77046600	-0.73921200	5.06593900
C	0.21136400	-3.92179800	1.57177000
H	0.65626700	-2.97914100	1.90747800
C	-1.18809500	-4.02641300	2.21762300
H	-1.85463600	-3.24195600	1.84910700
H	-1.65939400	-4.99422400	2.00945900
H	-1.10373500	-3.93147300	3.30720700
C	1.11323500	-5.07766200	2.07199700
H	0.71026400	-6.04800100	1.75699600
H	2.13218200	-4.99402400	1.67977500
H	1.17005600	-5.07316800	3.16733600
Ni	-0.01710600	0.40034900	-0.32663500
C	-3.70525000	-1.34664000	0.85816300
C	-2.65138900	-1.14657400	-0.06257100
C	-2.75327700	-1.64400300	-1.36596700
C	-3.90958800	-2.33850000	-1.70500000
C	-4.95071100	-2.53793600	-0.77503500
C	-4.86916500	-2.04488400	0.52427400
C	-2.06068300	-0.19151800	1.77354500
H	-1.94996100	-1.48306000	-2.07555800
H	-4.01619500	-2.73627700	-2.71008800
H	-5.83872400	-3.08459600	-1.07996900
H	-5.67518000	-2.19320600	1.23688300
H	-1.52091000	0.36935900	2.52208800
N	-1.63330000	-0.41539500	0.54960800
N	-3.29896100	-0.72190200	2.02766500
C	-4.04209300	-0.63577400	3.26975000
H	-4.99853600	-0.12628600	3.11195900
H	-4.23250900	-1.63440600	3.67843000
H	-3.45757000	-0.06442600	3.99402600
H	3.40103800	-3.41067400	0.31524900
H	4.53677900	-1.17539000	1.48934000
C	-0.66749000	1.89725100	-1.29813700
C	0.73559400	1.75305400	-1.46902300
C	-1.69459500	2.71190700	-1.58764400
C	-1.49249400	3.98320500	-2.47143500
C	-2.82075200	4.67121200	-2.85473300
H	-3.38867300	5.00488400	-1.97932400
H	-2.61317000	5.55848300	-3.46676700
H	-3.46634800	4.01021100	-3.44519000
C	-0.78015600	3.61139800	-3.79077100
H	0.19283400	3.15244300	-3.59997800
H	-1.38120600	2.89972600	-4.37002000
H	-0.62196400	4.50484100	-4.41084600
C	-0.62331400	5.00940400	-1.70710000
H	-0.42898500	5.89937800	-2.32282300
H	-1.12040200	5.33937400	-0.78708000
H	0.33926000	4.56960700	-1.42865700
C	-3.06559200	2.45164500	-0.97505000
H	-3.87277900	2.69091000	-1.68010200
H	-3.15211300	1.38201500	-0.76466900
C	-3.32245300	3.21835400	0.34027400
H	-3.20625800	4.29971400	0.18020300
H	-2.54178700	2.93474400	1.06083900
C	-4.70794800	2.95169200	0.94455000
H	-5.48259400	3.25234200	0.22455900
H	-4.83746900	1.86838900	1.08782500
C	-4.94253900	3.67813400	2.27408500
H	-4.85226700	4.76455100	2.15140200
H	-5.94074500	3.47223200	2.68007700
H	-4.20489100	3.37421800	3.02849600
H	1.14852300	1.37106100	-2.40855900
H	1.41166300	2.44498000	-0.95818700

1d

C	-0.22602800	-0.90528900	0.27647400
C	0.18361300	-2.68906300	1.70467900
C	-1.15984000	-2.49649100	1.68533700
N	-1.40496400	-1.41725000	0.82039300
N	0.74717400	-1.72279400	0.85244900
C	-2.72499300	-0.90723000	0.52890400
C	-3.26375700	0.10892000	1.35060000
C	-3.44446200	-1.45278600	-0.55869000
C	-4.55879300	0.56763600	1.06200000
C	-4.73377500	-0.95631700	-0.80701800
C	-5.28854400	0.04173600	-0.00486300
H	-4.99515300	1.34874800	1.67593100
H	-5.30502400	-1.35388500	-1.63949900

H	-6.28757400	0.41215100	-0.21338200
C	2.16612700	-1.58132800	0.63416500
C	2.76456600	-2.24552400	-0.46008800
C	2.91801700	-0.79436700	1.53606800
C	4.14821900	-2.09086200	-0.644454700
C	4.29853300	-0.67368900	1.30953200
C	4.90959400	-1.31156400	0.22830500
H	4.63280600	-2.59049200	-1.47720900
H	4.89885800	-0.07588600	1.98797800
H	5.97903900	-1.20831800	0.07091800
C	-2.86050200	-2.53484000	-1.46636500
H	-1.87134700	-2.79998000	-1.07963700
C	-3.72315300	-3.81831800	-1.45655000
H	-3.84013500	-4.21253700	-0.44039300
H	-4.72485100	-3.63145300	-1.86185400
H	-3.25430900	-4.59482600	-2.07272400
C	-2.66221500	-2.00689000	-2.90672700
H	-3.61948500	-1.72564300	-3.36245000
H	-2.00873300	-1.12766500	-2.91156900
H	-2.20496600	-2.78101200	-3.53521900
C	1.96479200	-3.13009100	-1.41647300
H	0.91239600	-3.07536000	-1.12168900
C	2.05277400	-2.63012200	-2.87631400
H	1.45414400	-3.27334700	-3.53231800
H	1.66700800	-1.60892000	-2.95989800
H	3.08502000	-2.64378200	-3.24697200
C	2.40700100	-4.60911600	-1.31015000
H	3.45361100	-4.73480900	-1.61317600
H	2.30784700	-4.98162900	-0.28414500
H	1.79066400	-5.23822500	-1.96335700
C	2.27894600	-0.08996900	-2.73339900
H	1.21048400	-0.32588100	2.73003600
C	2.40255300	1.44724900	2.62699700
H	3.45312700	1.76411900	2.62007600
H	1.92178900	1.81220300	1.71367500
H	1.91565600	1.92672000	3.48476400
C	2.86392200	-0.60326300	4.07022500
H	2.74220600	-1.68822200	4.16757300
H	3.93383300	-0.37735100	4.15287400
H	2.35504100	-0.12518900	4.91565600
C	-2.48641500	0.71515500	2.51832300
H	-1.49680500	0.24817000	2.54063500
C	-2.27021500	2.23421200	2.32651800
H	-1.75582400	2.44211100	1.38239800
H	-3.22359600	2.77644600	2.32263100
H	-1.66131700	2.63542800	3.14581300
C	-3.17472400	0.41803300	3.87153100
H	-4.17206000	0.87162500	3.91842500
H	-3.28855800	-0.66025200	4.03316600
H	-2.58154100	0.82691200	4.69829400
Ni	-0.07475900	0.47039100	-0.93916600
C	1.19125000	3.61353400	-1.18899300
C	-0.03545600	3.13419700	-1.71735600
C	-1.16811500	3.95125300	-1.70290700
C	-1.05476400	5.22972100	-1.15018100
C	0.16363500	5.69052600	-0.62517600
C	1.30834600	4.88801500	-0.63179600
C	1.42126700	1.50200700	-1.90631500
H	-2.10619800	3.59183500	-2.11581200
H	-1.92413200	5.88137600	-1.12781800
H	0.22049400	6.69175800	-0.20626100
H	2.24820800	5.24771200	-0.22223900
H	2.00693400	0.77514100	-2.46253100
N	0.13155600	1.83926000	-2.22324600
N	2.10913100	2.59455000	-1.35757500
C	3.50643200	2.63125500	-0.99512900
H	4.02125900	3.45175000	-1.51119400
H	3.63795900	2.76092700	0.08624300
H	3.97138800	1.68506600	-1.28170900
H	-1.95601900	-3.01404400	2.19185500
H	0.78780400	-3.40678600	2.23208500

1e

C	-1.24974100	0.80490900	0.28900900
C	-2.12755800	2.58686600	1.49783100
C	-3.17489300	1.93770100	0.93866700
N	-2.64426800	0.85301700	0.21726300
N	-0.96292100	1.90823700	1.09504200

C	-3.50938300	-0.09329200	-0.45662900
C	-3.67666000	-0.00711700	-1.85914500
C	-4.22390000	-1.03162500	0.32605900
C	-4.55542300	-0.91547900	-2.47031700
C	-5.09671900	-1.91050100	-0.33586900
C	-5.25591200	-1.86090200	-1.72004000
H	-4.69871300	-0.87769900	-3.54387100
H	-5.65409200	-2.64118000	0.24018100
H	-5.93099100	-2.55276500	-2.21404300
C	0.35405300	2.37910400	1.47283600
C	1.07710700	1.68183500	2.47138000
C	0.84439600	3.57061200	0.88656600
C	2.33509100	2.18402800	2.83756100
C	2.10595900	4.03261200	1.29788000
C	2.84946700	3.34368100	2.25412700
H	2.91669500	1.66863800	3.59222100
H	2.50620600	4.94293500	0.86494600
H	3.82409300	3.71515800	2.55528800
C	-4.11326700	-1.08620900	1.85200700
H	-3.25118400	-0.48061900	2.15027900
C	-5.37374500	-0.48137100	2.51972900
H	-5.54475800	0.55341700	2.20442700
H	-6.26709300	-1.06186600	2.25927200
H	-5.26937600	-0.49125800	3.61123400
C	-3.87283800	-2.51659100	2.38195900
H	-4.73192200	-3.17036600	2.19123300
H	-2.99280700	-2.96816400	1.91676500
H	-3.71330000	-2.49178100	3.46646600
C	0.48044300	0.47057000	3.19208400
H	-0.11817700	-0.08387100	2.46175900
C	1.53788000	-0.50298500	3.74946000
H	1.04431400	-1.40954000	4.11706700
H	2.25933000	-0.79709700	2.98131400
H	2.08871300	-0.06904600	4.59294400
C	-0.46286300	0.93005700	4.33453300
H	0.09508500	1.50173500	5.08656500
H	-1.27619900	1.56075400	3.96151900
H	-0.90889500	0.05993400	4.83168500
C	0.03254600	4.40390800	-0.11077400
H	-0.81275300	3.79774300	-0.45341600
C	0.84036100	4.81226100	-1.36265000
H	1.67458100	5.47675100	-1.10944400
H	1.24837900	3.93976200	-1.87929700
H	0.19231700	5.35208600	-2.06339200
C	-0.53771200	5.67296200	0.57314400
H	-1.14662200	5.42900100	1.45004700
H	0.27501800	6.32982400	0.90601000
H	-1.16312900	6.23691600	-0.12914600
C	-2.99664600	1.08467300	-2.68659900
H	-2.08290300	1.37712800	-2.16209800
C	-2.57979800	0.61337200	-4.09535600
H	-1.98252100	-0.30333800	-4.04891700
H	-3.44697000	0.42531000	-4.73967300
H	-1.97709500	1.38901200	-4.58155500
C	-3.90954600	2.33362500	-2.78557800
H	-4.84987800	2.08826300	-3.29454100
H	-4.15421700	2.73061500	-1.79430400
H	-3.41075800	3.12669300	-3.35584200
Ni	-0.01426000	-0.39671700	-0.68185500
C	1.68136800	0.23345200	-1.48799400
C	0.63424600	0.84680500	-2.13962600
H	0.41764600	1.90319700	-1.98669500
H	0.22512200	0.42555400	-3.06004800
C	2.97917900	0.13310000	-1.19021600
C	4.06271500	0.85116800	-2.04597400
C	5.13523700	1.49523800	-1.13483600
H	5.68208600	0.76011700	-0.53748400
H	5.87206600	2.03174500	-1.74594900
H	4.67936300	2.21687300	-0.44664200
C	3.47484000	1.98292100	-2.90989300
H	2.72319100	1.61460700	-3.61316700
H	3.00794900	2.75207600	-2.28666700
H	4.27645000	2.45804400	-3.48940000
C	4.73407200	-0.15834000	-3.01102200
H	5.50491900	0.34286700	-3.61210500
H	5.21088500	-0.98896100	-2.48510500
H	3.99148400	-0.58052400	-3.69788800
C	3.40828700	-0.62845500	0.06438200
H	3.76296300	0.10309300	0.80700900
H	2.50121400	-1.06720800	0.49615900

C	4.47438600	-1.73947200	-0.03988900
H	5.43082300	-1.33089800	-0.38751500
H	4.17071100	-2.48350600	-0.78677500
C	4.71560300	-2.43830900	1.30629700
H	5.01500800	-1.68841900	2.05325000
H	3.77146200	-2.86801000	1.67058500
C	5.77944600	-3.53919800	1.23422000
H	6.74518300	-3.13576100	0.90460400
H	5.93259900	-4.01464700	2.21016800
H	5.48905600	-4.32290100	0.52381400
H	-2.09099400	3.45412200	2.13236200
H	-4.23208200	2.13038300	0.98309800
C	-0.56674600	-2.30963600	-0.12303200
H	-1.65591500	-2.27302600	-0.15253200
C	0.09060300	-2.30842500	-1.37173700
C	-0.03343400	-2.91828000	1.16097200
H	1.04772700	-2.78048600	1.24397400
H	-0.46046000	-2.37717800	2.01686500
C	-0.40198300	-4.41160700	1.35798700
H	0.04456400	-4.76223700	2.30417000
H	-1.48739400	-4.47403500	1.52217400
C	-0.07025200	-5.39216100	0.25678100
H	-0.69708500	-6.28572200	0.26085800
C	0.86473700	-5.31725600	-0.69736200
H	0.90882400	-6.14046700	-1.41207300
C	1.86246600	-4.20925800	-0.92702700
H	2.74604700	-4.63426200	-1.42288500
H	2.22245300	-3.81278200	0.02511200
C	1.34395300	-3.05944100	-1.82306000
H	1.11295100	-3.49655600	-2.80561200
H	2.17082000	-2.36273300	-2.00184100
H	-0.58693900	-2.13344500	-2.21478700

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C	1.08797800	-0.76829400	-0.03152500
C	1.84583700	-2.94901600	-0.19590500
C	2.93611700	-2.16041100	-0.01575800
N	2.47023400	-0.83859400	0.08326000
N	0.72770500	-2.09776500	-0.20378100
C	3.34494400	0.29823100	0.26859300
C	3.87470800	0.94393600	-0.87109400
C	3.66365300	0.70844200	1.58201200
C	4.74596900	2.02505100	-0.66451500
C	4.53791900	1.79654800	1.73349600
C	5.07533000	2.44933500	0.62350800
H	5.16826700	2.53926700	-1.52164400
H	4.79827700	2.13472800	2.73115100
H	5.74967100	3.28877200	0.76199000
C	-0.62776600	-2.57007700	-0.37471600
C	-1.36609500	-2.95206700	0.76801800
C	-1.15918700	-2.66073200	-1.68112800
C	-2.66764700	-3.44048300	0.57193400
C	-2.46607100	-3.15430000	-1.82167000
C	-3.21301900	-3.54359200	-0.70894700
H	-3.25942400	-3.73880300	1.43080900
H	-2.90144000	-3.23272400	-2.81232200
H	-4.22087800	-3.92514500	-0.83942800
C	3.09344900	0.01640500	2.81996200
H	2.44739000	-0.80057900	2.48328800
C	4.21272700	-0.60278100	3.68953000
H	4.81250300	-1.31948200	3.11655300
H	4.89033800	0.16767500	4.07618000
H	3.77956400	-1.12908100	4.54844700
C	2.21129700	0.97924100	3.64805800
H	2.79300400	1.82717100	4.02918100
H	1.39100200	1.37108500	3.03787700
H	1.78076700	0.45341300	4.50882400
C	-0.80385200	-2.83061200	2.18409600
H	0.23931300	-2.50758700	2.10687200
C	-1.55740400	-1.74521600	2.98895200
H	-1.11781700	-1.63913600	3.98819800
H	-1.49891800	-0.77560600	2.48224200
H	-2.61590200	-2.00516500	3.11197800
C	-0.81444100	-4.18566200	2.92831400
H	-1.83579900	-4.55501400	3.07807300
H	-0.25882300	-4.95009500	2.37296900
H	-0.35247200	-4.07746400	3.91671500
C	-0.37039500	-2.23510900	-2.91941400

H	0.62996800	-1.93109700	-2.59466100
C	-1.02015700	-1.00891800	-3.60274300
H	-2.03232200	-1.24004800	-3.95623200
H	-1.08373900	-0.16346600	-2.90899200
H	-0.42363900	-0.69791400	-4.46898100
C	-0.19829100	-3.40329500	-3.91819400
H	0.28869600	-4.26421700	-3.44579000
H	-1.16429300	-3.73880800	-4.31385400
H	0.41720500	-3.08605500	-4.76823700
C	3.53852500	0.50165600	-2.29526900
H	2.80931400	-0.31217800	-2.23256500
C	2.87636200	1.63925900	-3.10569900
H	1.96981800	1.99405300	-2.60501900
H	3.55548800	2.49057000	-3.23417000
H	2.59937900	1.27972100	-4.10407000
C	4.78857500	-0.04605400	-3.02407700
H	5.55821200	0.72795100	-3.13042700
H	5.23229000	-0.88661500	-2.47793100
H	4.52152400	-0.39426700	-4.02897400
Ni	-0.00554300	0.80161000	-0.00998000
H	3.98244900	-2.40258400	0.05129900
H	1.75262900	-4.01419700	-0.31723600
C	-1.18235500	2.28382400	-0.09779000
C	0.11214900	2.72073900	0.16969000
C	-2.47716500	2.53525300	-0.30903400
C	-3.01368400	3.99699000	-0.29184000
C	-4.41793200	4.11388900	-0.92303900
H	-5.16967300	3.52140800	-0.39144800
H	-4.74743500	5.16002100	-0.89634800
H	-4.41576100	3.79607200	-1.97244100
C	-2.07470100	4.92663600	-1.09041700
H	-1.06358700	4.92788400	-0.67504900
H	-2.00865000	4.60884600	-2.13793800
H	-2.45049400	5.95813400	-1.07134600
C	-3.08157900	4.50096100	1.16986900
H	-3.43737700	5.53977600	1.20946200
H	-3.76127400	3.88932400	1.77398000
H	-2.09161400	4.46231500	1.63721200
C	-3.44432200	1.37405900	-0.49862400
H	-4.13575400	1.57690500	-1.32814900
H	-2.86660800	0.48790900	-0.78982400
C	-4.27102400	1.01232400	0.75384700
H	-4.81768900	1.89333800	1.11703700
H	-3.57879700	0.73025300	1.55932000
C	-5.27041800	-0.12578700	0.50775800
H	-5.96468600	0.17022400	-0.29226100
H	-4.73050900	-1.00651800	0.13378200
C	-6.06944300	-0.50918400	1.75840700
H	-6.64163600	0.34502900	2.14177100
H	-6.77980300	-1.31869800	1.55120300
H	-5.40478500	-0.84651000	2.56393600
H	0.75110700	3.13774800	-0.61425200
H	0.41151300	3.00176000	1.18444500

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C	-0.66064500	0.84561500	0.39766900
C	-1.97210900	2.16851400	1.81074400
C	-0.77802700	2.79363500	1.68807900
N	0.01516400	1.99713500	0.84355400
N	-1.90995100	1.00160400	1.02493300
C	1.35022300	2.39162500	0.46274700
C	2.42092000	2.14504300	1.35421000
C	1.53857600	3.08852500	-0.75387000
C	3.69434400	2.61955100	1.00196900
C	2.83347600	3.53761000	-1.06190900
C	3.90148200	3.30905600	-0.19334800
H	4.53218100	2.44511600	1.66821400
H	3.00225500	4.08048900	-1.98627300
H	4.89415700	3.66868900	-0.44673700
C	-3.07495500	0.16531400	0.85631600
C	-4.11869100	0.62246300	0.01612400
C	-3.18780600	-1.03593800	1.59058100
C	-5.29108500	-0.14645000	-0.05909200
C	-4.37831300	-1.77139500	1.47713200
C	-5.42394700	-1.33188200	0.66460500
H	-6.10648200	0.18755500	-0.69248700
H	-4.48873600	-2.69453600	2.03599900
H	-6.33928300	-1.91164900	0.59518100

C	0.38112600	3.40381300	-1.70153500
H	-0.49286800	2.84382500	-1.35721800
C	0.02835200	4.91046000	-1.65895400
H	-0.23359500	5.22842100	-0.64330300
H	0.87286600	5.52375600	-1.99677900
H	-0.82567300	5.12155400	-2.31390000
C	0.66707600	2.94481000	-3.14837800
H	1.51697200	3.48138700	-3.58741300
H	0.88227500	1.87169400	-3.17916900
H	-0.20713700	3.13489400	-3.78246500
C	-4.01663500	1.91999300	-0.78864900
H	-2.98631500	2.28103500	-0.71176500
C	-4.31446900	1.70338700	-2.29007300
H	-4.16338400	2.64024400	-2.83988700
H	-3.65516100	0.94381300	-2.72060600
H	-5.35130500	1.38734400	-2.45615600
C	-4.94584100	3.01501400	-0.21012100
H	-5.99728300	2.70823400	-0.26977500
H	-4.71667500	3.22403100	0.84053700
H	-4.83406600	3.94845000	-0.77486000
C	-2.08094500	-1.52088500	2.52511800
H	-1.18335700	-0.93548100	2.30363500
C	-1.73108900	-3.00603100	2.28458500
H	-2.56225700	-3.67031400	2.54970300
H	-1.48212500	-3.17977100	1.23202700
H	-0.87544700	-3.29645400	2.90861000
C	-2.45712100	-1.27325200	4.00590100
H	-2.64757000	-0.21055600	4.19364400
H	-3.36057900	-1.83150500	4.28113600
H	-1.64457500	-1.59586900	4.66880400
C	2.21291200	1.41914500	2.68438200
H	1.25259100	0.89599200	2.62483800
C	3.30085600	0.35868900	2.96211100
H	3.40632900	-0.32959600	2.11929300
H	4.27856400	0.81844600	3.14985000
H	3.03660600	-0.22023800	3.85561500
C	2.13890700	2.42262100	3.86230400
H	3.07606000	2.98620500	3.95055000
H	1.32413100	3.14188200	3.72989200
H	1.97166500	1.89191200	4.80763400
Ni	0.05558400	-0.45834900	-0.76280100
C	3.81656200	-2.36416500	-0.05388600
C	3.06279300	-1.28356100	-0.56849600
C	3.65626200	-0.37081500	-1.44711900
C	4.99053600	-0.57085300	-1.78819500
C	5.73022400	-1.65262600	-1.26839200
C	5.15776100	-2.56885300	-0.38972400
C	1.74691100	-2.39850500	0.71704800
H	3.08613900	0.46612200	-1.83526500
H	5.47669100	0.12284700	-2.46832100
H	6.77004400	-1.77458400	-1.55890200
H	5.72993200	-3.40103200	0.01007900
H	0.88115000	-2.74870300	1.26000900
N	1.76403900	-1.33870900	-0.06339800
N	2.94699800	-3.06276200	0.76870900
C	3.24136500	-4.26660900	1.51990200
H	3.54326900	-5.07756200	0.84791300
H	4.04421600	-4.08759700	2.24392500
H	2.34376800	-4.57616400	2.05971600
H	-0.41788000	3.71691700	2.10721300
H	-2.85443700	2.43309900	2.36701900
C	-1.16088700	-0.81600300	-2.31124400
C	-2.20173800	-1.77651600	-2.03011700
C	-1.97083600	-3.13145900	-1.97539300
C	-0.65521600	-3.62548900	-2.27184500
C	0.35531900	-2.75874400	-2.60248300
C	0.16043800	-1.33790100	-2.58902200
H	-1.46814500	0.14245600	-2.72934000
H	-3.21530600	-1.41203700	-1.87600100
H	-0.48273800	-4.70080800	-2.28230900
H	1.33220900	-3.14916600	-2.88572700
H	0.88237100	-0.72795700	-3.13521300
C	-3.08116800	-4.11279200	-1.67755700
H	-3.23379200	-4.81628000	-2.50850600
H	-2.85943200	-4.72215600	-0.78939900
H	-4.03033700	-3.59847200	-1.49418800

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C	-1.94701200	0.01272000	0.00036600
C	-4.16960900	-0.62937100	-0.13650300
C	-4.15690700	0.69518900	0.14747300
N	-2.80647500	1.08400900	0.21800900
N	-2.82686400	-1.04270100	-0.21332300
C	-2.40710000	2.45185000	0.48161800
C	-1.97806500	2.80258600	1.78361700
C	-2.51284300	3.40817900	-0.55705700
C	-1.63090700	4.14211000	2.01925300
C	-2.15794500	4.73509100	-0.26351400
C	-1.71574000	5.09928900	1.00785300
H	-1.29498500	4.43954000	3.00572600
H	-2.22742300	5.48876800	-1.03993400
H	-1.44248600	6.12982400	1.21239300
C	-2.45346400	-2.41744000	-0.47875200
C	-2.03627400	-2.77547900	-1.78262200
C	-2.57171500	-3.37195000	0.56025700
C	-1.71202000	-4.12051200	-2.01939200
C	-2.23998500	-4.70458900	0.26542300
C	-1.80843700	-5.07601200	-1.00749200
H	-1.38520800	-4.42361000	-3.00718700
H	-2.31908600	-5.45696600	1.04216100
H	-1.55282400	-6.11088800	-1.21292100
C	-3.04411900	3.05904800	-1.95068700
H	-2.98539600	1.97127400	-2.06997500
C	-4.53000800	3.47600200	-2.09672600
H	-5.16619900	2.99597200	-1.34651800
H	-4.63691200	4.56148100	-1.98243800
H	-4.90773400	3.19980100	-3.08843400
C	-2.21867600	3.69513700	-3.09243100
H	-2.33301400	4.78518800	-3.11509400
H	-1.15271500	3.46899100	-2.99870300
H	-2.56670500	3.31133300	-4.05864600
C	-2.00827400	-1.76429100	-2.93022600
H	-1.88098800	-0.76866400	-2.49548500
C	-0.83200700	-1.98337700	-3.90468900
H	-0.78457700	-1.15361800	-4.61941700
H	0.12233100	-2.03082500	-3.37061600
H	-0.94614400	-2.90609800	-4.48617700
C	-3.35532600	-1.78059600	-3.69698500
H	-3.53354400	-2.76461200	-4.14807800
H	-4.19753500	-1.55453200	-3.03367200
H	-3.34605600	-1.03451000	-4.50086400
C	-3.09251100	-3.01433900	1.95563700
H	-3.01588400	-1.92768500	2.07483900
C	-2.27385900	-3.66412700	3.09458000
H	-2.40621900	-4.75214200	3.11745700
H	-1.20461300	-3.45573700	2.99717200
H	-2.61224900	-3.27474800	4.06198400
C	-4.58451600	-3.40739800	2.10618400
H	-5.21515900	-2.91784400	1.35738300
H	-4.70887000	-4.49110800	1.99288500
H	-4.95504800	-3.12466800	3.09877800
C	-1.96059500	1.79040900	2.93060500
H	-1.84849300	0.79342300	2.49475300
C	-0.77806900	1.99202800	3.90122300
H	0.17515700	2.02547500	3.36414800
H	-0.87671800	2.91609700	4.48341700
H	-0.74062400	1.16141000	4.61554800
C	-3.30459500	1.82519400	3.70209100
H	-3.46728600	2.81137400	4.15435400
H	-4.15231400	1.61135000	3.04176500
H	-3.30294300	1.07864300	4.50560000
Ni	0.02459900	-0.00529500	-0.00335100
C	1.31293800	-1.28005900	0.71752500
C	0.35990600	-1.02560300	1.69407400
H	-0.41547900	-1.75325800	1.92086100
H	0.56688500	-0.32269500	2.50382800
C	2.25808000	-2.07788300	0.21073000
C	2.88358700	-3.22080400	1.06781500
C	3.24965300	-4.43839000	0.18710900
H	3.99608700	-4.19966800	-0.57609800
H	3.66741800	-5.23593900	0.81399600
H	2.36387300	-4.84149200	-0.31851700
C	1.91394200	-3.73238000	2.15305600
H	1.66437300	-2.95197500	2.87636400
H	0.97993100	-4.09574800	1.70928200
H	2.37647400	-4.56364900	2.70051200

C	4.15865900	-2.70842700	1.78104500
H	4.60534600	-3.50542100	2.39129600
H	4.91827000	-2.36622200	1.07196900
H	3.91522100	-1.87035500	2.44330600
C	2.70475500	-1.92332600	-1.23980300
H	2.50994300	-2.86525700	-1.77496400
H	2.05939800	-1.17309800	-1.70281600
C	4.16581600	-1.51393000	-1.51272700
H	4.86465300	-2.25423800	-1.10200100
H	4.37518200	-0.56793400	-0.99833100
C	4.45262000	-1.35145400	-3.01234100
H	4.21685500	-2.29252000	-3.53086800
H	3.77192400	-0.59592500	-3.43042300
C	5.90205600	-0.95389600	-3.31237000
H	6.60565500	-1.70719500	-2.93600900
H	6.07453600	-0.84633100	-4.38984900
H	6.15555200	0.00150400	-2.83695800
H	-4.98625800	-1.31186600	-0.29025300
H	-4.96017000	1.39254500	0.30496100
C	1.32706100	1.25274400	-0.73093800
C	0.37194100	1.00389600	-1.70610300
H	-0.39447500	1.73948300	-1.93781000
H	0.56963200	0.29235500	-2.51051700
C	2.27997400	2.04068300	-0.22343700
C	2.92389000	3.17258900	-1.08068600
C	3.26362600	4.40184300	-0.20561400
H	3.99263700	4.17489400	0.57788700
H	3.69270200	5.19461700	-0.83095600
H	2.36394300	4.80550800	0.27443300
C	1.98117800	3.66660600	-2.19692200
H	1.74897500	2.87487000	-2.91381800
H	1.03676400	4.03679000	-1.78205600
H	2.45698500	4.48939600	-2.74572500
C	4.21825300	2.65591900	-1.75534600
H	4.67445600	3.44603900	-2.36740300
H	4.96308100	2.32994100	-1.02360600
H	3.99594000	1.80584600	-2.40965600
C	2.71297300	1.88837500	1.23184100
H	2.51173800	2.83116800	1.76332800
H	2.06225900	1.13898800	1.68857600
C	4.17061000	1.47976400	1.52345800
H	4.87392400	2.22658600	1.13266600
H	4.39182200	0.53987600	1.00270800
C	4.43334100	1.30194600	3.02574400
H	4.18902000	2.23758800	3.55009500
H	3.74630300	0.54196200	3.42483200
C	5.87780900	0.90105200	3.34454000
H	6.58755500	1.65761300	2.98672400
H	6.03333500	0.78277500	4.42347100
H	6.13824500	-0.04983500	2.86382900

1i

C	0.86701200	-0.72654900	-0.00004800
C	2.80818100	-2.01767600	0.00019600
C	1.76075100	-2.88015200	0.00026100
N	0.58921700	-2.10332200	0.00008800
N	2.27110900	-0.71811000	0.00000700
C	-0.73833800	-2.66466100	0.00010800
C	-1.36612600	-2.94554800	1.23528100
C	-1.36604600	-2.94586000	-1.23503800
C	-2.64957800	-3.51426900	1.20882500
C	-2.64951200	-3.51454700	-1.20852400
C	-3.28820200	-3.79677800	0.00016600
H	-3.15299400	-3.73476200	2.14490100
H	-3.15288400	-3.73522400	-2.14458200
H	-4.28080100	-4.23735200	0.00019000
C	3.08323100	0.47295900	-0.00005200
C	3.48353900	1.03183000	-1.23511000
C	3.48366800	1.03186300	1.23495000
C	4.29106000	2.17998900	-1.20876400
C	4.29120700	2.18000400	1.20848300
C	4.69210700	2.75150200	-0.00017100
H	4.60690800	2.62989000	-2.14471300
H	4.60720400	2.62991600	2.14437800
H	5.31840500	3.63877700	-0.00020900
H	-0.69993000	-2.64004600	-2.57610700
C	0.28234000	-2.20530400	-2.36836600
C	-0.47897800	-3.92429000	-3.40851700

H	0.12534600	-4.65532500	-2.85889000
H	-1.43119400	-4.40314400	-3.66721600
H	0.04052900	-3.68613300	-4.34458500
C	-1.50131000	-1.58583700	-3.37389700
H	-2.50933900	-1.94561700	-3.61500600
H	-1.59159900	-0.65950100	-2.79626800
H	-0.99153700	-1.35586300	-4.31774800
C	3.04925400	0.43870300	-2.57449400
H	2.48705600	-0.47712700	-2.36696000
C	2.09544500	1.39810700	-3.32372000
H	1.76131200	0.94503800	-4.26539300
H	1.21295900	1.61052800	-2.71000900
H	2.59280500	2.34664500	-3.56314200
C	4.26013200	0.05366900	-3.45523600
H	4.85445500	0.93335700	-3.73105300
H	4.92225000	-0.64940800	-2.93664700
H	3.91774200	-0.42025200	-4.38310900
C	3.04951200	0.43878000	2.57438900
H	2.48718300	-0.47698800	2.36693800
C	2.09590200	1.39827000	3.32375400
H	2.59335900	2.34676800	3.56312500
H	1.21334300	1.61077100	2.71017700
H	1.76186000	0.94521500	4.26546500
C	4.26047900	0.05362900	3.45495300
H	4.92241500	-0.64957000	2.93629400
H	4.85496600	0.93325900	3.73060600
H	3.91818400	-0.42019000	4.38291400
C	-0.70006500	-2.63940800	2.57630500
H	0.28204100	-2.20433800	2.36847500
C	-1.50174600	-1.58542700	3.37408800
H	-1.59243400	-0.65916200	2.79640900
H	-2.50961900	-1.94554300	3.61534500
H	-0.99195200	-1.35519500	4.31786400
C	-0.47865300	-3.92353000	3.40878700
H	-1.43071500	-4.40267300	3.66752200
H	0.12589600	-4.65439700	2.85918400
H	0.04079800	-3.68516200	4.34483200
Ni	-0.30213500	0.64847300	-0.00011900
C	-3.46660400	3.31713700	-0.00010600
C	-2.94427900	2.00490500	-0.00009800
C	-3.80601700	0.90303000	-0.00009800
C	-5.17500000	1.15385800	-0.00008800
C	-5.68489500	2.46845300	-0.00007600
C	-4.84016200	3.57527300	-0.00007800
C	-1.25500200	3.35632800	-0.00007300
H	-3.40408300	-0.10488400	-0.00010500
H	-5.86933400	0.31840700	-0.00008300
H	-6.76049100	2.62196000	-0.00006100
H	-5.23449900	4.58720500	-0.00005900
H	-0.25286100	3.75937700	-0.00008400
N	-1.54624900	2.06613500	-0.00008300
N	-2.36432000	4.15959300	-0.00014000
C	-2.38400400	5.60886500	0.00018800
H	-2.89600400	5.98905800	-0.89074300
H	-2.89435700	5.98877300	0.89219500
H	-1.35617900	5.97791500	-0.00072800
H	1.73305500	-3.95631700	0.00032800
H	3.86973300	-2.19619400	0.00023100

Cartesian coordinates for the stationary points given in Fig. 1.

R1

C	-0.15563900	-0.36004900	-0.00001200
C	0.36926600	0.95617000	0.00000200
C	1.75650400	1.15031300	0.00001700
C	2.57534800	0.02516800	0.00001300
C	2.03507700	-1.27733000	-0.00000500
C	0.65904600	-1.49518400	-0.00001800
C	-1.75159600	1.16325000	0.00000500
H	2.16690000	2.15548600	0.00002000
H	3.65490200	0.14826600	0.00002000
H	2.70721500	-2.13109300	-0.00000600
H	0.24826100	-2.50089000	-0.00002400
H	-2.76151400	1.55713600	0.00001700
N	-0.66210700	1.88685000	-0.00002800

N	-1.53229200	-0.19766800	0.00000400
C	-2.53130400	-1.24672700	0.00001300
H	-2.43533900	-1.87766700	-0.89100100
H	-2.43527500	-1.87770800	0.89099100
H	-3.52457400	-0.79147100	0.00006100

R2

C	-1.32767800	1.64403200	0.00382300
C	-1.88036300	2.80663900	0.24302900
H	-2.46090700	3.33411900	-0.51314000
H	-1.78743100	3.29862700	1.21065700
C	-0.75298800	0.49134900	-0.25370600
C	-1.49110000	-0.84306300	0.02810000
C	-1.01975400	-1.95105700	-0.93648300
H	0.04236400	-2.18767000	-0.81257500
H	-1.58490800	-2.87137500	-0.74691900
H	-1.18615100	-1.66878100	-1.98281900
C	-3.01203000	-0.65986000	-0.15415200
H	-3.40347300	0.11543300	0.51170700
H	-3.25354400	-0.37071700	-1.18330400
H	-3.53616700	-1.59696100	0.06925700
C	-1.22368000	-1.28608800	1.48663900
H	-1.74457500	-2.22823700	1.70112400
H	-0.15752700	-1.44299200	1.67859700
H	-1.58410700	-0.52925400	2.19184800
C	0.66932100	0.51561400	-0.81484000
H	0.71932800	-0.10895800	-1.71708800
H	0.88412300	1.54007000	-1.14071100
C	1.78038100	0.07726800	0.15939700
H	1.63743300	-0.97047500	0.45489000
H	1.70373900	0.67110300	1.08064800
C	3.18405900	0.23736300	-0.44119100
H	3.24899800	-0.34629400	-1.37072400
C	3.33605200	1.28701300	-0.73004000
H	4.30052000	-0.19754000	0.51410100
H	4.19668600	-1.25400700	0.79118600
H	5.28921600	-0.06865100	0.05887100
H	4.28072000	0.39007200	1.44023500

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C	-0.22602800	-0.90528900	0.27647400
C	0.18361300	-2.68906300	1.70467900
C	-1.15984000	-2.49649100	1.68533700
N	-1.40496400	-1.41725000	0.82039300
N	0.74717400	-1.72279400	0.85244900
C	-2.72499300	-0.90723000	0.52890400
C	-3.26375700	0.10892000	1.35060000
C	-3.44446200	-1.45278600	-0.55869000
C	-4.55879300	0.56763600	1.06200000
C	-4.73377500	-0.95631700	-0.80701800
C	-5.28854400	0.04173600	-0.00486300
H	-4.99515300	1.34874800	1.67593100
H	-5.30502400	-1.35388500	-1.63949900
H	-6.28757400	0.41215100	-0.21338200
C	2.16612700	-1.58132800	0.63416500
C	2.76456600	-2.24552400	-0.46008800
C	2.91801700	-0.79436700	1.53606800
C	4.14821900	-2.09086200	-0.64454700
C	4.29853300	-0.67368900	1.30953200
C	4.90959400	-1.31156400	0.22830500
H	4.63280600	-2.59049200	-1.47720900
H	4.89885800	-0.07588600	1.98797800
H	5.97903900	-1.20831800	0.07091800
C	-2.86050200	-2.53484000	-1.46636500
H	-1.87134700	-2.79998000	-1.07963700
C	-3.72315300	-3.81831800	-1.45655000
H	-3.84013500	-4.21253700	-0.44039300
H	-4.72485100	-3.63145300	-1.86185400
H	-3.25430900	-4.59482600	-2.07272400
C	-2.66221500	-2.00689000	-2.90672700
H	-3.61948500	-1.72564300	-3.36245000
H	-2.00873300	-1.12766500	-2.91156900
H	-2.20496600	-2.78101200	-3.53521900
C	1.96479200	-3.13009100	-1.41647300
H	0.91239600	-3.07536000	-1.12168900

C	2.05277400	-2.63012200	-2.87631400
H	1.45414400	-3.27334700	-3.53231800
H	1.66700800	-1.60892000	-2.95989800
H	3.08502000	-2.64378200	-3.24697200
C	2.40700100	-4.60911600	-1.31015000
H	3.45361100	-4.73480900	-1.61317600
H	2.30784700	-4.98162900	-0.28414500
H	1.79066400	-5.23822500	-1.96335700
C	2.27894600	-0.08996900	2.73339900
H	1.21048400	-0.32588100	2.73003600
C	2.40255300	1.44724900	2.62699700
H	3.45312700	1.76411900	2.62007600
H	1.92178900	1.81220300	1.71367500
H	1.91565600	1.92672000	3.48476400
C	2.86392200	-0.60326300	4.07022500
H	2.74220600	-1.68822200	4.16757300
H	3.93383300	-0.37735100	4.15287400
H	2.35504100	-0.12518900	4.91565600
C	-2.48641500	0.71515500	2.51832300
H	-1.49680500	0.24817000	2.54063500
C	-2.27021500	2.23421200	2.32651800
H	-1.75582400	2.44211100	1.38239800
H	-3.22359600	2.77644600	2.32263100
H	-1.66131700	2.63542800	3.14581300
C	-3.17472400	0.41803300	3.87153100
H	-4.17206000	0.87162500	3.91842500
H	-3.28855800	-0.66025200	4.03316600
H	-2.58154100	0.82691200	4.69829400
Ni	-0.07475900	0.47039100	-0.93916600
C	1.19125000	3.61353400	-1.18899300
C	-0.03545600	3.13419700	-1.71735600
C	-1.16811500	3.95125300	-1.70290700
C	-1.05476400	5.22972100	-1.15018100
C	0.16363500	5.69052600	-0.62517600
C	1.30834600	4.88801500	-0.63179600
C	1.42126700	1.50200700	-1.90631500
H	-2.10619800	3.59183500	-2.11581200
H	-1.92413200	5.88137600	-1.12781800
H	0.22049400	6.69175800	-0.20626100
H	2.24820800	5.24771200	-0.22223900
H	2.00693400	0.77514100	-2.46253100
N	0.13155600	1.83926000	-2.22324600
N	2.10913100	2.59455000	-1.35757500
C	3.50643200	2.63125500	-0.99512900
H	4.02125900	3.45175000	-1.51119400
H	3.63795900	2.76092700	0.08624300
H	3.97138800	1.68506600	-1.28170900
H	-1.95601900	-3.01404400	2.19185500
H	0.78780400	-3.40678600	2.23208500

TS₁₀₋₁₁

C	0.97427200	-0.67409300	0.02074600
C	2.96674900	-1.81871900	-0.17437700
C	1.98976500	-2.74691200	0.00183700
N	0.78247200	-2.04251500	0.12141900
N	2.34109800	-0.56132800	-0.16014600
C	-0.50821700	-2.66727900	0.32235100
C	-0.91964600	-2.96452600	1.64180200
C	-1.30874200	-2.96478700	-0.80415500
C	-2.16720000	-3.58394700	1.81342900
C	-2.54630100	-3.58780300	-0.57539600
C	-2.97232700	-3.89566700	0.71690000
H	-2.51249200	-3.81754600	2.81513100
H	-3.18371300	-3.82577400	-1.41983800
H	-3.93505200	-4.37309500	0.87023100
C	3.05577800	0.68587000	-0.32771400
C	3.21729200	1.21072400	-1.62880900
C	3.58405300	1.32652600	0.81474200
C	3.93200700	2.41159000	-1.76363300
C	4.29176500	2.52371200	0.62460900
C	4.46504900	3.06288500	-0.65079100
H	4.06583300	2.84094300	-2.75090400
H	4.70564500	3.03937400	1.48503200
H	5.01311900	3.99141600	-0.77693900
C	-0.86860700	-2.65182600	-2.23449300
H	0.05036200	-2.05880200	-2.18197800
C	-0.54383100	-3.95269700	-3.00831600
H	0.23418900	-4.53765300	-2.50354400

H	-1.43356700	-4.58697600	-3.10244800
H	-0.19160300	-3.71520900	-4.01908400
C	-1.91400300	-1.80029500	-2.99135000
H	-2.85835700	-2.34378500	-3.11808300
H	-2.12571100	-0.86126300	-2.46873900
H	-1.53741300	-1.55693800	-3.99233700
C	2.64923000	0.52366600	-2.87048600
H	2.11320600	-0.37375200	-2.54519400
C	1.62554900	1.42471000	-3.59968000
H	1.21155600	0.89847000	-4.46794400
H	0.79779400	1.69288300	-2.93541800
H	2.09235600	2.34963500	-3.95942700
C	3.77586100	0.07181500	-3.82960100
H	4.34085300	0.92995100	-4.21273800
H	4.48350000	-0.59895400	-3.32840500
H	3.35122500	-0.45978600	-4.68934800
C	3.40380600	0.76869000	2.26482000
H	2.81945000	-0.15424400	2.15364600
C	2.60329800	1.74491500	3.11928900
H	3.13475800	2.69517400	3.24906000
H	1.62491000	1.95996200	2.67646300
H	2.44560300	1.30915100	4.11325900
C	4.76126400	0.40883900	2.87470400
H	5.31454700	-0.31424800	2.26446200
H	5.39294300	1.29657900	2.99726500
H	4.60469900	-0.03016200	3.86722800
C	-0.07294200	-2.60919200	2.86406800
H	0.88529100	-2.21465800	2.51009800
C	-0.74759100	-1.49382300	3.69757000
H	-0.91668800	-0.60034700	3.08634200
H	-1.71603100	-1.82487400	4.09114800
H	-0.11366800	-1.21559600	4.54833800
C	0.23365600	-3.84761600	3.73721800
H	-0.68084700	-4.27633300	4.16350400
H	0.73174200	-4.63158300	3.15544600
H	0.89034800	-3.57063700	4.57035700
Ni	-0.41215600	0.63648500	-0.00022200
C	-3.72572400	2.92035100	0.26810000
C	-3.83334700	2.25536500	-0.98175800
C	-5.00843400	2.38548100	-1.73547900
C	-6.03875900	3.16891700	-1.22210200
C	-5.91635300	3.81884500	0.02273200
C	-4.75781000	3.70372600	0.79069200
C	-1.88172900	1.73305700	-0.19005800
H	-5.09981200	1.88242400	-2.69391100
H	-6.95869100	3.28365100	-1.78969500
H	-6.74193500	4.42142000	0.39244700
H	-4.66939900	4.20381100	1.75150200
H	-0.39667600	2.05491000	-0.39194600
N	-2.67188900	1.55821200	-1.24982400
N	-2.47024600	2.59512200	0.74191000
C	-1.90579900	3.01589900	2.00507200
H	-1.95401300	4.10721400	2.10179800
H	-2.43670300	2.56528500	2.85366900
H	-0.85990000	2.70174100	2.03721800
H	2.03279900	-3.82085800	0.05372000
H	4.02921700	-1.92449700	-0.30749100

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C	1.11422600	0.00019100	0.22613000
C	2.96466900	-0.67873100	1.41661000
C	2.96449200	0.67995000	1.41640700
N	1.83244300	1.08448600	0.69007300
N	1.83272500	-1.08377900	0.69040300
C	1.46869200	2.46994000	0.47751600
C	1.98789500	3.14671600	-0.64858700
C	0.62623100	3.10365600	1.41824000
C	1.64309200	4.49743300	-0.81317700
C	0.31077300	4.45491700	1.20429300
C	0.81285300	5.14641200	0.10159400
H	2.02634200	5.04331800	-1.66887800
H	-0.33654400	4.96713300	1.90828200
H	0.55596600	6.19083100	-0.04589100
C	1.46932800	-2.46937500	0.47817300
C	0.62672100	-3.10297000	1.41884300
C	1.98897100	-3.14638600	-0.64758400
C	0.31157600	-4.45435300	1.20520100
C	1.64446000	-4.49721600	-0.81188200

C	0.81407200	-5.14607300	0.10283200
H	-0.33582300	-4.96648900	1.90917300
H	2.02806600	-5.04328200	-1.66730800
H	0.55741200	-6.19058100	-0.04442200
C	0.07172700	2.38268100	2.64711500
H	0.38318000	1.33433100	2.59525800
C	0.65491500	2.97597900	3.95216100
H	1.75023100	2.92910900	3.95916600
H	0.36323000	4.02590600	4.07494100
H	0.28313900	2.42049900	4.82136500
C	-1.47410800	2.39613100	2.67241100
H	-1.86480300	3.41855600	2.73964600
H	-1.88517000	1.92533200	1.77416300
H	-1.83795800	1.84306400	3.54705400
C	0.07180100	-2.38177100	2.64740000
H	0.38301700	-1.33335900	2.59530800
C	-1.47402400	-2.39556900	2.67244400
H	-1.83815200	-1.84227700	3.54683300
H	-1.88505500	-1.92517500	1.77396800
H	-1.86451700	-3.41805200	2.73997800
C	0.65493500	-2.97456200	3.95271300
H	0.36353500	-4.02454000	4.07572200
H	1.75023500	-2.92736200	3.95988100
H	0.28284600	-2.41895800	4.82170200
C	2.90930300	-2.46826500	-1.66209100
H	2.96907600	-1.40581100	-1.40627600
C	2.34437100	-2.55427800	-3.09786200
H	2.27375700	-3.59293900	-3.44265100
H	1.34909500	-2.10196500	-3.14704600
H	3.00161000	-2.01705100	-3.79230500
C	4.34167200	-3.05039400	-1.59220100
H	4.76754600	-2.94617500	-0.58735500
H	4.34830800	-4.11637500	-1.84996900
H	4.99963600	-2.52929100	-2.29784900
C	2.90795000	2.46842900	-1.66323100
H	2.96796100	1.40605500	-1.40712600
C	2.34245300	2.55397200	-3.09881400
H	1.34720500	2.10156300	-3.14749500
H	2.27161000	3.59253900	-3.44384900
H	2.99948000	2.01661900	-3.79335800
C	4.34026000	3.05076800	-1.59409600
H	4.34668200	4.11664800	-1.85228300
H	4.76654300	2.94698500	-0.58937900
H	4.99801800	2.52947900	-2.29980300
Ni	-0.44716600	-0.00027400	-0.85021500
C	-4.39470100	-0.00097900	-1.47483700
C	-3.89785100	-0.00010000	-0.14469200
C	-4.79133400	0.00061300	0.93150500
C	-6.15778900	0.00023400	0.65160700
C	-6.63613100	-0.00074000	-0.67143300
C	-5.75982900	-0.00136400	-1.75872600
C	-2.16635600	-0.00063900	-1.48299300
H	-4.42372300	0.00135600	1.95358700
H	-6.87063000	0.00070100	1.47216800
H	-7.70777700	-0.00101000	-0.85159900
H	-6.13219200	-0.00210700	-2.77953600
H	0.36054500	-0.00072900	-2.05831600
N	-2.51025000	0.00016600	-0.19878300
N	-3.26633700	-0.00134500	-2.29406700
C	-3.26025900	-0.00247500	-3.74218500
H	-3.76369900	-0.89403800	-4.13499500
H	-3.76431100	0.88812900	-4.13638100
H	-2.22093200	-0.00237800	-4.07469600
H	3.64345500	1.39000700	1.85499000
H	3.64382100	-1.38848600	1.85539100

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C	-0.72991700	-1.24851000	-0.04962800
C	-2.29084200	-2.94198500	-0.19981700
C	-1.43935600	-3.27161400	0.79817000
N	-0.48657300	-2.24220100	0.88216400
N	-1.86349100	-1.70187900	-0.70886400
C	0.64289400	-2.35892400	1.78454300
C	1.74780800	-3.13598500	1.36448400
C	0.55443700	-1.79982400	3.08069200
C	2.79327800	-3.33099400	2.28092500
C	1.63042700	-2.02730800	3.95448900
C	2.73733200	-2.78102100	3.56159300

H	3.65323800	-3.92479300	1.99005700
H	1.59754900	-1.61239200	4.95465500
H	3.55401200	-2.94598400	4.25789900
C	-2.59446000	-1.04801000	-1.77617500
C	-3.84858100	-0.46627300	-1.47383900
C	-2.08567200	-1.10279900	-3.09694800
C	-4.58515800	0.08373000	-2.53683400
C	-2.85822900	-0.52354700	-4.11636900
C	-4.09545300	0.06287200	-3.84176600
H	-5.55139900	0.53317700	-2.33547900
H	-2.49541000	-0.54408300	-5.13717600
H	-4.67958600	0.49640900	-4.64769900
C	-0.68518100	-1.03621000	3.55369100
H	-1.14572100	-0.56369400	2.68047000
C	-1.70957000	-2.00683900	4.19584700
H	-2.02552900	-2.79079600	3.49922000
H	-1.28154700	-2.49332700	5.08160200
H	-2.60365700	-1.45534900	4.51021400
C	-0.36102000	0.10980200	4.53283600
H	0.03058600	-0.25774000	5.48987400
H	0.35600200	0.80781800	4.09438200
H	-1.27809200	0.66957200	4.74601200
C	-4.44296900	-0.46112200	-0.06262500
H	-3.64986800	-0.73495400	0.64038800
C	-4.96525400	0.92806100	0.36464100
H	-5.30900300	0.88892300	1.40458500
H	-4.18438600	1.68867300	0.30111500
H	-5.81545000	1.24931100	-0.24937200
C	-5.57888500	-1.50886200	0.05863400
H	-6.40998700	-1.25910800	-0.61221600
H	-5.23841700	-2.51862600	-0.19494000
H	-5.96669600	-1.52884200	1.08373500
C	-0.78520200	-1.83782000	-3.43320200
H	-0.12434300	-1.76925400	-2.56321000
C	-0.02183100	-1.22322200	-4.62516000
H	-0.54173900	-1.38771800	-5.57672000
H	0.12197500	-0.14446000	-4.50000500
H	0.96602100	-1.68978800	-4.70948200
C	-1.06558800	-3.33872100	-3.70270800
H	-1.53431700	-3.82281800	-2.83962400
H	-1.73283800	-3.45897400	-4.56518300
H	-0.12932000	-3.86678700	-3.92010100
C	1.80274000	-3.81730700	-0.00582900
H	0.99068200	-3.41272500	-0.61732500
C	3.11635400	-3.53306600	-0.76612700
H	3.24928800	-2.45925000	-0.92386600
H	3.99184700	-3.91656200	-0.22915900
H	3.09098600	-4.02287100	-1.74715600
C	1.57717900	-5.34328000	0.13464100
H	2.37265000	-5.80324100	0.73325000
H	0.62091300	-5.56597500	0.62122100
H	1.57627800	-5.82191500	-0.85207100
Ni	0.31095600	0.28583600	-0.48666100
C	-2.23262800	3.45234900	0.54060300
C	-1.76160300	2.93339400	1.77052400
C	-2.10657300	3.57479100	2.96655500
C	-2.91116900	4.71245000	2.90244700
C	-3.37464000	5.21214800	1.67104600
C	-3.04314300	4.58746100	0.46672400
C	-0.95691800	1.61220400	0.22094500
H	-1.74670500	3.19116800	3.91746100
H	-3.18657000	5.22645400	3.82010300
H	-3.99880800	6.10204200	1.65570900
H	-3.39879500	4.97911500	-0.48305000
H	1.32883100	-0.76000200	-0.86883100
N	-0.99527300	1.80136600	1.53726700
N	-1.72333900	2.59851200	-0.42463700
C	-2.02004300	2.71327700	-1.83564000
H	-3.10032100	2.81111000	-1.99195600
H	-1.53001800	3.58834900	-2.28586500
H	-1.68389500	1.81026100	-2.34548700
H	-1.40289100	-4.12729100	1.44789900
H	-3.15085400	-3.45010800	-0.59657100
C	2.10420500	1.53277800	-0.93040200
C	1.11882500	1.64815300	-1.84227600
H	0.52566800	2.55628500	-1.88469200
H	1.07084600	0.98750900	-2.70811100
C	3.24416500	1.82752400	-0.33138300
C	3.67510300	1.35428800	1.07036400
C	4.67909800	2.33692800	1.71140600

H	4.25733700	3.34510700	1.79909400
H	4.92340900	1.99224000	2.72292800
H	5.61970700	2.40572200	1.15417600
C	4.33113100	-0.04195700	0.96862800
H	3.62320100	-0.76411500	0.55506900
H	5.22400000	-0.03096300	0.33434900
H	4.62891400	-0.39185400	1.96483000
C	2.44782900	1.26328000	1.99381100
H	2.74900900	0.90754000	2.98659100
H	1.95541700	2.23391500	2.10491000
H	1.70047700	0.56653400	1.60331700
C	4.18459600	2.70125100	-1.17596600
H	3.60148100	3.14958600	-1.98806900
H	4.55083700	3.53502600	-0.56364000
C	5.38758300	1.96575900	-1.79785900
H	5.02050800	1.10755200	-2.37791700
H	6.03137000	1.55329800	-1.01038200
C	6.22859700	2.87687700	-2.70326900
H	5.58956700	3.28618600	-3.49863400
H	6.58118700	3.74061900	-2.12156100
C	7.42904100	2.15906100	-3.32961400
H	7.10637400	1.30888100	-3.94325600
H	8.00755100	2.83311800	-3.97184800
H	8.10600900	1.77142200	-2.55827700

TS₁₂₋₁₃

C	-0.68032000	-1.18350400	0.00423800
C	-2.31468700	-2.77273500	-0.38067100
C	-1.52678500	-3.24345900	0.61291800
N	-0.52691600	-2.28036800	0.83464900
N	-1.80391900	-1.51563300	-0.74459700
C	0.55649900	-2.57958800	1.75250100
C	1.58213200	-3.44086900	1.29812300
C	0.49282500	-2.11194100	3.08515700
C	2.55745200	-3.84289800	2.22482100
C	1.49783000	-2.54307400	3.96689100
C	2.51452200	-3.40245900	3.54700600
H	3.35474500	-4.50583000	1.90551100
H	1.48155400	-2.20229100	4.99514500
H	3.27478400	-3.72585500	4.25148900
C	-2.43259000	-0.73528800	-1.79208200
C	-3.67998700	-0.12359100	-1.52325100
C	-1.83863600	-0.70446500	-3.07817700
C	-4.31488100	0.55379400	-2.57836200
C	-2.51187600	-0.00159000	-4.08998900
C	-3.73672300	0.62265800	-3.84471600
H	-5.27333400	1.02920400	-2.40158300
H	-2.08246300	0.04439000	-5.08377600
H	-4.24347500	1.15325200	-4.64494600
C	-0.64181900	-1.21052100	3.57382300
H	-0.97282800	-0.58938100	2.73502600
C	-1.84305600	-2.05555900	4.06913600
H	-2.23700900	-2.70679000	3.28117100
H	-1.55310000	-2.68742500	4.91865500
H	-2.65531600	-1.39622100	4.39727500
C	-0.19922900	-0.22414700	4.67302300
H	0.03459900	-0.72926100	5.61906700
H	0.67423100	0.35415900	4.35705300
H	-1.01144600	0.48359000	4.86782700
C	-4.38059000	-0.22690600	-0.16543200
H	-3.65003900	-0.58396500	0.56731700
C	-4.91033100	1.13046100	0.34674900
H	-5.32821600	1.00644700	1.35222100
H	-4.11661600	1.87741300	0.40591700
H	-5.71017900	1.52183600	-0.29369300
C	-5.54600100	-1.24792900	-0.22781600
H	-6.31533500	-0.91230100	-0.93395300
H	-5.21227900	-2.24100200	-0.54725600
H	-6.01333300	-1.34839000	0.75877200
C	-0.55843600	-1.48272000	-3.39849100
H	0.04742000	-1.52530600	-2.48733600
C	0.31217800	-0.82167800	-4.48741700
H	-0.16141900	-0.86659900	-5.47541800
H	0.52106900	0.22857900	-4.25798800
H	1.27035400	-1.34803000	-4.56194400
C	-0.90039400	-2.93808500	-3.81119000
H	-1.45230400	-3.46266700	-3.02449600
H	-1.51299900	-2.94699900	-4.72114500

H	0.01840900	-3.50157800	-4.01403800
C	1.65466300	-3.95685100	-0.14136300
H	0.86003300	-3.47313300	-0.71772200
C	2.99238600	-3.58648500	-0.82255400
H	3.14015100	-2.50191700	-0.83033900
H	3.84674600	-4.04596200	-0.31192900
H	2.99573000	-3.94040000	-1.86073100
C	1.41422300	-5.48438900	-0.20367200
H	2.19051900	-6.02947000	0.34637400
H	0.44464400	-5.75499800	0.22952400
H	1.43169700	-5.83124700	-1.24369000
Ni	0.36037300	0.42405400	-0.27110700
C	-2.15558300	3.51768000	0.90779500
C	-1.80184000	2.81570000	2.08531400
C	-2.20691700	3.31060400	3.33074100
C	-2.95003500	4.49051700	3.36697900
C	-3.29516000	5.17428500	2.18627500
C	-2.90419900	4.69652100	0.93362900
C	-0.95018700	1.67092600	0.42695300
H	-1.93853700	2.78528400	4.24340800
H	-3.26954100	4.89326000	4.32497500
H	-3.87327900	6.09265600	2.24974100
H	-3.16856200	5.22969900	0.02386600
H	1.58625100	-0.41639200	-0.56571400
N	-1.07443100	1.68244000	1.75182400
N	-1.61636200	2.77154300	-0.12813800
C	-1.77845300	3.09511800	-1.52795000
H	-2.83538800	3.26940700	-1.75940700
H	-1.21186600	3.99496000	-1.80454200
H	-1.43182500	2.25447400	-2.12800800
H	-1.56259300	-4.15871200	1.17620900
H	-3.17802400	-3.19509000	-0.86162200
C	2.22226700	1.23529500	-0.74589600
C	1.18490400	1.82300200	-1.43579100
H	0.93059700	2.85713900	-1.22612500
H	0.83948700	1.43394300	-2.39601900
C	3.47570900	1.40295400	-0.31840700
C	4.10733700	0.81200800	0.95555000
C	4.48602100	1.97853800	1.90792700
H	3.60331200	2.57962400	2.15361900
H	4.88783300	1.57081100	2.84354100
H	5.24767200	2.64498200	1.49120800
C	5.38057200	0.00230400	0.61471600
H	5.14661300	-0.83295000	-0.05633900
H	6.14900800	0.61742500	0.13434800
H	5.81767200	-0.41490200	1.53005500
C	3.14024200	-0.09291500	1.72862300
H	3.60753200	-0.41846900	2.66523000
H	2.21268500	0.43389500	1.97662000
H	2.87494300	-0.98629900	1.16320400
C	4.42342600	2.26007200	-1.17474600
H	5.10167800	2.80659100	-0.50907100
H	5.07190600	1.57227900	-1.74004300
C	3.82227800	3.26851400	-2.16079700
H	3.17593100	3.97363200	-1.62094800
H	3.18002200	2.75263600	-2.88489300
C	4.90290000	4.05267000	-2.91926900
H	5.54457200	4.58086300	-2.19955300
H	5.55864300	3.34725600	-3.45001200
C	4.32244400	5.05952400	-3.91813300
H	3.68999000	5.79948300	-3.41225300
H	5.11480700	5.60364800	-4.44510100
H	3.70434900	4.55736400	-4.67284800

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C	-0.50906000	-1.27335300	0.45565200
C	-1.81457500	-2.83795900	1.54461900
C	-0.63540500	-2.77096600	2.20961200
N	0.15901800	-1.83181200	1.53474500
N	-1.73553700	-1.92542300	0.48199900
C	1.55308000	-1.62881300	1.88092900
C	2.47109100	-2.65130100	1.54020900
C	1.93602800	-0.46997200	2.59755500
C	3.81552300	-2.46989300	1.90456000
C	3.29495500	-0.34070100	2.92899100
C	4.22568000	-1.32323600	2.58418800
H	4.54230100	-3.23745500	1.65935900
H	3.62567000	0.53657900	3.47102800

H	5.26891200	-1.19992600	2.85862900
C	-2.80236000	-1.79146700	-0.49027400
C	-4.01355800	-1.16771100	-0.10279900
C	-2.62920300	-2.36373500	-1.77282700
C	-5.04539000	-1.10281700	-1.05357100
C	-3.69070200	-2.25775500	-2.68655200
C	-4.88634100	-1.63227000	-2.33459700
H	-5.98297700	-0.62923600	-0.78536300
H	-3.58162300	-2.68357600	-3.67861600
H	-5.69708900	-1.56626600	-3.05358700
C	0.91290200	0.56820800	3.05997100
H	0.14984000	0.68706000	2.28312100
C	0.20710400	0.09257900	4.35696100
H	-0.29896700	-0.86875600	4.21877100
H	0.92844100	-0.01616300	5.17725700
H	-0.54702300	0.82811700	4.65987100
C	1.51070900	1.97144000	3.27891600
H	2.16810100	2.01242300	4.15744900
H	2.07578000	2.30772700	2.40416400
H	0.69518200	2.68376500	3.43742000
C	-4.24981400	-0.61701500	1.30618300
H	-3.27449900	-0.49727900	1.78936800
C	-4.93177100	0.76864100	1.30563000
H	-4.94862600	1.17144100	2.32440900
H	-4.39975500	1.48281200	0.67485000
H	-5.97133600	0.70784000	0.96103300
C	-5.09834000	-1.60404900	2.14935800
H	-6.09303000	-1.73093000	1.70465900
H	-4.63930700	-2.59544900	2.22242800
H	-5.22941800	-1.21573300	3.16615800
C	-1.37271500	-3.13500100	-2.18263700
H	-0.65729900	-3.08888100	-1.35656500
C	-0.68208000	-2.50671100	-3.41392200
H	-1.33233500	-2.53047400	-4.29650300
H	-0.41120100	-1.46356000	-3.21684700
H	0.23294600	-3.05958500	-3.65833300
C	-1.69542700	-4.62830200	-2.43066900
H	-2.15326700	-5.08749300	-1.54714700
H	-2.38819400	-4.75304100	-3.27127000
H	-0.77793300	-5.18029200	-2.66743800
C	2.04802600	-3.96208500	0.86628800
H	0.99183100	-3.88341400	0.59143800
C	2.82729700	-4.25694700	-0.43401100
H	2.67186100	-3.46975800	-1.17700800
H	3.90477400	-4.34263500	-0.25228200
H	2.48706400	-5.20648200	-0.86452300
C	2.18160300	-5.14932500	1.85257500
H	3.22749300	-5.30206900	2.14375200
H	1.60332100	-4.98052500	2.76790500
H	1.82218500	-6.07459800	1.38674300
Ni	0.01570400	0.18943200	-0.75785300
C	-2.75819900	3.14981600	-0.44709100
C	-2.11142600	3.13320000	0.81331700
C	-2.46378600	4.07904800	1.78275100
C	-3.44748600	5.01716100	1.46769900
C	-4.08140000	5.01869100	0.21145800
C	-3.74831800	4.08025400	-0.76843100
C	-1.24482000	1.49300000	-0.32773300
H	-1.97614800	4.07643400	2.75405500
H	-3.73153800	5.76340000	2.20551100
H	-4.84158000	5.76542300	-0.00307700
H	-4.23841800	4.08562800	-1.73860300
H	2.05441000	-0.07204400	-2.98173300
N	-1.19068500	2.09628800	0.85313500
N	-2.19818500	2.09586300	-1.15161500
C	-2.60143800	1.69575500	-2.48178900
H	-3.69070800	1.58227600	-2.52980600
H	-2.29060200	2.43188200	-3.23458000
H	-2.14423900	0.73391700	-2.71274700
H	-0.27974800	-3.29938800	3.07618000
H	-2.68638600	-3.44292200	1.71400400
C	2.02528300	0.71399300	-2.22615100
C	0.72827500	1.40200900	-2.07612400
H	0.79347400	2.43894800	-1.74347500
H	0.13077500	1.34732200	-2.99183400
C	3.18295000	0.98867700	-1.55773800
C	4.50986100	0.30628500	-1.96776000
C	5.62953100	0.51022500	-0.92405200
H	5.35590400	0.08589700	0.04857500
H	6.54255300	0.00578000	-1.26260400

H	5.87672500	1.56682700	-0.77885200
C	4.98508500	0.90868200	-3.31658800
H	4.24552500	0.73463500	-4.10563800
H	5.14302400	1.98990200	-3.24102000
H	5.93297000	0.45054300	-3.62868200
C	4.33223900	-1.21628200	-2.14785400
H	5.28174900	-1.67362500	-2.45424700
H	4.02038700	-1.67763200	-1.20668900
C	3.59021400	-1.46379900	-2.91364700
C	3.19904800	2.09955000	-0.52333400
H	2.19875900	2.19241600	-0.08779900
H	3.86466300	1.83761500	0.30715100
C	3.61549900	3.48350900	-1.07347900
H	2.97508900	3.73617500	-1.92945300
H	4.64302500	3.44288200	-1.46130900
C	3.51965900	4.59309300	-0.01779600
H	2.48965700	4.64012600	0.36189100
H	4.15115800	4.32998500	0.84341600
C	3.93203300	5.96916700	-0.55155100
H	3.29669300	6.27345900	-1.39251800
H	3.84936300	6.74004300	0.22340600
H	4.97035900	5.96328100	-0.90672800

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C	-0.41015100	-2.05088800	0.63778800
C	-1.71739400	-3.57554700	1.78374900
C	-0.53087100	-3.49585500	2.43988500
N	0.25729200	-2.57016600	1.74085300
N	-1.63900400	-2.69642400	0.69130400
C	1.60357000	-2.21063600	2.13107900
C	2.68644800	-2.95524200	1.60902700
C	1.78885300	-1.14586300	3.04164200
C	3.98123300	-2.60328200	2.02152300
C	3.10490500	-0.83597100	3.42125200
C	4.19055100	-1.55361200	2.91755100
H	4.83168900	-3.15761900	1.63830900
H	3.27800400	-0.02178000	4.11641500
H	5.19949600	-1.29626200	3.22458400
C	-2.71990200	-2.51259000	-0.25155400
C	-3.73834500	-1.57936400	0.05312800
C	-2.74448100	-3.30060400	-1.42374200
C	-4.79773800	-1.45068100	-0.85961700
C	-3.82538700	-3.13037700	-2.30414100
C	-4.84215400	-2.21594800	-2.02686100
H	-5.59497800	-0.74529300	-0.65328000
H	-3.87144500	-3.72362200	-3.21160800
H	-5.67194200	-2.10172700	-2.71768500
C	0.62094500	-0.36107500	3.63940500
H	-0.29357900	-0.67081100	3.12333900
C	0.44754700	-0.69830700	5.14108000
H	0.29475000	-1.77281700	5.29850800
H	1.33091300	-0.39696300	5.71711000
H	-0.41888800	-0.16607100	5.55109500
C	0.76628500	1.16236900	3.42432200
H	1.66229300	1.55565700	3.92039300
H	0.81258200	1.41045800	2.35888700
H	-0.10110100	1.67869800	3.85420700
C	-3.73069600	-0.76501700	1.34771200
H	-2.71037500	-0.78389800	1.74528600
C	-4.10498200	0.71665200	1.13097300
H	-3.98333800	1.26952900	2.06926400
H	-3.46568500	1.18780600	0.37963300
H	-5.14939700	0.83272800	0.81688200
C	-4.66480300	-1.40799500	2.40396800
H	-5.70310700	-1.41642100	2.05013500
H	-4.37610500	-2.44140500	2.62584100
H	-4.62994500	-0.83711500	3.33937500
C	-1.66410900	-4.33476000	-1.74233500
H	-0.89032900	-4.26315400	-0.97164000
C	-0.97946800	-4.05415600	-3.09905500
H	-1.69040200	-4.11654800	-3.93160200
H	-0.52797000	-3.05623200	-3.10624400
H	-0.18646800	-4.78919900	-3.28155200
C	-2.23655700	-5.77169600	-1.69699100
H	-2.68092300	-5.99156600	-0.71954000
H	-3.01260200	-5.91496400	-2.45838800
H	-1.44246000	-6.50435100	-1.88410900
C	2.48946600	-4.12641800	0.64586100

H	1.42748100	-4.17306700	0.38378800
C	3.27377600	-3.93053700	-0.67145400
H	2.98465500	-2.99547000	-1.16296400
H	4.35580300	-3.90309400	-0.49729100
H	3.06821900	-4.75855800	-1.36047000
C	2.86436400	-5.46992100	1.31642400
H	3.92447500	-5.48958100	1.59607800
H	2.27493100	-5.64006400	2.22466700
H	2.68139100	-6.30459700	0.62910700
Ni	0.28707800	-0.79651700	-0.57549600
C	-1.73293900	2.54580400	-1.33316100
C	-0.90996500	2.91322900	-0.23537500
C	-1.15816000	4.11562000	0.43996600
C	-2.21471100	4.91503200	0.00415700
C	-3.02041300	4.53522000	-1.08529600
C	-2.79280400	3.34036300	-1.77344900
C	-0.17006100	0.98531500	-0.90967000
H	-0.53516200	4.40816900	1.28047700
H	-2.42193900	5.85238900	0.51422400
H	-3.83411400	5.18344800	-1.40000100
H	-3.41636800	3.05031900	-2.61508700
H	3.09041300	0.15091400	-0.52304100
N	0.05833200	1.95314100	-0.02292400
N	-1.24169900	1.32653700	-1.75989500
C	-1.78900000	0.53455700	-2.83942300
H	-2.86229200	0.36655000	-2.69366900
H	-1.63779800	1.02525500	-3.81080800
H	-1.29281600	-0.43822200	-2.84585600
H	-0.17423700	-3.99830500	3.32202800
H	-2.59712600	-4.16255600	1.98093100
C	2.63758000	0.81701500	-1.25450500
C	1.35557100	0.32538000	-1.81862300
H	1.07556100	0.78317000	-2.76616900
H	1.41342800	-0.78314800	-2.03130700
C	3.26351300	1.97502500	-1.54882200
C	4.63116600	2.29164400	-0.88607600
C	5.12063700	3.72626200	-1.17850900
H	4.44113700	4.48118800	-0.76687400
H	6.10142700	3.88017000	-0.71271000
H	5.23476400	3.91892600	-2.25080800
C	5.70015800	1.30435400	-1.41633900
H	5.42304700	0.26761100	-1.19794400
H	5.82078900	1.39503300	-2.50240000
H	6.67534800	1.50117200	-0.95124200
C	4.53027300	2.14799600	0.65141100
H	5.48763900	2.41177500	1.12020100
H	3.75611800	2.81052200	1.05346400
H	4.28166800	1.12737000	0.95661700
C	2.66778500	2.94350900	-2.55580200
H	1.57622100	2.85704100	-2.54359600
H	2.87683200	3.97690700	-2.25868400
C	3.16362300	2.73612300	-4.00403100
H	2.92842500	1.70944500	-4.31964000
H	4.25915300	2.81694400	-4.04113400
C	2.55004300	3.73227400	-4.99677900
H	1.45402600	3.65802000	-4.95252600
H	2.79607900	4.75602800	-4.68072000
C	3.01985700	3.51586000	-6.43933100
H	2.75613300	2.51214400	-6.79580300
H	2.56456000	4.24214300	-7.12275800
H	4.10915700	3.61869000	-6.52170600

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C	-1.43731900	0.29935000	0.12658000
C	-3.34101300	-0.69523600	0.08965900
C	-3.62128400	0.68554100	-0.03083000
C	-4.39167000	-1.61983300	0.09707800
C	-4.92137800	1.18215100	-0.14302600
C	-5.69264000	-1.13487500	-0.01491600
H	-4.18495100	-2.68186000	0.18857800
C	-5.95362000	0.24445600	-0.13293100
H	-5.12830300	2.24499200	-0.23220500
H	-6.52622400	-1.83186200	-0.01112200
H	-6.98163300	0.58622800	-0.21716900
C	-2.17149400	2.74095300	-0.08369300
H	-2.65163800	3.14982500	-0.97997100
H	-2.58642600	3.24659500	0.79669500
H	-1.10340000	2.95525600	-0.13652000

N	-1.97214600	-0.89742600	0.18580900
C	0.03722300	0.59669000	0.20887200
C	0.87609700	-0.65560100	0.30786500
H	0.21130100	1.24103000	1.08713200
H	0.33462700	1.20411500	-0.65749800
C	2.13934300	-0.79980900	-0.12405500
H	0.35677500	-1.48690900	0.76819600
N	-2.38232900	1.30866800	-0.00743100
C	2.88381300	-2.14519400	-0.00764000
C	2.10002000	-3.19084600	0.80857000
C	3.10447400	-2.72309000	-1.42868800
C	4.25827900	-1.94698400	0.67543000
H	1.90215100	-2.84118300	1.82805200
H	1.14135300	-3.44009800	0.34175400
H	2.68350400	-4.11630400	0.87928900
C	3.69309600	-2.05218200	-2.06399300
H	3.64290600	-3.67739800	-1.37228600
H	2.14484000	-2.90314100	-1.92610500
H	4.78924900	-2.90463200	0.73883600
H	4.90173200	-1.25366800	0.12339000
H	4.13990300	-1.56145200	1.69495600
C	2.88883500	0.35715100	-0.77478900
C	3.41414900	1.41636800	0.21747400
H	2.23585900	0.85968900	-1.50270700
H	3.73734400	-0.01846600	-1.35771700
C	4.16744900	2.56196900	-0.47185900
H	2.57447800	1.82815000	0.79374200
H	4.07473300	0.93651500	0.95139900
C	4.68068000	3.62139100	0.50943000
H	5.01309000	2.14890600	-1.04018400
H	3.50820100	3.03664000	-1.21309200
H	5.21845700	4.42261600	-0.01040700
H	3.85398800	4.08114400	1.06531000
H	5.36664800	3.18144300	1.24381400

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C	-1.83506900	-0.73891000	0.03790100
C	-3.28133800	-2.30936000	-0.85479600
C	-3.15930300	-2.58470200	0.46857700
N	-2.28124100	-1.62886400	1.00604000
N	-2.47662600	-1.18781400	-1.11031900
C	-1.97173200	-1.56778400	2.42013000
C	-0.84974100	-2.27286400	2.91249700
C	-2.83978600	-0.84569700	3.26955200
C	-0.61796300	-2.24263100	4.29679600
C	-2.56146100	-0.84763000	4.64589500
C	-1.46368600	-1.53967000	5.15645100
H	0.23465500	-2.77331600	4.70439300
H	-3.21264500	-0.30235900	5.32111900
H	-1.26554100	-1.53128000	6.22387300
C	-2.40477500	-0.54914500	-2.40750800
C	-3.31739800	0.48993100	-2.70185600
C	-1.45468700	-1.00815400	-3.34921500
C	-3.25701700	1.07109400	-3.97870600
C	-1.44508100	-0.39942600	-4.61437000
C	-2.33467400	0.62945900	-4.92752600
H	-3.94167800	1.87448100	-4.22971600
H	-0.72804300	-0.73029200	-5.35712600
H	-2.30666800	1.08866000	-5.91087800
C	-4.06736400	-0.09737100	2.74812800
H	-4.03561100	-0.11704900	1.65438600
C	-5.37508900	-0.79670900	3.19125800
H	-5.41015400	-1.83495500	2.84188400
H	-5.46610300	-0.80745400	4.28408600
H	-6.24692400	-0.27003400	2.78499300
C	-4.06664300	1.38847900	3.17231000
H	-4.13219600	1.49931700	4.26108300
H	-3.15598200	1.89064900	2.83129100
H	-4.92845700	1.90560800	2.73358200
C	-4.35128100	0.98955800	-1.69202900
H	-4.26742200	0.37527900	-0.79004600
C	-4.07271400	2.45238100	-1.27371900
H	-4.81325200	2.78295200	-0.53526800
H	-3.07733900	2.54687900	-0.82561400
H	-4.12918300	3.13061000	-2.13374400
C	-5.79355800	0.82989900	-2.22761300
H	-5.96293700	1.45034700	-3.11555700
H	-6.00511900	-0.21058700	-2.49946600
H	-6.51703500	1.13771400	-1.46343100
C	-0.47826300	-2.14039200	-3.03208200

H	-0.41648700	-2.23134600	-1.94218500
C	0.94973400	-1.85752900	-3.54818200
H	1.00833700	-1.93068800	-4.64116300
H	1.28556200	-0.85667700	-3.25658100
H	1.64997900	-2.57986400	-3.11812200
C	-0.99225400	-3.49181600	-3.58762800
H	-1.97342600	-3.75184000	-3.17505400
H	-1.08407900	-3.45159100	-4.68008300
H	-0.29188600	-4.29586600	-3.33376000
C	0.06978800	-3.07494500	1.99173100
H	-0.01821400	-2.65220300	0.98483100
C	1.55685800	-2.98278900	2.39412300
H	1.86779800	-1.94101700	2.52863100
H	1.76236900	-3.52354800	3.32602600
H	2.17751600	-3.41956900	1.60600900
C	-0.37116800	-4.55875700	1.92037500
H	-0.31265600	-5.02800000	2.91042700
H	-1.40026100	-4.65867600	1.55854400
H	0.28391500	-5.11493100	1.23982800
Ni	-0.66813400	0.77290600	0.24120600
C	5.17061800	-1.37783400	-0.41781400
C	4.56614800	-2.60034800	-0.80337000
C	5.36975200	-3.70910900	-1.09887100
C	6.75024200	-3.56342500	-0.99969000
C	7.33450500	-2.33925300	-0.61399600
C	6.55563300	-1.22346000	-0.31574500
C	2.97055200	-1.22235500	-0.46096700
H	4.91585900	-4.64991900	-1.39589900
H	7.39557000	-4.40858000	-1.22344400
H	8.41651600	-2.26459700	-0.54764300
H	7.00948300	-0.28226100	-0.01864100
H	1.99603900	-0.75653600	-0.35581300
N	3.18347200	-2.46718600	-0.81896200
N	4.11528500	-0.50636400	-0.20419900
C	4.19514700	0.88040200	0.21525600
H	4.65018800	0.96066600	1.20891000
H	4.79451200	1.46152900	-0.49457800
H	3.18798700	1.30188500	0.25207600
H	-3.60815400	-3.35047700	1.07646400
H	-3.85699600	-2.78650400	-1.62824300
C	0.36160800	2.30341500	0.60831600
C	0.02053000	1.65923700	1.80771400
C	0.90407700	3.40452400	0.07213500
C	0.91707000	3.68035100	-1.44147500
C	-0.07913500	4.82255600	-1.76282700
H	0.16988700	5.74547300	-1.22688500
H	-0.07300600	5.05197600	-2.83669500
H	-1.09827200	4.53483300	-1.48068400
C	0.49734300	2.43577000	-2.24332100
H	1.18194700	1.59884500	-2.06355100
H	-0.51341900	2.10650000	-1.97238700
H	0.49819500	2.65140900	-3.31939100
C	2.32720200	4.10259000	-1.91831500
H	2.31880500	4.31115500	-2.99574500
H	2.68158400	5.00728100	-1.41270300
H	3.05950800	3.30652800	-1.73831000
C	1.47363000	4.47926600	1.00457600
H	1.55826000	5.43891100	0.47781900
H	0.76254300	4.64553100	1.82512600
C	2.84207600	4.13909100	1.62394100
H	3.58070000	3.97930900	0.82520900
H	2.75600800	3.18660300	2.16499300
C	3.35976100	5.22145800	2.58104700
H	3.44501000	6.17494500	2.03993700
H	2.61544500	5.38746300	3.37293700
C	4.71074000	4.87309900	3.21538000
H	5.48518600	4.73614800	2.44999500
H	5.05193900	5.66300800	3.89475900
H	4.64842000	3.94203400	3.79270000
H	0.74167600	1.03523900	2.34455100
H	-0.79173900	2.02952500	2.44145900

TS₁₄₋₁₅

C	0.42547300	-1.46914600	0.04940700
C	0.88584600	-3.66984000	-0.48852500
C	1.71516000	-3.32798300	0.52530000
N	1.44103400	-1.98545300	0.84224300

N	0.09257900	-2.54425000	-0.76696800
C	2.16082700	-1.29834700	1.89470000
C	3.49737900	-0.89570200	1.65425500
C	1.54307100	-1.13665000	3.15719500
C	4.20017200	-0.30054800	2.71493500
C	2.29193600	-0.53270300	4.18041900
C	3.60568800	-0.11630400	3.96407100
H	5.22470600	0.01795300	2.55912400
H	1.84431300	-0.40009400	5.15934700
H	4.16932200	0.34278100	4.77051200
C	-0.98320500	-2.59606700	-1.74004800
C	-2.15685500	-3.31374200	-1.40244700
C	-0.80779200	-1.98886800	-3.00647100
C	-3.17075300	-3.40333000	-2.36981100
C	-1.86033200	-2.10312000	-3.92982100
C	-3.02825100	-2.80019000	-3.61848600
H	-4.08010900	-3.94798700	-2.13998800
H	-1.76233300	-1.64254600	-4.90519500
H	-3.82537100	-2.87584300	-4.35168000
C	0.13910800	-1.66244800	3.46105200
H	-0.35102100	-1.89315400	2.51110900
C	0.21836200	-2.97394000	4.28165000
H	0.79353200	-3.74126800	3.75133600
H	0.70090100	-2.80109100	5.25128700
H	-0.78743600	-3.36910500	4.46853600
C	-0.74385700	-0.62081600	4.18253800
H	-0.36013900	-0.37921300	5.18067100
H	-0.80849000	0.30894400	3.60763600
H	-1.75940900	-1.01427700	4.30837900
C	-2.34264300	-4.02042500	-0.05550000
H	-1.55996800	-3.66722100	0.62438600
C	-3.70168500	-3.70350300	0.61085900
H	-3.74672000	-4.17123700	1.60162500
H	-3.84810800	-2.62669500	0.73496800
H	-4.54128100	-4.09546100	0.02540800
C	-2.18176900	-5.55383200	-0.21016900
H	-2.95937100	-5.95976500	-0.86833600
H	-1.21039100	-5.82045700	-0.63986200
H	-2.26999500	-6.04888100	0.76436700
C	0.49320100	-1.28474800	-3.39629100
H	0.90130100	-0.79391000	-2.50774100
C	0.29848000	-0.17126600	-4.44350300
H	0.05233900	-0.57348000	-5.43475300
H	-0.48797700	0.52619800	-4.13979100
H	1.22515700	0.40277900	-4.53088300
C	1.53608600	-2.31535400	-3.90140800
H	1.75473100	-3.07863700	-3.14651500
H	1.17303800	-2.82363900	-4.80381800
H	2.47505000	-1.80721700	-4.15076400
C	4.20606100	-1.13892800	0.31894200
H	3.44005700	-1.34355500	-0.43637000
C	5.01463800	0.08371400	-0.16725100
H	4.40320500	0.98736700	-0.20273000
H	5.88067600	0.27822800	0.47697900
H	5.39539200	-0.10469300	-1.17738800
C	5.14099400	-2.37301700	0.40693300
H	5.93633100	-2.20149200	1.14270600
H	4.60511700	-3.28150100	0.70030300
H	5.61366000	-2.55785600	-0.56482000
Ni	-0.38632000	0.26273700	-0.00968200
C	2.71320100	3.00149700	-0.34019100
C	2.57464200	2.53620700	-1.67217600
C	3.43794400	3.01715100	-2.66572100
C	4.41145400	3.94570000	-2.30268800
C	4.53596100	4.39622300	-0.97361100
C	3.68905600	3.92961400	0.03238300
C	1.04873200	1.50283600	-0.51799600
H	3.34012300	2.66995000	-3.69058100
H	5.09027300	4.33321500	-3.05805000
H	5.30642100	5.12189900	-0.72651200
H	3.78959300	4.27761700	1.05700600
H	-0.45399400	1.70673800	-0.32549000
N	1.53422500	1.62698800	-1.74965000
N	1.73011800	2.34124900	0.37281600
C	1.48306400	2.48728600	1.79218700
H	2.31929700	2.09708400	2.38281500
H	1.32643300	3.54208800	2.04814500
H	0.58320900	1.92403800	2.04716600
H	2.46354400	-3.89371300	1.04969600
H	0.77614700	-4.59026200	-1.03330200

C	-2.16539900	1.15620500	0.09015300
C	-2.22451800	-0.16817700	0.54608800
C	-2.95774200	2.19696100	-0.20040200
C	-2.50716400	3.51927000	-0.87617600
C	-3.69216000	4.47082700	-1.16046000
H	-4.24084400	4.74537000	-0.25307700
H	-3.30816800	5.39690900	-1.60381600
H	-4.40373500	4.04083200	-1.87417400
C	-1.84005500	3.22042100	-2.24110500
H	-0.93788100	2.61204200	-2.14794200
H	-2.53797600	2.68821800	-2.89885300
H	-1.55883200	4.15881300	-2.73692500
C	-1.51905900	4.28494000	0.03604000
H	-1.20408500	5.22019500	-0.44423400
H	-1.98690000	4.53782700	0.99519800
H	-0.61880600	3.70215600	0.24302500
C	-4.42484200	2.02288600	0.20577500
H	-5.09001600	2.51936800	-0.50942600
H	-4.67136300	0.95578000	0.16904900
C	-4.74359900	2.53839000	1.62439900
H	-4.46738300	3.59846600	1.71235900
H	-4.11195500	1.99816300	2.34354000
C	-6.21997100	2.36756100	2.00619500
H	-6.84612600	2.91344700	1.28590600
H	-6.49787000	1.30822800	1.90788100
C	-6.53742400	2.84944200	3.42605500
H	-6.30271500	3.91457200	3.54502800
H	-7.59787700	2.71349200	3.66872100
H	-5.95139000	2.29759900	4.17162600
H	-2.25415200	-0.38857000	1.61515000
H	-2.69718500	-0.92072600	-0.08359500

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C	0.08302700	1.32732800	-0.25157200
C	0.60950300	3.07936800	-1.66378100
C	-0.60740100	3.34690600	-1.13928200
N	-0.93302800	2.27368000	-0.29133000
N	1.03614500	1.85679400	-1.11680600
C	-2.20481100	2.24870100	0.40391300
C	-3.37759000	1.97369400	-0.34205000
C	-2.25278200	2.61735000	1.76867900
C	-4.60870300	2.04602800	0.33043600
C	-3.51054000	2.66519000	2.39189100
C	-4.67777200	2.38071500	1.68320800
H	-5.52244200	1.84070900	-0.21577900
H	-3.57531300	2.94741300	3.43716800
H	-5.64118800	2.43116300	2.18113000
C	2.35494900	1.33638800	-1.43801000
C	3.48131200	1.93670300	-0.82126700
C	2.48403600	0.33617000	-2.43255800
C	4.75557400	1.48897300	-1.20561300
C	3.78490000	-0.07419500	-2.77179500
C	4.90796700	0.49095900	-2.16694000
H	5.63483900	1.93014400	-0.74953200
H	3.91753400	-0.84064900	-3.52516800
H	5.90160400	0.15865900	-2.45137600
C	-1.00891700	3.04663900	2.54762100
H	-0.12941000	2.75427700	1.96807800
C	-0.97589000	4.58699800	2.70743800
H	-0.99298100	5.08828500	1.73304300
H	-1.83939100	4.94103000	3.28354100
H	-0.06576400	4.89722900	3.23489600
C	-0.89640500	2.35283600	3.92257700
H	-1.70755300	2.64899000	4.59789300
H	-0.92200600	1.26336600	3.81698300
H	0.04888100	2.62779200	4.40509100
C	3.36644500	3.07878900	0.19412100
H	2.33201800	3.11018400	0.55277800
C	4.27774600	2.88510600	1.42844900
H	4.07555100	3.67227600	2.16461500
H	4.10950600	1.91739300	1.90872200
H	5.33877400	2.95424800	1.16200100
C	3.68360200	4.44323400	-0.46970600
H	4.71531600	4.46007400	-0.84090000
H	3.02028900	4.65118100	-1.31501900
H	3.57131700	5.25635200	0.25747600
C	1.27630000	-0.23923800	-3.17487500
H	0.43160100	-0.28912700	-2.48099400

C	1.49245400	-1.68293100	-3.66975500
H	2.22601300	-1.73852000	-4.48460600
H	1.81355400	-2.33886500	-2.85553300
H	0.54343600	-2.07501300	-4.04739800
C	0.88639800	0.67171700	-4.36814700
H	0.64402500	1.69008000	-4.04641800
H	1.70525600	0.73055900	-5.09666900
H	0.00683600	0.26117700	-4.87783200
C	-3.35651500	1.67165500	-1.84362200
H	-2.33079100	1.40849200	-2.12216200
C	-4.25522800	0.47804500	-2.23403600
H	-4.00473600	-0.42105700	-1.66842200
H	-5.31761800	0.70209000	-2.07769200
H	-4.12315400	0.25148600	-3.29808200
C	-3.77840200	2.92052000	-2.66085400
H	-4.81120600	3.20410500	-2.42396100
H	-3.14014900	3.78676400	-2.45900400
H	-3.72504700	2.70378800	-3.73415500
N	0.19257000	-0.26530900	0.76822300
C	-3.03101700	-2.51314100	-0.55160100
C	-2.06405200	-2.68613900	-1.57213100
C	-2.34417900	-3.53718700	-2.64862600
C	-3.57566300	-4.19159700	-2.67604100
C	-4.52441700	-4.00931200	-1.65230100
C	-4.26681700	-3.16439600	-0.57053200
C	-1.16831900	-1.30020800	-0.13380000
H	-1.61061200	-3.68330800	-3.43728500
H	-3.80955900	-4.85878300	-3.50205600
H	-5.47326800	-4.53741300	-1.70211300
H	-5.00075000	-3.02712400	0.21973900
H	0.61641000	-0.61477100	3.41103900
N	-0.94273700	-1.92250400	-1.28961000
N	-2.45200900	-1.62273200	0.33705900
C	-3.07820100	-1.17053300	1.55851100
H	-4.03446500	-0.67770200	1.34988300
H	-3.26004200	-2.00757400	2.24551200
H	-2.41762200	-0.44973800	2.04264300
H	-1.27302400	4.17880600	-1.27967300
H	1.21372000	3.62464600	-2.36586800
C	1.20466200	-0.79754300	2.51602800
C	1.75595200	0.34649600	1.86959100
C	1.13982500	-2.06798100	1.94289200
C	0.44083400	-3.23150900	2.69161300
C	1.52427500	-4.16272300	3.30000700
H	2.20263200	-3.61270600	3.96257100
H	1.04082600	-4.95056900	3.89068100
H	2.12245000	-4.65612500	2.52757800
C	-0.43883300	-4.08708800	1.75112000
H	-1.29739300	-3.52348500	1.38434100
H	0.11208300	-4.44912400	0.87867400
H	-0.80933300	-4.96581500	2.29385400
C	-0.44357400	-2.74882600	3.86014300
H	-0.97512400	-3.60445700	4.29224200
H	0.14662000	-2.29510700	4.66498700
H	-1.19455000	-2.02320400	3.53338000
C	2.11185800	-2.45441400	0.82328900
H	1.82645200	-3.42923900	0.41601400
H	2.01534500	-1.75905900	-0.02088900
C	3.60279100	-2.50213900	1.23340800
H	3.73460800	-3.15249000	2.10612200
H	3.93201500	-1.50436100	1.54905700
C	4.50549200	-2.99806900	0.09572100
H	4.18534000	-4.00528600	-0.20794000
H	4.36721700	-2.35435400	-0.78323000
C	5.98932800	-3.02817500	0.47809400
H	6.16444100	-3.68268000	1.34120800
H	6.60928200	-3.39533200	-0.34837900
H	6.34887700	-2.02649100	0.74518500
H	1.71514700	1.28967900	2.40893400
H	2.62489400	0.24408500	1.22650200

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C	1.16857400	-0.87501600	0.05420800
C	2.79492300	-1.58147800	1.51010800
C	2.08372600	-2.67604900	1.14043800
N	1.08059600	-2.23890500	0.25922000
N	2.23365700	-0.48283700	0.84306500
C	0.15605100	-3.15614700	-0.38099900

C	-0.96583900	-3.62048700	0.34812000
C	0.44935900	-3.60959300	-1.68822500
C	-1.80975600	-4.54776400	-0.28464100
C	-0.43291700	-4.53346900	-2.27216600
C	-1.55177200	-4.99680200	-1.58096100
H	-2.67877200	-4.92010900	0.24477500
H	-0.23280100	-4.89868200	-3.27370000
H	-2.21944900	-5.71406000	-2.04820000
C	2.81174200	0.84915300	0.90716800
C	3.88752100	1.14894400	0.03862900
C	2.33226300	1.76656700	1.87052200
C	4.47619500	2.41865300	0.14579500
C	2.95943300	3.02157900	1.93130100
C	4.01637300	3.34695400	1.07974200
H	5.30175500	2.67957100	-0.50746200
H	2.61508500	3.75195400	2.65357800
H	4.48427000	4.32408600	1.14764300
C	1.70633800	-3.18794100	-2.45158100
H	2.18918400	-2.37802600	-1.89640600
C	2.71342500	-4.36161100	-2.53285300
H	2.98471800	-4.72515000	-1.53510500
H	2.29212600	-5.20398200	-3.09445400
H	3.63044300	-4.04147200	-3.04152300
C	1.38774900	-2.63849400	-3.85982000
H	0.92633700	-3.40017500	-4.49909800
H	0.71382700	-1.77809700	-3.80170000
H	2.31158300	-2.31009500	-4.35008200
C	4.45232400	0.13808300	-0.96183800
H	3.77593400	-0.72264200	-0.99648000
C	4.53414200	0.70713500	-2.39607700
H	4.88421700	-0.06981500	-3.08635200
H	3.55600800	1.05668300	-2.73812200
H	5.23875100	1.54448500	-2.45905100
C	5.83728400	-0.37846600	-0.49945100
H	6.56527300	0.44035700	-0.45650100
H	5.78596100	-0.83350200	0.49636000
H	6.21691600	-1.13185300	-1.19992600
C	1.21995800	1.40609700	2.85564100
H	0.59412400	0.63585900	2.39576800
C	0.27632600	2.58707200	3.15960900
H	0.77535300	3.38585800	3.72231200
H	-0.13613300	3.00397700	2.23700000
H	-0.56273700	2.23138400	3.76749600
C	1.82089100	0.84219500	4.16828100
H	2.43426100	-0.04790000	3.98679200
H	2.45214900	1.59143700	4.66245900
H	1.01886600	0.56287500	4.86195900
C	-1.24885600	-3.18802000	1.78902400
H	-0.76114200	-2.22049200	1.95035700
C	-2.75371800	-2.99575500	2.07922400
H	-3.23110500	-2.34505400	1.34314500
H	-3.28795600	-3.95377500	2.09597100
H	-2.88158200	-2.53387000	3.06405500
C	-0.66049200	-4.20727500	2.79926700
H	-1.12774000	-5.19100600	2.66798400
H	0.42072900	-4.33074600	2.68441100
H	-0.85426300	-3.87397900	3.82552100
N	0.34782200	0.25309900	-1.17667300
C	-3.46185100	-0.04930500	-0.03612000
C	-2.86884400	0.54142200	1.10663800
C	-3.67794000	0.95969200	2.16970700
C	-5.05547900	0.77499900	2.06216700
C	-5.62901500	0.18464900	0.91958300
C	-4.84115000	-0.23914500	-0.15172500
C	-1.24223900	0.08190000	-0.24182200
H	-3.23459000	1.41730800	3.04962500
H	-5.70343500	1.09395800	2.87440900
H	-6.70725800	0.05883500	0.86863700
H	-5.28711100	-0.69234300	-1.03276100
H	-1.27157800	1.51137800	-3.76117600
N	-1.48979000	0.58653300	0.95119500
N	-2.40328200	-0.34689300	-0.87992600
C	-2.52062100	-0.98409300	-2.17630700
H	-3.21264600	-0.42549200	-2.81549800
H	-1.53772300	-0.99670800	-2.64963100
H	-2.87655900	-2.01581100	-2.07233300
H	2.19374200	-3.71268100	1.40230500
H	3.64090500	-1.47259200	2.16502600
C	-0.62499700	2.06213100	-3.07630400
C	0.67681100	1.38744600	-2.81620400

C	-1.10513900	3.22645800	-2.57128600
C	-2.46425700	3.79815100	-3.05034900
C	-3.02040400	4.86696000	-2.08341500
H	-2.35767400	5.73500500	-1.99732800
H	-3.98824300	5.23151100	-2.44931500
H	-3.17783400	4.45845100	-1.07825500
C	-3.54319400	2.69630400	-3.16729900
H	-3.28003700	1.93877900	-3.91323200
H	-3.69702600	2.19250400	-2.20676700
H	-4.49991400	3.13517100	-3.47952500
C	-2.29085600	4.45205500	-4.44570400
H	-3.24141600	4.86861600	-4.80746100
H	-1.55719800	5.26530000	-4.41780000
H	-1.93997000	3.71562300	-5.17738700
C	-0.24825300	4.02675500	-1.60506200
H	-0.86780300	4.49119000	-0.82805600
H	0.41954000	3.33798800	-1.07253500
C	0.62055800	5.12592600	-2.25697100
H	-0.02228600	5.85673800	-2.76783000
H	1.24464100	4.67161200	-3.03919600
C	1.51211400	5.86373800	-1.24966400
H	0.88027900	6.31074100	-0.46811600
C	2.15713600	5.13544000	-0.73795900
H	2.37839800	6.95460900	-1.88956600
H	1.75914800	7.71731400	-2.37834600
H	3.00371100	7.46254000	-1.14510100
H	3.04475600	6.53407400	-2.65332500
H	0.97554800	0.78376400	-3.68181600
H	1.48368700	2.09453700	-2.59068700

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C	1.97350400	0.35107400	-0.06212100
C	4.21674100	-0.06937500	0.25837500
C	4.00477600	1.23260600	0.58530600
N	2.63975500	1.47856500	0.38763300
N	2.97643100	-0.59723400	-0.13270700
C	2.01389800	2.76497700	0.62385000
C	1.55483000	3.07072900	1.92481000
C	1.91468500	3.67962900	-0.45113200
C	0.96877000	4.33131800	2.12479600
C	1.32201500	4.92536400	-0.19330400
C	0.84973600	5.24760700	1.08004200
H	0.60258500	4.59351900	3.11119600
H	1.23224200	5.64964200	-0.99536300
H	0.39206400	6.21565300	1.25819800
C	2.81501000	-1.96460500	-0.58350800
C	2.87470400	-2.23349200	-1.96921900
C	2.65545100	-2.98652800	0.38107100
C	2.75626000	-3.57096600	-2.38055200
C	2.55008900	-4.30679100	-0.08514100
C	2.59721700	-4.59791300	-1.44999000
H	2.79585600	-3.80739300	-3.43878900
H	2.42668000	-5.11341500	0.62830100
H	2.51275600	-5.62642700	-1.78699800
C	2.47688600	3.37453000	-1.84130200
H	2.67127600	2.29763400	-1.89814900
C	3.82723700	4.10221400	-2.05789500
H	4.56131300	3.81939500	-1.29514300
H	3.69537500	5.18984200	-2.01077400
H	4.24325800	3.85278800	-3.04133600
C	1.48790300	3.71982500	-2.97655300
H	1.30047600	4.79790600	-3.03843500
H	0.52480500	3.21841400	-2.83391400
H	1.90096500	3.40262000	-3.94128400
C	3.08458300	-1.13807600	-3.01525200
H	3.16254300	-0.17921500	-2.49272300
C	1.88405000	-1.03386500	-3.98415900
H	2.04644400	-0.22329200	-4.70472800
H	0.95697200	-0.82645700	-3.43831600
H	1.74556600	-1.96240400	-4.55063600
C	4.40583100	-1.34761300	-3.79265200
H	4.38792900	-2.28198300	-4.36581100
H	5.26490900	-1.38706600	-3.11337100
H	4.56563900	-0.52457900	-4.49922500
C	2.64285100	-2.69586000	1.88316600
H	2.39828200	-1.63637400	2.01644200
C	1.57374700	-3.50646000	2.64663200
H	1.80844600	-4.57782300	2.66116100

H	0.57985100	-3.37636800	2.21154700
H	1.52975600	-3.16843200	3.68785000
C	4.04197700	-2.94699100	2.50167500
H	4.81553800	-2.33192900	2.02904300
H	4.33139100	-3.99884100	2.38752900
H	4.02982200	-2.71272300	3.57256300
C	1.72156200	2.11529200	3.10736800
H	2.07418100	1.15346300	2.72093500
C	0.39015700	1.84168800	3.84189500
H	-0.32400600	1.33852200	3.18214200
H	-0.05711300	2.76573300	4.22820200
H	0.57484200	1.18215200	4.69904700
C	2.79802100	2.65233700	4.08385000
H	2.48734000	3.60756500	4.52424300
H	3.75897700	2.81270000	3.57998300
H	2.95518500	1.93965500	4.90179700
Ni	0.06360600	0.33853300	-0.53183500
C	-1.90754500	-2.67095100	1.30540200
C	-1.85202700	-1.66711200	2.30460900
C	-2.42802100	-1.90796100	3.55705000
C	-3.04387900	-3.14062900	3.77752800
C	-3.08825200	-4.12708000	2.77535500
C	-2.51657100	-3.90882600	1.51933400
C	-0.83526300	-0.84374000	0.57134400
H	-2.39410800	-1.14618600	4.33116800
H	-3.50002500	-3.34557700	4.74290000
H	-3.57777200	-5.07579600	2.97996100
H	-2.55346500	-4.67204700	0.74630800
H	-2.41037000	-0.29071900	-2.80413000
N	-1.18543600	-0.55217100	1.81458400
N	-1.25234400	-2.12524000	0.21283200
C	-1.05591200	-2.79285300	-1.05386600
H	-2.01628200	-3.01098400	-1.53679000
H	-0.50433600	-3.73101500	-0.91927100
H	-0.47491900	-2.13751600	-1.70454700
H	4.67832500	1.99406900	0.93738000
H	5.11371100	-0.66284600	0.25982800
C	-2.68125700	0.24510800	-1.89679300
C	-1.56589600	0.97638200	-1.26489800
C	-3.95466100	0.15051400	-1.44962900
C	-5.01421800	-0.71637600	-2.15602400
C	-6.29227100	0.11140600	-2.43726600
H	-6.73434700	0.51073500	-1.51891200
H	-7.05172200	-0.51623100	-2.92066000
H	-6.07813100	0.95490800	-3.10428700
C	-4.52609600	-1.28479300	-3.50285200
H	-3.66979600	-1.95723400	-3.37792700
H	-4.23394400	-0.48785700	-4.19644800
H	-5.32987600	-1.86238000	-3.97478800
C	-5.39157600	-1.91370000	-1.24639700
H	-6.14212400	-2.54612700	-1.73823700
H	-5.81126900	-1.58774900	-0.28941500
H	-4.51394600	-2.53135100	-1.02589500
C	-4.37733700	0.88358000	-0.18152900
H	-3.59025000	0.78109700	0.57518900
H	-5.26609400	0.41096000	0.25408900
C	-4.68141300	2.38558100	-0.37965400
H	-3.80526100	2.87894800	-0.82087100
H	-5.49486700	2.50795900	-1.10722400
C	-5.05838500	3.09437400	0.92794800
H	-4.24232800	2.96980200	1.65366600
H	-5.93550100	2.60010400	1.37040100
C	-5.35480300	4.58649400	0.74168600
H	-4.48385800	5.11464500	0.33327200
H	-5.61931100	5.06559400	1.69189700
H	-6.18978800	4.74189700	0.04677500
H	-1.88401500	1.73705600	-0.54405400
H	-0.92893100	1.46454000	-2.04796700

Cartesian coordinates for the stationary points given in Fig. 2.

NaO_tBu

O	-0.75431600	0.00003700	-0.12712400
C	0.61635600	0.00000200	-0.00372200

C	1.27221200	0.00211500	-1.40769900
C	1.08202900	1.25930500	0.76964000
C	1.08226000	-1.26146700	0.76595700
H	0.94773700	-0.88380000	-1.96761500
H	0.94744700	0.88950500	-1.96510600
H	2.37025500	0.00224200	-1.36677100
H	0.62054300	1.27114500	1.76552500
H	2.17252100	1.30878900	0.89538700
H	0.75581800	2.16103700	0.23629100
H	2.17275500	-1.31105800	0.89163500
H	0.62068300	-1.27633400	1.76176600
H	0.75629300	-2.16171000	0.22995400
Na	-2.69515100	0.00001500	-0.01901200

TS_{1h-17}

C	0.88910200	-1.27793300	-0.00020000
C	1.30626300	-3.57014100	-0.21900500
C	2.47929000	-2.98271000	0.12405500
N	2.23253200	-1.60588400	0.25653900
N	0.34446000	-2.54482300	-0.29456000
C	3.25565200	-0.64662200	0.59555200
C	4.05315900	-0.10225800	-0.43839400
C	3.45338200	-0.30019200	1.95191200
C	5.06855200	0.79944200	-0.08144700
C	4.47590300	0.61294400	2.25522500
C	5.27913700	1.15637200	1.25159400
H	5.69562100	1.22867500	-0.85603200
H	4.64213000	0.90094400	3.28815900
H	6.06670500	1.85850400	1.50754000
C	-1.03300500	-2.75709900	-0.63777400
C	-1.95601400	-3.08829300	0.38598900
C	-1.43612800	-2.62217200	-1.99088300
C	-3.30857800	-3.24367500	0.03144300
C	-2.80122700	-2.78192200	-2.29134900
C	-3.73131800	-3.08319700	-1.29127000
H	-4.03485000	-3.49249100	0.79777400
H	-3.13608500	-2.67888200	-3.31824200
H	-4.78008600	-3.20167200	-1.54383000
C	2.59174100	-0.87442800	3.07578200
H	1.89572600	-1.59152600	2.62950300
C	3.44323100	-1.63564500	4.11810100
H	4.01975000	-2.44183500	3.64962800
H	4.15024600	-0.96792200	4.62462400
H	2.79618700	-2.07831700	4.88499600
C	1.73909200	0.22842200	3.74562300
H	2.37074800	0.99744800	4.20687200
H	1.08984400	0.71146900	3.00720900
H	1.10748400	-0.20459700	4.53122600
C	-1.52060200	-3.28507300	1.83792500
H	-0.45007500	-3.06801600	1.89534100
C	-2.23541000	-2.30579100	2.79643800
H	-1.87767600	-2.45488400	3.82195600
H	-2.02918300	-1.26652500	2.51658800
H	-3.32160700	-2.45805000	2.79760400
C	-1.72874800	-4.75194900	2.28442900
H	-2.78953700	-5.02958800	2.26303200
H	-1.18593600	-5.44717400	1.63393100
H	-1.36618900	-4.89024300	3.30966500
C	-0.43960900	-2.32798200	-3.11229800
H	0.54705900	-2.20922200	-2.65554600
C	-0.76237200	-1.00587300	-3.84558300
H	-1.75384700	-1.03257600	-4.31496600
H	-0.72049600	-0.15869900	-3.15049900
H	-0.02507200	-0.82490600	-4.63643700
C	-0.36183000	-3.51265100	-4.10502800
H	-0.09446500	-4.44427200	-3.59339800
H	-1.31956700	-3.67138300	-4.61533400
H	0.39675200	-3.31381600	-4.87097800
C	3.84274900	-0.46874200	-1.90756200
H	2.93763300	-1.08102300	-1.97019100
C	3.60660900	0.78057500	-2.78640800
H	2.76615400	1.37214000	-2.40981100
H	4.49175400	1.42746500	-2.81688400
H	3.38212600	0.47803300	-3.81654900
C	5.02139600	-1.31169500	-2.45025100
H	5.96099500	-0.74704300	-2.41245600
H	5.15777900	-2.22964300	-1.86685000
H	4.84037500	-1.59431400	-3.49442900
Ni	0.16900400	0.37258000	-0.00690200
C	-0.31908600	4.40109500	-0.55200000

C	0.41175600	3.23569300	-0.24597700
C	1.80384600	3.29960200	-0.11333600
C	2.42446600	4.53439800	-0.29829900
C	1.68298000	5.69002900	-0.60836100
C	0.29532600	5.64157500	-0.73878800
C	-1.73678200	2.64247600	-0.33544300
H	2.37692900	2.41057400	0.12969400
H	3.50434000	4.60659400	-0.19831200
H	2.19933300	6.63667700	-0.74479200
H	-0.27877800	6.53371300	-0.97381100
H	-3.09149700	1.95947800	-0.11371900
N	-0.48437700	2.16581800	-0.12557800
N	-1.64287000	3.99451200	-0.60263100
C	-2.75863700	4.86273000	-0.91524000
H	-2.89662300	5.62886300	-0.14163500
H	-2.59800600	5.36609200	-1.87636000
H	-3.66176300	4.25529700	-0.98313100
H	3.45626400	-3.40409200	0.28773800
H	1.06269000	-4.60049300	-0.41378100
O	-3.97893700	1.25382300	-0.03669900
C	-4.89292000	1.50079600	1.02437600
C	-5.74448800	0.23330400	1.20096100
C	-4.13229700	1.81031400	2.32868300
C	-5.80989300	2.68357200	0.65625800
H	-6.26628300	-0.00437800	0.26644800
H	-5.10798100	-0.62064400	1.46409500
H	-6.49356400	0.35641200	1.99288100
H	-3.50615300	2.70146600	2.21097600
H	-4.82193200	1.98539400	3.16385700
H	-3.47506600	0.97461300	2.59692500
H	-6.57637300	2.85572500	1.42251300
H	-5.22806500	3.60625300	0.55291300
H	-6.31117400	2.48684700	-0.29800500
Na	-2.38669700	-0.15676500	-0.51945100

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C	-1.04797500	-1.19952200	0.03410900
C	-1.60718100	-3.45076300	0.34072900
C	-2.73616200	-2.80879500	-0.05023800
N	-2.40321600	-1.45600700	-0.23653600
N	-0.58548400	-2.48359400	0.39118300
C	-3.35504800	-0.45100600	-0.64248900
C	-4.12509700	0.20276800	0.34759100
C	-3.51092300	-0.16569100	-2.01820300
C	-5.07269400	1.14915600	-0.07386100
C	-4.46680200	0.79418200	-2.38748800
C	-5.24382900	1.44403000	-1.42753900
H	-5.67777700	1.66305300	0.66598600
H	-4.60006400	1.03571300	-3.43704700
H	-5.97961200	2.18159800	-1.73331400
C	0.77312900	-2.75620000	0.76590400
C	1.68775100	-3.19076900	-0.22564100
C	1.16915500	-2.57060200	2.11495400
C	3.02686200	-3.39588000	0.15336400
C	2.52020700	-2.78669600	2.44178000
C	3.44400900	-3.18735700	1.47106500
H	3.74704500	-3.72233200	-0.58958300
H	2.84901500	-2.64837400	3.46653100
H	4.48230500	-3.34759500	1.74358200
C	-2.66564400	-0.84706300	-3.09354200
H	-2.03559000	-1.59295500	-2.59915700
C	-3.54040300	-1.58765900	-4.13109000
H	-4.19091100	-2.32676900	-3.64917100
H	-4.17817700	-0.89208200	-4.68941000
H	-2.90567900	-2.11101300	-4.85632400
C	-1.71934000	0.16648000	-3.77914000
H	-2.28419300	0.95952000	-4.28429000
H	-1.05674700	0.63099100	-3.04050100
H	-1.10052200	-0.33907000	-4.53109400
C	1.26081300	-3.43248400	-1.67348000
H	0.19026600	-3.21977000	-1.74360800
C	1.97877200	-2.47373500	-2.65084200
H	1.64023400	-2.65692800	-3.67749000
H	1.75376700	-1.42999500	-2.40273900
H	3.06663600	-2.61401000	-2.62763500
C	1.47433200	-4.90889200	-2.08217900
H	2.53580800	-5.18341400	-2.05792600
H	0.93583400	-5.58907000	-1.41246800
H	1.10952600	-5.07467100	-3.10254300

C	0.17825500	-2.16540200	3.20587700
H	-0.78954900	-1.99459300	2.72623100
C	0.58155700	-0.84356400	3.89832700
H	1.55477700	-0.92726300	4.39841300
H	0.62434700	-0.02374100	3.17152700
H	-0.16073000	-0.57675500	4.65977900
C	0.00064500	-3.30432300	4.23880400
H	-0.32357200	-4.23330400	3.75601200
H	0.93672200	-3.51033700	4.77205800
H	-0.75447900	-3.02446400	4.98257400
C	-3.95606600	-0.09500800	1.83726000
H	-3.08587400	-0.74967300	1.94734100
C	-3.66530300	1.18456200	2.65345600
H	-2.78785100	1.70830000	2.26075900
H	-4.51420200	1.87883800	2.63562700
H	-3.47187400	0.92527700	3.70151700
C	-5.18627900	-0.84512500	2.40203900
H	-6.09439000	-0.23601600	2.31485900
H	-5.36091600	-1.78582800	1.86690500
H	-5.03789300	-1.07873500	3.46340300
Ni	-0.20130300	0.38661800	0.01843600
C	0.77155000	4.32808800	0.57150300
C	-0.09537500	3.27462900	0.21787000
C	-1.45425200	3.53078100	-0.00150700
C	-1.90672700	4.84173300	0.14475000
C	-1.03130100	5.88463700	0.50180700
C	0.32525000	5.64343600	0.72015400
C	1.94799600	2.38010700	0.44364000
H	-2.12871100	2.72654100	-0.28011500
H	-2.95741300	5.06440200	-0.02275400
H	-1.41746400	6.89531700	0.60633500
H	1.00147100	6.44901200	0.99358500
H	3.58575800	1.55037900	0.01764500
N	0.64878900	2.09130800	0.15347700
N	2.01941200	3.73947100	0.70480000
C	3.22014500	4.44998600	1.08758900
H	3.48481800	5.21533900	0.34632300
H	3.08973800	4.94252400	2.05933800
H	4.03685100	3.73042600	1.16563200
H	-3.73415500	-3.17757600	-0.21442400
H	-1.43168400	-4.48471700	0.58397700
O	4.27116200	0.80585100	-0.10381600
C	5.11774800	1.02821100	-1.24345300
C	5.94820200	-0.24879900	-1.40849600
C	4.25959500	1.28447000	-2.49340500
C	6.03700700	2.22898900	-0.96544100
H	6.53781300	-0.44006400	-0.50490300
H	5.29323500	-1.11090600	-1.57979400
H	6.63456800	-0.16459500	-2.25868000
H	3.62514200	2.16681600	-2.35451800
H	4.88757900	1.45035100	-3.37703900
H	3.60578000	0.42837400	-2.69402100
H	6.74143300	2.39044600	-1.79033600
H	5.44976100	3.14621300	-0.84232900
H	6.61058300	2.06224700	-0.04719600
Na	2.34004000	-0.18645400	0.53191700

TS₁₇₋₁₈

C	0.74788900	-1.28939300	-0.00307000
C	1.00221500	-3.60331600	0.24189700
C	2.14929800	-3.12965000	-0.30724000
N	1.99790200	-1.74019600	-0.45955200
N	0.15091200	-2.49759300	0.42321500
C	3.00717700	-0.87802300	-1.02215800
C	3.01384900	-0.64823800	-2.41713600
C	3.96576800	-0.29189300	-0.16505300
C	4.01070400	0.18967000	-2.94172800
C	4.94390600	0.53607000	-0.73858700
C	4.96828000	0.77658400	-2.11294000
H	4.03399300	0.38642200	-4.00883300
H	5.68816900	1.00093100	-0.09977900
H	5.73136100	1.42210200	-2.53749100
C	-1.16670800	-2.54411200	0.99187400
C	-1.32619300	-2.32292300	2.38257500
C	-2.27801700	-2.77524800	0.14107700
C	-2.63302300	-2.29971300	2.90332500
C	-3.56357700	-2.74790500	0.71078000
C	-3.74337800	-2.50165900	2.07657400

H	-2.77993600	-2.13517100	3.96588200	C	1.56827700	-0.68740600	0.19311300
H	-4.42910200	-2.91963300	0.08082300	C	2.82699800	-2.46983700	1.03287300
H	-4.74401500	-2.49072200	2.49844800	C	3.70404400	-1.56427700	0.52992600
C	3.95925600	-0.52349500	1.34506500	N	2.94830800	-0.49383500	0.02209300
H	3.11808400	-1.18389700	1.57736700	N	1.53793600	-1.94576900	0.82556600
C	5.25288600	-1.22804200	1.81698800	C	3.52910700	0.68000200	-0.58212200
H	5.39849600	-2.18319200	1.29873100	C	3.69196000	0.72117100	-1.98553500
H	6.13735700	-0.60697300	1.63017700	C	3.93149000	1.75155600	0.24788200
H	5.20644500	-1.42739000	2.89454200	C	4.26619700	1.87183600	-2.54876000
C	3.72741300	0.79638500	2.11607400	C	4.50189100	2.87932900	-0.36383600
H	4.53373500	1.51643300	1.93035000	C	4.66816400	2.94213500	-1.74814300
H	2.77997600	1.25719000	1.81771000	H	4.39610300	1.93035200	-3.62472100
H	3.69235200	0.60350900	3.19556000	H	4.81314800	3.71763600	0.25105200
C	-0.13211900	-2.12465500	3.31495700	H	5.10968800	3.82402500	-2.20239200
H	0.76743400	-2.08736300	2.69436000	C	0.31842400	-2.59748300	1.21832700
C	-0.20771200	-0.78597700	4.08323900	C	-0.28865400	-2.24679200	2.45094700
H	0.68129600	-0.66473900	4.71338000	C	-0.24994200	-3.56614700	0.35616300
H	-0.24292000	0.05631800	3.38369200	C	-1.50975500	-2.86193600	2.78124200
H	-1.08663600	-0.74251400	4.73931700	C	-1.47030700	-4.15372100	0.73291900
C	0.00994800	-3.31968400	4.28837500	C	-2.10112200	-3.80073200	1.92855600
H	-0.86219600	-3.40237000	4.94862700	H	-1.99414900	-2.61177900	3.71910100
H	0.11180500	-4.26623800	3.74532100	H	-1.93149500	-4.88944600	0.08275700
H	0.89763100	-3.19064700	4.91868900	H	-3.04224500	-4.26685000	2.20390400
C	-2.09449100	-3.06590000	-1.34788300	C	3.73964200	1.72685000	1.76420300
H	-1.10016800	-2.70338600	-1.62673500	H	3.35969100	0.73779800	2.03871800
C	-3.11727700	-2.32953300	-2.23978200	C	5.07314500	1.93794500	2.51768000
H	-4.13508700	-2.71521100	-2.09796900	H	5.82030100	1.19152100	2.22358200
H	-3.12177600	-1.25373100	-2.03656300	H	5.49477100	2.93077400	2.32001300
H	-2.85886900	-2.47968000	-3.29465300	H	4.91378700	1.85464500	3.59942500
C	-2.13746100	-4.59205300	-1.61200800	C	2.67681400	2.76002900	2.20683600
H	-1.36877600	-5.12126100	-1.03823400	H	2.98356800	3.78115700	1.94834100
H	-3.11412800	-5.00861300	-1.33550600	H	1.71545300	2.55252000	1.72368000
H	-1.96962500	-4.79765900	-2.67584500	H	2.53285100	2.71612100	3.29359700
C	1.96453200	-1.25674600	-3.34685200	C	0.36169900	-1.26478600	3.42542600
H	1.35346000	-1.94597400	-2.75539500	H	1.19016900	-0.78060500	2.90066600
C	1.01546900	-0.16686600	-3.89911900	C	-0.60141100	-0.14369100	3.87482700
H	0.51058000	0.35221700	-3.07711100	H	-0.07441200	0.55430800	4.53594900
H	1.56699900	0.57238400	-4.49368200	H	-0.97103200	0.42459200	3.01406600
H	0.25204100	-0.61871900	-4.54510700	H	-1.45936700	-0.53856400	4.43340600
C	2.60654400	-2.07217200	-4.49249900	C	0.94544700	-2.02124300	4.64419900
H	3.19830000	-1.43413200	-5.15981300	H	0.15480100	-2.52385000	5.21494300
H	3.26761200	-2.85528200	-4.10331100	H	1.67127700	-2.78118000	4.33214900
H	1.82789700	-2.55174100	-5.09784600	H	1.45357400	-1.32028700	5.31692100
Ni	0.04389000	0.36698000	0.09053900	C	0.40793500	-3.95610400	-0.96826400
C	0.35805200	3.93305200	0.47050300	H	1.39796400	-3.49155500	-0.99724100
C	-0.10743600	3.08596400	1.50285100	C	-0.38725900	-3.40266100	-2.17494200
C	0.16288300	3.39506500	2.83861200	H	-1.40655600	-3.80950000	-2.19478300
C	0.90080800	4.54760900	3.11497400	H	-0.43685200	-2.30791000	-2.12414300
C	1.36171900	5.38084200	2.07997300	H	0.10540900	-3.67789500	-3.11523300
C	1.09772900	5.08798600	0.74071100	C	0.60795200	-5.48392400	-1.08802100
C	-0.80852300	2.19805900	-0.43567500	H	1.18637000	-5.87665500	-0.24416000
H	-0.19257400	2.74952000	3.63782300	H	-0.34908500	-6.01818400	-1.11732500
H	1.12312100	4.80802400	4.14659500	H	1.14782100	-5.72148300	-2.01209700
H	1.93553700	6.27040600	2.32709500	C	3.24354800	-0.42524700	-2.89049700
H	1.46059500	5.73279700	-0.05511100	H	2.89244000	-1.23892300	-2.24805900
H	-2.41693800	1.55293900	-1.10679300	C	2.05056800	0.00371600	-3.77645300
N	-0.83161100	2.03712400	0.92618400	H	1.21326500	0.33721800	-3.15285500
N	-0.08416200	3.36039300	-0.70930600	H	2.33086600	0.82367600	-4.44936700
C	0.22268600	3.85076400	-2.03468100	H	1.71204700	-0.83813500	-4.39362200
H	-0.13489800	4.87997900	-2.16996500	C	4.40765200	-0.97518300	-3.74628200
H	1.30305700	3.82975000	-2.22557700	H	4.79092600	-0.21777000	-4.44059300
H	-0.27416700	3.20046400	-2.75701400	H	5.24213400	-1.30683500	-3.11755200
H	3.05017000	-3.64031600	-0.60178900	H	4.06834200	-1.83057100	-4.34310100
H	0.71674400	-4.60322000	0.52059700	Ni	0.18977600	0.47945700	-0.08395900
O	-3.34199200	1.12483000	-1.02332200	C	-2.39574500	3.69144800	0.01196300
C	-4.35780100	2.00345800	-1.53616100	C	-3.19326200	2.66317600	0.57312300
C	-5.68172600	1.24339800	-1.40684000	C	-4.47968600	2.96294500	1.04062900
C	-4.39494500	3.29948200	-0.70868500	C	-4.93808400	4.27634200	0.93186100
C	-4.05606600	2.31218800	-3.01153300	C	-4.13491700	5.28538500	0.36922400
H	-5.64111600	0.30495700	-1.97022100	C	-2.84853000	5.00789100	-0.09895100
H	-5.88688000	1.00450400	-0.35585200	C	-1.26493600	1.71802900	-0.00086800
H	-6.51698900	1.84160300	-1.78833200	H	-5.09848100	2.18783500	1.48753400
H	-3.43044700	3.81561000	-0.75453600	H	-5.93276300	4.52819900	1.29156500
H	-5.17005000	3.98273400	-1.07630900	H	-4.52065700	6.29934300	0.30017000
H	-4.60848900	3.07674700	0.34385500	H	-2.22922000	5.79029300	-0.52978500
H	-4.83330400	2.94863100	-3.45131300	H	-2.80205700	-1.68227900	-2.12602100
H	-3.09662600	2.83345500	-3.10558100	N	-2.48740200	1.47425500	0.54779000
H	-3.99738500	1.38402400	-3.58968800	N	-1.20951300	3.07559600	-0.33637400
Na	-2.48279900	0.31069700	0.91690500				

C	-0.08121600	3.74505100	-0.94757800
H	-0.35909400	4.18138700	-1.91605200
H	0.29994000	4.54634900	-0.30156100
H	0.70767800	3.00502900	-1.10085500
H	4.77961600	-1.57664900	0.48416400
H	2.99137300	-3.42038700	1.51109000
O	-3.42357300	-1.63770700	-1.37978100
C	-4.68818800	-1.10932300	-1.88221900
C	-5.56371200	-0.92457200	-0.64186100
C	-4.43040600	0.22895800	-2.58407700
C	-5.29362600	-2.14177600	-2.84102000
H	-5.67688100	-1.87379700	-0.10529000
H	-5.12407100	-0.18204500	0.03285500
H	-6.56001700	-0.57205300	-0.92801900
H	-3.77047800	0.09286900	-3.45119100
H	-5.36816500	0.66351000	-2.94830600
H	-3.95912800	0.93861300	-1.89771700
H	-6.26232700	-1.80005500	-3.22261000
H	-4.63610300	-2.30564800	-3.70425800
H	-5.43912400	-3.10082100	-2.33263100
Na	-2.19302100	-0.77133200	0.38932200

TS₁₈₋₁₉

C	0.51090300	2.57462500	0.28858600
C	-0.81815900	4.33203600	1.07429100
C	-1.45172300	3.18442500	1.40468300
N	-0.66983100	2.12140700	0.91916700
N	0.36605100	3.97700300	0.39223100
C	-1.15118600	0.76075400	0.88941600
C	-2.13399100	0.41454200	-0.06995300
C	-0.66698300	-0.17592600	1.83349500
C	-2.59640200	-0.91222800	-0.09103800
C	-1.15642600	-1.48974300	1.76340800
C	-2.10493900	-1.85888800	0.80684100
H	-3.35062700	-1.20170700	-0.81586600
H	-0.79774400	-2.23123600	2.46713300
H	-2.46945300	-2.88115700	0.77223700
C	1.20319100	4.98198700	-0.21829500
C	2.11404000	5.71350600	0.58454400
C	1.00695300	5.29229800	-1.59057200
C	2.82228600	6.77274400	-0.01621400
C	1.75289300	6.34525200	-2.14397400
C	2.64475100	7.08702100	-1.36619600
H	3.49735900	7.36908100	0.58824400
H	1.61954600	6.59944800	-3.18853500
H	3.18369400	7.92136500	-1.80644700
C	0.29690000	0.24690100	2.94288400
H	0.93887300	1.03456500	2.53345700
C	-0.48693700	0.83521300	4.14429600
H	0.20885700	1.16593300	4.92505700
H	-1.09485100	1.69609600	3.84691400
H	-1.15386800	0.08061800	4.58044600
C	1.22325500	-0.88822300	3.41807300
H	0.66964800	-1.69415700	3.91576300
H	1.78873400	-1.31253300	2.58243700
H	1.94252900	-0.49368700	4.14408400
C	2.31768900	5.41435000	2.07184400
H	2.04856200	4.36389100	2.23099700
C	3.78424400	5.60923600	2.52151600
H	3.92552500	5.18291000	3.52005300
H	4.48944700	5.12133700	1.84186600
H	4.04816800	6.67265400	2.57993600
C	1.39988700	6.28963500	2.96383900
H	1.58459300	6.06903500	4.02194600
H	1.60439400	7.35479700	2.79829000
H	0.34071800	6.10942400	2.76473900
C	-0.04251600	4.56919100	-2.43679400
H	-0.13950500	3.55385900	-2.03892700
C	0.34477800	4.44552700	-3.92429100
H	0.31017100	5.41468400	-4.43825400
H	1.34227600	4.01768000	-4.05014900
H	-0.36595100	3.78558200	-4.43399000
C	-1.41806400	5.27602000	-2.31138500
H	-1.76724000	5.31358700	-1.27494900
H	-1.35788000	6.30386800	-2.69098300
H	-2.17003000	4.74098700	-2.90396200
C	-2.75040700	1.43979200	-1.02646200
H	-2.19940600	2.37819700	-0.91957700

C	-2.64637000	1.02470800	-2.51040700
H	-1.60148500	0.93885600	-2.82037100
H	-3.14366000	0.06663000	-2.70357900
H	-3.12664100	1.78015900	-3.14421600
C	-4.22552400	1.71944300	-0.64521500
H	-4.83898500	0.81731400	-0.75763700
H	-4.31412900	2.05575500	0.39401600
H	-4.64639900	2.49745000	-1.29338800
Ni	1.91249500	1.49458800	-0.21637600
C	2.90066000	1.78636300	-4.04331300
C	1.90909600	0.79828000	-4.28592900
C	1.50640200	0.44738400	-5.57146900
C	2.11602600	1.11207300	-6.64424200
C	3.09491800	2.09213900	-6.42355500
C	3.49666800	2.44018800	-5.12985000
C	2.25704200	1.05268200	-2.06318200
H	0.75369400	-0.31714500	-5.74556300
H	1.82808800	0.85851100	-7.66097600
H	3.55314900	2.58813900	-7.27569500
H	4.25854600	3.19840700	-4.96345900
N	1.50688900	0.36545900	-3.02988800
N	3.10948300	1.91773100	-2.68804700
C	0.64110600	-0.76343000	-2.77503700
H	0.20763900	-0.66708300	-1.77737100
H	-0.17368000	-0.78168100	-3.50537300
H	1.18418200	-1.71752200	-2.84107200
H	-2.38228100	3.01739400	1.91878600
H	-1.09363700	5.35879100	1.23693500
C	3.58178600	0.61996400	0.37259600
C	3.09616800	-0.03679800	-0.88550000
C	4.76333200	0.30177400	0.95379900
C	5.23750500	0.89988300	2.30192600
C	4.30931700	2.01624600	2.80037800
H	3.28365600	1.65923100	2.91515600
H	4.66680000	2.39951200	3.76597500
H	4.27602900	2.85244600	2.09631200
C	6.66907300	1.47896600	2.19575500
H	7.40105200	0.72541600	1.88565900
H	6.70903900	2.30369400	1.47155700
H	6.99751400	1.87417300	3.16625300
C	5.24540900	-0.21119400	3.38450600
H	5.54505000	0.20271900	4.35656700
H	4.24814600	-0.64943000	3.49390100
H	5.94309900	-1.02147900	3.14713700
C	5.68258500	-0.77376000	0.35022300
H	6.34004600	-1.20704500	1.11463600
H	5.07185000	-1.60900200	-0.01921100
C	6.57677900	-0.28198300	-0.81017400
H	7.20960100	0.54548600	-0.45963700
H	5.94786300	0.13319700	-1.61087100
C	7.47047000	-1.38187800	-1.40026000
H	8.10702200	-1.79673800	-0.60539500
H	6.83876100	-2.21177900	-1.74803500
C	8.34923400	-0.89202100	-2.55628100
H	9.01912700	-0.08566900	-2.23096500
H	8.97298500	-1.69914300	-2.95827900
H	7.73772600	-0.50285100	-3.38015300
H	3.84648300	-0.31107800	-1.63120100
H	2.44197600	-0.89915100	-0.70523300
Na	4.24674400	2.82436600	-0.87930800
H	4.71957900	5.53657900	-0.88823200
O	5.36707500	4.80727100	-0.90425700
C	6.61113200	5.29404700	-1.48010900
C	7.56492700	4.09911800	-1.45571200
C	6.34751000	5.76303900	-2.91651800
C	7.14061100	6.43907800	-0.60722500
H	7.71040400	3.74113400	-0.43085000
H	7.17336800	3.27377900	-2.06139300
H	8.54166500	4.38107300	-1.86264500
H	5.62882900	6.59148500	-2.93175700
H	7.27202900	6.11263000	-3.38973000
H	5.93813800	4.94519400	-3.51870000
H	8.09761600	6.81182200	-0.98886100
H	6.43679100	7.28073300	-0.59641000
H	7.28648300	6.09990600	0.42349900

ZTS₁₈₋₁₉

C	0.47123700	2.51889200	0.14634700
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C -0.90985900 4.21055600 0.98788200
C -1.47860700 3.03309100 1.33121300
N -0.66677400 2.00768300 0.81296900
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C	3.08773700	-2.59967000	3.42494200
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TS₁₉₋₂₀

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C	-4.09098700	-0.19882400	-2.03082800
C	-2.99944300	-2.38486800	-1.67316200
C	-4.41641900	-0.60715800	-3.33431800
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C	-4.04731600	-1.86564700	-3.80967800
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C	-1.37785600	-2.09219600	4.84656400
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C	-6.04967200	1.12402300	-1.11532800
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C	5.14688100	-1.58947400	0.48492100
C	4.03364300	-2.35835900	0.89102100
C	4.20681300	-3.69710800	1.26281100
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H	5.65518500	-5.26398800	1.50424300
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N	2.88780900	-1.57787300	0.84728100
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C	5.40656900	0.79830400	-0.29077400
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H	2.69641300	5.93470900	-0.34461400
C	2.00926300	6.01156300	1.70582900
H	1.87065700	5.34629800	2.56717100
H	2.69499900	6.81201100	2.00771600
H	1.03775800	6.47064400	1.48471700
H	1.72963700	0.79318600	1.18659900
H	3.01079100	1.70702400	0.42312200
Na	0.79230100	-1.98747200	-0.18672500
H	1.42725200	-0.30233700	-1.71876100
O	1.50002400	-1.46188100	-2.18341500
C	2.37355800	-1.88501800	-3.21512700
C	1.65351800	-1.82937900	-4.57945300
C	3.64291800	-1.01204700	-3.26883700
C	2.78283500	-3.34451800	-2.92724200
H	0.72099100	-2.40330200	-4.53383100
H	1.39882800	-0.79859200	-4.84656800
H	2.27617100	-2.24335500	-5.38339100
H	4.20659800	-1.10192600	-2.33474300
H	4.29995400	-1.31605700	-4.09355300
H	3.38175000	0.04170600	-3.41334000
H	3.45751300	-3.73972600	-3.69772800
H	3.29358600	-3.41231300	-1.95941200
H	1.89503900	-3.98851200	-2.89527100
C	1.23238100	-0.73232300	-1.00654900
C	2.33745200	-0.92176200	-3.03399800
C	1.49381000	-1.97878900	-2.93825900
N	0.82001900	-1.85763500	-1.71758900
N	2.18000600	-0.17206500	-1.86169500
C	-0.14503500	-2.86233700	-1.29933000
C	0.30398500	-3.92993000	-0.48344100
C	-1.46773400	-2.79663900	-1.80344200
C	-0.62645500	-4.92525100	-0.14815100
C	-2.35600400	-3.81627600	-1.42359000
C	-1.94265600	-4.86643200	-0.60623300
H	-0.31904400	-5.75119300	0.48207900
H	-3.38650500	-3.76905600	-1.74772300
H	-2.65229500	-5.63457900	-0.31782600
C	3.01234100	0.98670400	-1.60507600
C	2.47875600	2.28449300	-1.79609300
C	4.36876800	0.76811800	-1.26975100
C	3.34207100	3.37354700	-1.60016700
C	5.19018400	1.89562500	-1.10025900
C	4.68245300	3.18432600	-1.25450900
H	2.96762000	4.38134700	-1.73154300
H	6.23632700	1.75836900	-0.84837000
H	5.33158900	4.04335900	-1.11659000
C	-1.94483500	-1.69459000	-2.75976500
H	-1.36160200	-0.78710100	-2.54578700
C	-1.68394600	-2.07565000	-4.24212100
H	-0.62288400	-2.21067800	-4.46699800
H	-2.20796100	-3.00735300	-4.48688500
H	-2.06968800	-1.28819100	-4.90054300
C	-3.44885800	-1.35643100	-2.59889400
H	-4.06557600	-2.09761000	-3.12432700
H	-3.79121400	-1.34504600	-1.55123700
H	-3.65443300	-0.38493400	-3.06522600
C	1.03687000	2.49953200	-2.26393000
H	0.41538500	1.73562100	-1.78161300
C	0.46121300	3.87393100	-1.86753600
H	-0.61373900	3.89663600	-2.07500200
H	0.60745000	4.07978000	-0.80209400
H	0.92297000	4.68832300	-2.43927500
C	0.91839000	2.31580500	-3.79938500
H	1.53578500	3.05593300	-4.32341000
H	1.23644800	1.31876200	-4.11778100
H	-0.12201400	2.45508600	-4.11614900
C	4.97480200	-0.63272600	-1.14030300
H	4.15905300	-1.36171100	-1.17536000
C	5.71091000	-0.84581500	0.20058900
H	6.57898000	-0.18378000	0.29742700
H	5.04846000	-0.66103400	1.05028600
H	6.07435500	-1.87835700	0.26458200
C	5.92581500	-0.93457900	-2.32525600
H	5.41669500	-0.83702700	-3.29042500
H	6.77923800	-0.24601600	-2.32790300
H	6.31663700	-1.95596100	-2.24835000
C	1.76233400	-4.05593900	-0.03323500
H	2.18609600	-3.04616900	0.01705100
C	1.91882600	-4.68664600	1.36707700
H	1.29664600	-4.17926700	2.10941100
H	1.65162700	-5.74997400	1.36532100
H	2.96397600	-4.61578700	1.69005000
C	2.58675500	-4.86885400	-1.06511400
H	2.19124700	-5.88803800	-1.15307500
H	2.56269700	-4.40986200	-2.05866600
H	3.63462500	-4.93721000	-0.74797900
Ni	0.73103300	-0.07907900	0.75967400
C	-3.20092500	4.08885000	-0.10602900
C	-3.42019400	2.72575300	-0.39695700
C	-4.50703000	2.34044000	-1.19062400
C	-5.33146000	3.34606700	-1.69001800
C	-5.09015400	4.70486400	-1.40641600
C	-4.02115700	5.10300600	-0.60491000
C	-1.67907900	2.80057500	0.88711900
H	-4.70643400	1.29020200	-1.37960200
H	-6.18575000	3.07801100	-2.30508100
H	-5.75620100	5.45990200	-1.81470300
H	-3.84515500	6.15107500	-0.38049700
N	-2.44782800	1.95485900	0.23016300
N	-2.08754400	4.11192900	0.72401800
C	-1.49522300	5.31661700	1.27458300

H	-1.03404200	5.92154200	0.48504600
H	-2.26313600	5.91618000	1.77485000
H	-0.73089000	5.05266400	2.00577400
H	1.31414400	-2.80026000	-3.60737500
H	3.03219900	-0.63814700	-3.80426600
C	-0.37614300	0.93722400	2.02352400
C	-0.49920200	2.43157600	1.74056500
C	0.71388000	0.36347100	2.73089400
C	0.43204400	-0.86843100	3.65227400
C	1.73139000	-1.65093100	3.94110700
H	2.46774200	-1.04719800	4.48211200
H	1.51440100	-2.52894600	4.56225200
H	2.19576700	-2.00101800	3.01229700
C	-0.58442700	-1.86161100	3.04633700
H	-1.58997600	-1.43734100	2.95081000
H	-0.26991800	-2.21433500	2.05792000
H	-0.68242400	-2.73602200	3.70216800
C	-0.16026700	-0.37959800	5.00016700
H	-0.37240100	-1.23384800	5.65545000
H	0.52343000	0.28404800	5.54119500
H	-1.10105800	0.15984800	4.84043800
C	1.85544500	1.27699400	3.21320000
H	1.59276900	2.32402100	3.02126900
H	1.90980100	1.20280700	4.30882900
C	3.28419800	1.07605000	2.67366600
H	3.29972900	1.25296300	1.59045900
H	3.60679500	0.03843900	2.82349700
C	4.27280100	2.02310500	3.37402200
H	3.95059600	3.06219100	3.21115000
H	4.21514300	1.85752600	4.45988200
C	5.72744600	1.86972400	2.91967300
H	5.83071900	2.07529000	1.84813400
H	6.38654500	2.56071200	3.45875900
H	6.09488000	0.85202200	3.10039400
H	0.41276800	2.81833300	1.26810200
H	-0.59166200	2.97643200	2.69611400
Na	-2.36289200	-0.41404300	0.36067500
H	-1.35440000	0.49129700	2.21094700
O	-4.11610400	-1.47012400	0.53851600
C	-5.25360000	-1.86620200	1.20001100
C	-5.48205500	-3.39257100	1.02812200
C	-5.14676400	-1.56032600	2.71891000
C	-6.49631000	-1.12070900	0.64185600
H	-5.57699400	-3.63309900	-0.03873500
H	-4.61650100	-3.94032300	1.42132500
H	-6.38414800	-3.75516100	1.54200800
H	-4.99845000	-0.48213900	2.86665700
H	-6.03702000	-1.86449600	3.28859200
H	-4.27756300	-2.08344400	3.13899200
H	-7.43241300	-1.40169100	1.14635000
H	-6.35602800	-0.03819400	0.75411700
H	-6.60753800	-1.33738800	-0.42852700

Cartesian coordinates for the stationary points given in Fig. 3

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C	1.59229200	-0.53629400	0.58237300
C	3.39882200	-0.42192700	-0.61241700
C	3.81108900	-0.51130300	0.73425400
C	4.35390800	-0.33563500	-1.63150000
C	5.15581800	-0.51422600	1.10814100
C	5.69829000	-0.33865100	-1.26835100
H	4.04956500	-0.27042400	-2.67244700
C	6.09365700	-0.42653000	0.08052800
H	5.46539100	-0.57655100	2.14718700
H	6.46021600	-0.27126100	-2.03965200
H	7.15168100	-0.42386200	0.32625800
C	2.59649000	-0.67211700	2.92668800
H	1.58478600	-0.90304100	3.25839900
H	3.26575200	-1.46785300	3.26915500
H	2.90869100	0.27572800	3.37902900
N	2.01291800	-0.43873300	-0.67199600
C	0.13378200	-0.55469000	0.93604700
C	-0.60951300	-1.60786000	0.12135200

H	-0.25848400	0.46503300	0.72582000
H	-0.00777500	-0.72858400	2.00931100
C	-1.93265700	-1.85514800	0.15699400
H	0.03177800	-2.22759500	-0.49797800
N	2.63735400	-0.58923300	1.47673500
C	-2.54204500	-3.04787200	-0.61227700
C	-1.58075100	-3.64824700	-1.65752600
C	-2.88491600	-4.16315100	0.40969400
C	-3.83764000	-2.63820500	-1.35060800
H	-1.26200100	-2.89787500	-2.39137300
H	-0.68458300	-4.08085700	-1.20004400
H	-2.08621100	-4.45259500	-2.20398300
H	-3.60144300	-3.82220900	1.16434600
H	-3.33018200	-5.02493900	-0.10292900
H	-1.98307100	-4.50516900	0.93015000
H	-4.26149200	-3.50777700	-1.86731500
H	-4.60207600	-2.25790700	-0.66683500
H	-3.64131800	-1.86414100	-2.10146000
C	-2.85881900	-1.03073500	1.03839000
C	-3.43371300	0.24779700	0.38361900
H	-2.32088100	-0.73257800	1.94832000
H	-3.69441500	-1.65464600	1.38151600
C	-4.36508900	1.00468700	1.34189900
H	-2.61449000	0.90599900	0.05969100
H	-3.99819100	-0.02481900	-0.51781100
C	-5.04944800	2.20931100	0.68736000
H	-5.13260400	0.31896800	1.73266400
H	-3.78704200	1.34346000	2.21390700
H	-5.69875800	2.73546700	1.39739500
H	-4.31020700	2.92579600	0.31249100
H	-5.66940000	1.89748000	-0.16281100
O	-0.72742400	2.04241500	-0.59743500
C	-0.62490000	3.40997900	-0.41584500
C	-0.94982200	3.77541500	1.05492800
C	0.81207500	3.90388400	-0.73315700
C	-1.61485200	4.15460700	-1.34662000
H	-1.96018200	3.43377200	1.30845800
H	-0.24628100	3.26738300	1.72705800
H	-0.89150900	4.85507400	1.25034700
H	1.06044700	3.68163200	-1.78176400
H	0.94494900	4.98430700	-0.58216800
H	1.53423300	3.37759800	-0.09549500
H	-1.57846400	5.24668700	-1.22880200
H	-1.38828700	3.91657600	-2.39479600
H	-2.63887800	3.81934500	-1.14503300
Na	0.20780700	0.60748000	-1.75875400

TS₂₁₋₂₂

C	1.43103900	-0.49726200	0.51956300
C	3.34026400	-0.81280500	-0.49365000
C	3.64696000	-0.46692600	0.84289900
C	4.37611700	-1.08386700	-1.39298700
C	4.95569100	-0.37741900	1.31110100
C	5.69121900	-0.99971200	-0.93180300
H	4.15701500	-1.36021700	-2.42123700
C	5.97841700	-0.65314700	0.39877500
H	5.18117200	-0.10177000	2.33745400
H	6.51030700	-1.20735400	-1.61508500
H	7.01268000	-0.59557500	0.72613800
C	2.23342100	0.03581000	2.86986800
H	1.25332100	-0.31477600	3.19826300
H	2.99972000	-0.47706200	3.45910800
H	2.30635400	1.11407800	3.05790100
N	1.96626200	-0.81023300	-0.67217800
C	0.00009500	-0.30272300	0.71843400
C	-0.84100000	-1.37334200	0.10641500
H	-0.24498900	0.88805600	-0.00843800
H	-0.28097200	-0.04500900	1.74203800
C	-2.17194000	-1.58224300	0.23954900
H	-0.27406900	-2.08157300	-0.49737500
N	2.41605900	-0.27913800	1.46678200
C	-2.86849900	-2.81133700	-0.37942400
C	-1.99202700	-3.55227100	-1.40921200
C	-3.21325100	-3.81819900	0.74879300
C	-4.17865400	-2.40603200	-1.09647400
H	-1.69709900	-2.89407500	-2.23742500
H	-1.08231600	-3.96597600	-0.96119700
H	-2.55375200	-4.38938800	-1.83959700

H	-3.86623900	-3.37342500	1.50740700
H	-3.73215100	-4.69482000	0.34005100
H	-2.30249600	-4.16341300	1.25095600
H	-4.67484500	-3.29345500	-1.50893000
H	-4.88724900	-1.91993300	-0.41895000
H	-3.97993100	-1.71625200	-1.92576900
C	-3.01461200	-0.65700900	1.10499700
C	-3.52407400	0.61424300	0.38951500
H	-2.42648800	-0.34240400	1.97868700
H	-3.87834900	-1.19785900	1.51349900
C	-4.29200300	1.55368300	1.32911600
H	-2.67251600	1.14216100	-0.05583700
H	-4.18058200	0.32670900	-0.44286000
C	-4.85744400	2.78789600	0.61762100
H	-5.11402400	1.00276800	1.81007100
H	-3.62622500	1.87488000	2.14357900
H	-5.39307900	3.44389800	1.31413300
H	-4.05797300	3.37711200	0.15173600
H	-5.55903600	2.50041300	-0.17553500
O	-0.46203800	1.71241800	-0.92619600
C	-0.04067200	3.04656900	-0.70161100
C	-0.40594700	3.48167300	0.73192900
C	1.48402200	3.17111500	-0.90592000
C	-0.77390600	3.94252200	-1.71539200
H	-1.48312000	3.37312200	0.89850300
H	0.11537600	2.86048100	1.47007700
H	-0.13182900	4.52731800	0.91798400
H	1.75623200	2.89084600	-1.93270200
H	1.83999000	4.19515600	-0.73582900
H	2.02200300	2.50566700	-0.22086200
H	-0.49666800	4.99834900	-1.60306000
H	-0.53083600	3.63389700	-2.74008700
H	-1.85769900	3.85145000	-1.58438600
Na	0.27919300	0.01081200	-2.04160900

22

C	1.24013400	-0.79503300	0.66610300
C	3.14351800	-1.15190500	-0.37199600
C	3.47690800	-0.73130200	0.94090400
C	4.16824100	-1.45778600	-1.27287600
C	4.79159400	-0.60539400	1.37365100
C	5.49540700	-1.33842800	-0.84321600
H	3.93307500	-1.79527600	-2.27955700
C	5.80584900	-0.92204000	0.45759200
H	5.03369700	-0.27301700	2.37975800
H	6.30110000	-1.57670300	-1.53308000
H	6.84491200	-0.83950000	0.76431600
C	2.08000900	-0.24039300	2.98905900
H	1.16217200	-0.72341100	3.33692900
H	2.92443200	-0.65224700	3.55029300
H	2.01296700	0.83551000	3.20213700
N	1.77076900	-1.16659800	-0.53262700
C	-0.14050200	-0.64835400	0.93017400
C	-1.10178100	-1.42854200	0.17697600
H	-0.06981100	1.35793800	-0.11480700
H	-0.44731900	-0.17345200	1.85764400
C	-2.46777500	-1.40894200	0.20677000
H	-0.63364500	-2.18080000	-0.46162600
N	2.25828600	-0.51494000	1.58097000
C	-3.31925400	-2.43426300	-0.56433700
C	-2.52398100	-3.19737500	-1.64319600
C	-3.88438900	-3.48620400	0.42686200
C	-4.50739500	-1.74250800	-1.27652900
H	-2.09002300	-2.51171300	-2.38562100
H	-1.71281400	-3.79829200	-1.21902700
H	-3.18881000	-3.88088800	-2.18404800
H	-4.49043800	-3.01845700	1.21055300
H	-4.52203100	-4.21350000	-0.09297100
H	-3.06939500	-4.03183500	0.91530400
H	-5.12567700	-2.48338300	-1.79896900
H	-5.15770800	-1.21188200	-0.57370500
H	-4.15416700	-1.01544500	-2.01868100
C	-3.19007000	-0.45125000	1.14100800
C	-3.40381000	0.97495100	0.58737900
H	-2.63059400	-0.36974800	2.08458700
H	-4.17075600	-0.85721800	1.42268200
C	-4.06983500	1.91661400	1.59978500
H	-2.43859700	1.39256800	0.27389600
H	-4.02183900	0.92649700	-0.31956600
C	-4.31784200	3.32505300	1.04897700

H	-5.02509300	1.48045100	1.92660600
H	-3.44387100	1.98108600	2.50174600
H	-4.79461200	3.97134400	1.79540400
H	-3.37762000	3.80338800	0.74694900
H	-4.97066400	3.29652700	0.16760500
O	-0.09029000	1.80017700	-0.99983200
C	0.66952900	3.03530800	-0.96119800
C	0.01143700	3.98587600	0.04770600
C	2.12194400	2.73416900	-0.56955600
C	0.58550400	3.60333600	-2.37972900
H	-1.03339600	4.16930700	-0.22327100
H	0.03408100	3.55664300	1.05667800
H	0.53638800	4.94731100	0.08138700
H	2.58390400	2.03858500	-1.27814200
H	2.72008600	3.65230300	-0.55027000
H	2.17289000	2.27708100	0.42506800
H	1.11563600	4.55916500	-2.44513900
H	1.04241200	2.91462500	-3.10076300
H	-0.45874600	3.76553700	-2.66767100
Na	0.10437800	-0.28757100	-1.82311400

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C	2.07613900	0.66002100	0.08711800
C	3.77821400	-0.70658300	0.34410000
C	4.29302000	0.46405200	-0.26879700
C	4.64321600	-1.76678900	0.63204200
C	5.63548500	0.60244700	-0.60337600
C	5.99706100	-1.63300300	0.30319900
H	4.26830900	-2.66665400	1.11368100
C	6.48878600	-0.46892700	-0.30220700
H	6.01608300	1.50046400	-1.08281500
H	6.68134100	-2.44833900	0.52426000
H	7.54492900	-0.39281700	-0.54598600
C	3.25852500	2.68843500	-0.86429400
H	3.09704700	2.77939300	-1.94720200
H	2.49039800	3.26886100	-0.34530700
H	4.23873700	3.11110100	-0.62248000
N	2.41518100	-0.58139700	0.53642200
C	0.77199400	1.20698100	0.06810600
C	-0.24468500	0.81717100	1.00217400
H	-2.08889300	-1.10575800	-0.00394000
H	0.59536900	2.05952500	-0.57936900
C	-1.54907500	1.24972000	1.08700000
H	0.10306200	0.12758400	1.77430200
N	3.20275200	1.31653200	-0.41319700
C	-2.43688700	0.94911500	2.31066900
C	-1.92008900	-0.23548700	3.15306600
C	-2.48418200	2.19439300	3.23661900
C	-3.88639900	0.61394700	1.88167600
H	-1.81737300	-1.14669400	2.54979900
H	-0.94865800	-0.02213800	3.61135400
H	-2.62329500	-0.45224000	3.96600600
H	-2.87272900	3.07449300	2.71213300
H	-3.13119000	2.01564700	4.10622200
H	-1.48012100	2.43836500	3.60073400
H	-4.52737600	0.46611500	2.76020900
H	-4.33553100	1.40977000	1.27867600
H	-3.92233300	-0.31005200	1.28922400
C	-2.04128600	2.29919000	0.09888400
C	-2.43401800	1.75918000	-1.29206000
H	-1.26098300	3.06384000	-0.04338500
H	-2.90260700	2.84262800	0.50758700
C	-2.82474900	2.85949400	-2.28761900
H	-1.59482100	1.17984400	-1.70203800
H	-3.27472300	1.05756800	-1.18518900
C	-3.22338200	2.31879900	-3.66505900
H	-3.65541900	3.44724700	-1.87071900
H	-1.98461400	3.55980800	-2.39862900
H	-3.49460500	3.12806600	-4.35309800
H	-2.39986300	1.75588100	-4.12275500
H	-4.08488000	1.64279900	-3.59170900
O	-1.67534100	-1.91542900	-0.36893900
C	-2.67487800	-2.87726800	-0.79893200
C	-3.37371600	-3.46295600	0.43466400
C	-3.67419100	-2.18437000	-1.73262500
C	-1.88701100	-3.95718000	-1.54430800
H	-2.64237700	-3.92586100	1.10582000
H	-3.90460800	-2.68401800	0.99301100
H	-4.10511700	-4.22491400	0.14231000
H	-3.15659600	-1.73245800	-2.58499400

H	-4.41044100	-2.90071000	-2.11378700
H	-4.22095900	-1.39375200	-1.20540100
H	-2.55646500	-4.74308200	-1.90837000
H	-1.36484200	-3.52824700	-2.40736400
H	-1.14865500	-4.42441500	-0.88159600
Na	0.47496700	-1.45378700	-0.19368100

TS₂₃₋₂₄

C	2.06168200	0.53962200	0.21024400
C	3.70704900	-0.88395000	0.03296100
C	4.28311600	0.40725300	-0.02323000
C	4.52762500	-2.01355500	-0.05574100
C	5.65467800	0.60860100	-0.16707100
C	5.90217300	-1.82081400	-0.19746300
H	4.10121100	-3.01210200	-0.00553000
C	6.45848900	-0.53102000	-0.25095800
H	6.08646000	1.60416000	-0.21526800
H	6.55768800	-2.68463000	-0.26615400
H	7.53308800	-0.41636300	-0.36121100
C	3.32510400	2.73483100	0.19266700
H	3.41293100	3.20345100	-0.79520500
H	2.43734400	3.12396700	0.69508400
H	4.20639000	2.99751900	0.78632400
N	2.33128700	-0.77728900	0.15539800
C	0.74275600	1.10443200	0.32895900
C	-0.26890600	0.46326900	1.02130600
H	-1.96748200	-0.49473200	0.15866900
H	0.55476300	2.04998100	-0.17052700
C	-1.68681600	0.69067600	0.99041300
H	0.06194700	-0.38858300	1.61969900
N	3.21879600	1.29210700	0.09547800
C	-2.44074700	0.42445600	2.33902800
C	-1.94780300	-0.87099400	3.02352000
C	-2.21432400	1.60157900	3.31851200
C	-3.96029800	0.26756700	2.10913700
H	-1.95139800	-1.71438900	2.32379000
H	-0.93608300	-0.76659200	3.43177000
H	-2.60404900	-1.12689200	3.86427600
H	-2.59875000	2.54461600	2.91330000
H	-2.72306500	1.42221800	4.27542200
H	-1.14524800	1.73625200	3.52312100
H	-4.47552300	0.11280300	3.06552200
H	-4.40778500	1.15059100	1.64144400
H	-4.17828000	-0.59410700	1.47023200
C	-2.11021600	1.97459100	0.25131400
C	-2.11500500	1.89990800	-1.28772900
H	-1.46015000	2.81436800	0.55424600
H	-3.11731200	2.27386300	0.56307200
C	-2.39928400	3.25416100	-1.95100800
H	-1.15321800	1.51513900	-1.65259200
H	-2.86973600	1.17347200	-1.61017900
C	-2.43526800	3.18504100	-3.48167500
H	-3.35840300	3.64538100	-1.58114800
H	-1.63678600	3.98198800	-1.63621300
H	-2.64087000	4.16647400	-3.92526400
H	-1.47767700	2.83179100	-3.88533500
H	-3.21333200	2.49363700	-3.82858900
O	-1.82421600	-1.51359300	-0.52763700
C	-2.87190100	-2.31908400	-1.04201000
C	-3.40580500	-3.26711100	0.05065100
C	-4.01824900	-1.45348700	-1.59758500
C	-2.27749000	-3.15888400	-2.19097600
H	-2.58682900	-3.87499100	0.45431300
H	-3.84222300	-2.70119800	0.87981400
H	-4.17558400	-3.94508600	-0.33904800
H	-3.65473000	-0.81184500	-2.40741900
H	-4.83094600	-2.07543500	-1.99285600
H	-4.43543700	-0.81057300	-0.81557600
H	-3.02696300	-3.81086400	-2.65661200
H	-1.86898800	-2.50091100	-2.96815400
H	-1.46895300	-3.80334700	-1.81671400
Na	0.32125100	-1.62059300	-0.59683000

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C	1.96690500	0.64988800	0.12563600
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C	3.55217700	-0.80733600	-0.14240800
C	4.18293100	0.42819500	0.12523600
C	4.32648200	-1.95369900	-0.35985800
C	5.57104400	0.56394400	0.18464500
C	5.71147900	-1.82750200	-0.30115000
H	3.85620600	-2.91258600	-0.56098700
C	6.32485400	-0.58791700	-0.03271400
H	6.04834800	1.51810900	0.38707500
H	6.33480600	-2.70199000	-0.46373800
H	7.40865000	-0.52792300	0.00483000
C	3.31549200	2.73862100	0.64868500
H	3.61114400	3.33710300	-0.22069800
H	2.37833100	3.12551000	1.05031300
H	4.08550800	2.83036200	1.42052200
N	2.17641900	-0.63665700	-0.14829800
C	0.65315400	1.28386300	0.21313200
C	-0.43240400	0.62174800	0.65645600
H	-2.37525600	0.22217500	0.17013100
H	0.57743100	2.31001400	-0.13737300
C	-1.87086000	1.06292500	0.67523700
H	-0.29051900	-0.38911600	1.02978500
N	3.14990500	1.33929800	0.29409400
C	-2.46014200	1.06089700	2.14352100
C	-2.04876500	-0.23941000	2.87199900
C	-1.95929900	2.27760800	2.94396300
C	-4.00132800	1.08493500	2.07223200
H	-2.18254100	-1.11165100	2.22109300
H	-0.99962500	-0.21259100	3.19102700
H	-2.65586900	-0.37380300	3.77519000
H	-2.31054200	3.22392400	2.51616400
H	-2.32086100	2.22978300	3.97860400
H	-0.86296200	2.30731200	2.97692500
H	-4.42524900	1.06594900	3.08360200
H	-4.38808800	1.98132200	1.57577100
H	-4.38101300	0.20899100	1.53339200
C	-2.13724100	2.35890400	-0.11851700
C	-2.10312900	2.17037600	-1.64417900
H	-1.42313700	3.14276400	0.17366200
H	-3.12347700	2.75371400	0.14983600
C	-2.37005800	3.46587500	-2.42246800
H	-1.13267200	1.75774400	-1.95277600
H	-2.85257800	1.41688800	-1.92438600
C	-2.35517600	3.26893200	-3.94215600
H	-3.34197700	3.87841400	-2.11630900
H	-1.61989600	4.22071300	-2.14366600
H	-2.54758000	4.20938100	-4.47145000
H	-1.38441100	2.88713700	-4.28281200
H	-3.12019800	2.54756100	-4.25420200
O	-1.67903300	-2.16996100	-0.22868900
C	-2.61091800	-3.15147400	-0.49813800
C	-2.73744800	-4.12239700	0.70425200
C	-3.99768000	-2.51393600	-0.77285300
C	-2.20533600	-3.97841600	-1.75007800
H	-1.76150200	-4.58072200	0.91272700
H	-3.04144300	-3.56704300	1.59952300
H	-3.46607000	-4.92807400	0.53542000
H	-3.92209500	-1.81770900	-1.61763900
H	-4.77579500	-3.25496800	-1.00375000
H	-4.32084200	-1.94170700	0.10555300
H	-2.92825900	-4.76330200	-2.01309200
H	-2.10042900	-3.30954500	-2.61554400
H	-1.23514500	-4.46845900	-1.57319900
Na	0.29538000	-1.90911100	-0.77395000

P2

C	1.30035700	-0.02065700	0.03421900
C	3.27300500	-0.53138800	-0.65046900
C	3.45254400	0.43769100	0.36801200
C	4.39177500	-1.06965300	-1.30236800
C	4.71588000	0.88333400	0.76437900
C	5.65273200	-0.62740300	-0.91555800
H	4.26199900	-1.81140400	-2.08457200
C	5.81295600	0.33459200	0.10288500
H	4.84891800	1.61792700	1.55371100
H	6.53543800	-1.03033900	-1.40462400
H	6.81374600	0.65334200	0.38109800
C	1.85594300	1.70442100	1.84409400
H	1.84753100	1.22354700	2.83019300

H	2.60473600	2.50120500	1.84960500
H	0.88164300	2.16236300	1.66362100
N	1.93179100	-0.79357900	-0.83109800
C	-0.14662000	0.02744200	0.21177600
C	-0.99043100	-0.68211300	-0.55795200
H	-2.87491100	-0.82163000	-1.47879400
H	-0.52678900	0.66174200	1.00708900
C	-2.49793600	-0.75406600	-0.44546400
H	-0.53375200	-1.29107800	-1.33512100
N	2.17267600	0.76280000	0.78669600
C	-2.96078600	-2.10770100	0.23668000
C	-2.22982000	-3.29899700	-0.41976600
C	-2.65600200	-2.10451200	1.74598500
C	-4.47479500	-2.31188300	0.01803300
H	-2.36709300	-3.30083900	-1.50887800
H	-1.15453300	-3.28584300	-0.21554700
H	-2.62826100	-4.24531900	-0.03466200
H	-3.22147800	-1.32848100	2.27442500
H	-2.92835200	-3.06933900	2.19079800
H	-1.58963000	-1.93836400	1.93494500
H	-4.78686400	-3.28175300	0.42392800
H	-5.08023700	-1.54550200	0.51285100
H	-4.72601800	-2.30339900	-1.05013300
C	-3.12702300	0.51118700	0.17927100
C	-3.03131000	1.75488600	-0.71833500
H	-2.66631300	0.72601300	1.15255300
H	-4.18563600	0.32367600	0.39179100
C	-3.64301200	3.01004800	-0.08185000
H	-1.98155200	1.95015400	-0.97377300
H	-3.54199500	1.54860700	-1.67073200
C	-3.57275100	4.24210700	-0.99063000
H	-4.69131300	2.81027500	0.18293000
H	-3.12784200	3.22496700	0.86584000
H	-4.01374900	5.12193400	-0.50803000
H	-2.53465000	4.48721400	-1.24708400
H	-4.11254200	4.07178300	-1.93024200

Cartesian coordinates for the stationary points given in Fig. 5.

T_{1h}

C	0.04812400	2.95701600	0.03750000
C	0.77452500	5.14391400	0.28053600
C	-0.54813500	5.19594300	-0.00709500
N	-0.98833000	3.86624200	-0.14244300
N	1.13556800	3.78411800	0.29585900
C	-2.37046000	3.53822600	-0.42826800
C	-2.73718800	3.20199800	-1.75300400
C	-3.32378100	3.62778000	0.61472800
C	-4.09142100	2.93645800	-2.00960100
C	-4.66577200	3.35889600	0.29980600
C	-5.04758900	3.01296200	-0.99635400
H	-4.40141500	2.67397600	-3.01429700
H	-5.41775500	3.42013700	1.07841900
H	-6.09050000	2.80888800	-1.21798000
C	2.49612800	3.34865300	0.54235700
C	2.83913900	2.85837000	1.82458200
C	3.45433800	3.48350600	-0.49092600
C	4.17243100	2.47885400	2.04435100
C	4.77526500	3.09522100	-0.21337800
C	5.13163500	2.59190100	1.03742500
H	4.46366300	2.09360100	3.01437300
H	5.53056000	3.18616000	-0.98607200
H	6.15663300	2.29058400	1.22914400
C	-2.95221900	4.04912200	2.03950800
H	-1.86936200	3.92674900	2.15433500
C	-3.29249200	5.54158300	2.28407300
H	-2.77702600	6.19985500	1.57773600
H	-4.37054600	5.71267500	2.17761900
H	-3.00019400	5.83829600	3.29849600
C	-3.63428300	3.18244300	3.12281700
H	-4.71680500	3.35284300	3.15460400
H	-3.46529800	2.11491900	2.95457700
H	-3.23455700	3.44122200	4.11025700
C	1.82530600	2.80874200	2.96915600
H	0.82875900	2.71428000	2.52774200

C	2.02084200	1.59604700	3.90304300
H	1.18583900	1.53610300	4.61076200
H	2.05885600	0.65992300	3.33705100
H	2.94106200	1.67664500	4.49405700
C	1.86410200	4.12743900	3.78311800
H	2.85039800	4.27102800	4.24149300
H	1.65456600	4.99705600	3.15051300
H	1.11655100	4.10288000	4.58534000
C	3.11406600	4.07872900	-1.86053800
H	2.02494500	4.05051100	-1.97796900
C	3.72742700	3.28429300	-3.03612300
H	4.81970800	3.37466000	-3.05849000
H	3.47818800	2.22080900	-2.98168800
H	3.34860800	3.67775900	-3.98679500
C	3.56422800	5.55938600	-1.94888500
H	3.10156600	6.17526800	-1.17119000
H	4.65224700	5.63780900	-1.83553800
H	3.29273600	5.98275100	-2.92331100
C	-1.72291900	3.19506500	-2.89779300
H	-0.73259700	3.02652300	-2.46499800
C	-1.96804900	2.06295100	-3.91763200
H	-2.03990000	1.08995400	-3.42112900
H	-2.88633300	2.22193900	-4.49553300
H	-1.13800700	2.02330500	-4.63246600
C	-1.70280500	4.57087000	-3.61124500
H	-2.68024200	4.79164400	-4.05772000
H	-1.45809500	5.38032900	-2.91463100
H	-0.95425500	4.57417800	-4.41284900
Ni	-0.00866300	0.98730400	-0.04967300
C	1.23568800	-0.28258200	-0.85128600
C	0.95083700	0.69006500	-1.79751300
H	1.66925100	1.47249500	-2.03037200
H	0.21264800	0.50606500	-2.58025400
C	2.03711300	-1.24096700	-0.38270500
C	3.13577100	-1.86756200	-1.29344400
C	3.75403500	-0.83479800	-2.24890400
H	3.00578700	-0.43159600	-2.93504400
H	4.18730000	-0.00735800	-1.67880200
H	4.54390800	-1.30144400	-2.84563900
C	2.53791200	-3.03106400	-2.10898600
H	3.29228600	-3.47647100	-2.77118200
H	2.14534300	-3.81384300	-1.45478500
H	1.71646500	-2.66543800	-2.73322800
C	1.95402500	-1.72543700	1.05586800
H	2.92331700	-1.53309300	1.53451300
H	1.21254600	-1.10741200	1.56932200
C	1.59214300	-3.20417400	1.28398000
H	2.33589800	-3.84959100	0.80289300
H	0.62578900	-3.41870200	0.80995400
C	1.51439200	-3.56362100	2.77442900
H	2.47881500	-3.33788900	3.25237300
H	0.77284500	-2.91748500	3.26645400
C	1.15365300	-5.03225000	3.02366200
H	1.89401400	-5.70390000	2.57066200
H	1.10905100	-5.26064100	4.09526500
H	0.17681400	-5.27771800	2.58907600
H	1.48762100	5.92522300	0.47384400
H	-1.21349300	6.03199600	-0.12845400
C	-1.25108000	-0.34057500	0.63552000
C	-0.99955700	0.57863900	1.64781400
H	-1.73566300	1.33447500	1.91226600
H	-0.28468600	0.35105600	2.44125100
C	-2.03947500	-1.28521700	0.11668000
C	-3.13335200	-1.96975400	0.99381700
C	-3.78792300	-0.98698300	1.97522800
H	-3.05700300	-0.63794600	2.70761200
H	-4.18872000	-0.11157200	1.45689500
H	-4.59878800	-1.48349300	2.52004400
C	-2.51014600	-3.13210400	1.79198400
H	-3.26804600	-3.61009300	2.42528700
H	-2.10129500	-3.88880800	1.11767500
H	-1.70122500	-2.76385000	2.43115800
C	-1.93566300	-1.71302200	-1.33838500
H	-2.89580300	-1.50256000	-1.82982200
H	-1.18681800	-1.07616100	-1.81710000
C	-1.57623200	-3.18391600	-1.61967900
H	-2.32814600	-3.84061500	-1.16890100
H	-0.61372900	-3.41836100	-1.14659400
C	-1.48697500	-3.48390500	-3.12247400
H	-2.44858500	-3.23996600	-3.59720100

H	-0.74298800	-2.81852400	-3.58498400
C	-1.12409800	-4.94160000	-3.42721900
H	-1.86639100	-5.63012900	-3.00431500
H	-1.07326100	-5.12788800	-4.50675600
H	-0.14940800	-5.20377900	-2.99721500
O	-4.10688400	-2.55641900	0.11437100
Si	-5.76913000	-2.42102100	-0.24611100
C	-6.54509700	-0.71106300	0.11075700
H	-7.53930300	-0.66747800	-0.35115100
H	-6.66209000	-0.50127900	1.17805100
H	-5.94154000	0.09163200	-0.32705400
C	-5.84698300	-2.70773800	-2.12828100
H	-5.33030100	-1.89802200	-2.65600700
H	-5.36041400	-3.64765400	-2.40927200
H	-6.88080400	-2.73771600	-2.49159300
C	-6.75530700	-3.81668300	0.68415000
C	-8.22478900	-3.80275000	0.21273600
H	-8.31280900	-3.97339800	-0.86714400
H	-8.79145200	-4.59997800	0.71557900
H	-8.72429100	-2.85374300	0.44521400
C	-6.72073200	-3.59562100	2.20862500
H	-7.29978700	-4.37831500	2.72032600
H	-5.69846700	-3.63655300	2.60159800
H	-7.15546000	-2.62957800	2.49475100
C	-6.13098000	-5.18921600	0.36221000
H	-6.66933400	-5.98808400	0.89330000
H	-6.17894700	-5.41928300	-0.70919400
H	-5.07918800	-5.23305300	0.66601900
O	4.17273800	-2.33403000	-0.41101100
Si	5.50705500	-3.38628400	-0.61160500
C	4.96510800	-5.21248200	-0.47727200
H	5.84024800	-5.87357600	-0.46789200
H	4.39363700	-5.39937100	0.43808400
H	4.33888500	-5.50703900	-1.32645700
C	6.43233700	-3.17704100	-2.27238300
H	5.79200600	-3.40802100	-3.13060600
H	6.82383200	-2.16343000	-2.40765700
H	7.28152900	-3.87068000	-2.30494800
C	6.66890100	-2.89815500	0.86214000
C	7.97374900	-3.71873100	0.80681800
H	8.53990200	-3.53261100	-0.11432100
H	8.62639100	-3.44906100	1.64981600
H	7.78754300	-4.79817000	0.87465900
C	5.95660900	-3.16976700	2.20219600
H	6.59907400	-2.86837100	3.04280300
H	5.01914600	-2.60833000	2.27809700
H	5.72462000	-4.23375900	2.33420800
C	7.00677400	-1.39630300	0.76882200
H	7.65137000	-1.09851600	1.60923300
H	7.54552700	-1.15569300	-0.15667200
H	6.10035000	-0.78224400	0.80015300

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C	0.88910200	-1.27793300	-0.00020000
C	1.30626300	-3.57014100	-0.21900500
C	2.47929000	-2.98271000	0.12405500
N	2.23253200	-1.60588400	0.25653900
N	0.34446000	-2.54482300	-0.29456000
C	3.25565200	-0.64662200	0.59555200
C	4.05315900	-0.10225800	-0.43839400
C	3.45338200	-0.30019200	1.95191200
C	5.06855200	0.79944200	-0.08144700
C	4.47590300	0.61294400	2.25522500
C	5.27913700	1.15637200	1.25159400
H	5.69562100	1.22867500	-0.85603200
H	4.64213000	0.90094400	3.28815900
H	6.06670500	1.85850400	1.50754000
C	-1.03300500	-2.75709900	-0.63777400
C	-1.95601400	-3.08829300	0.38598900
C	-1.43612800	-2.62217200	-1.99088300
C	-3.30857800	-3.24367500	0.03144300
C	-2.80122700	-2.78192200	-2.29134900
C	-3.73131800	-3.08319700	-1.29127000
H	-4.03485000	-3.49249100	0.79777400
H	-3.13608500	-2.67888200	-3.31824200
H	-4.78008600	-3.20167200	-1.54383000
C	2.59174100	-0.87442800	3.07578200
H	1.89572600	-1.59152600	2.62950300
C	3.44323100	-1.63564500	4.11810100

H	4.01975000	-2.44183500	3.64962800
H	4.15024600	-0.96792200	4.62462400
H	2.79618700	-2.07831700	4.88499600
C	1.73909200	0.22842200	3.74562300
H	2.37074800	0.99744800	4.20687200
H	1.08984400	0.71146900	3.00720900
H	1.10748400	-0.20459700	4.53122600
C	-1.52060200	-3.28507300	1.83792500
H	-0.45007500	-3.06801600	1.89534100
C	-2.23541000	-2.30579100	2.79643800
H	-1.87767600	-2.45488400	3.82195600
H	-2.02918300	-1.26652500	2.51658800
H	-3.32160700	-2.45805000	2.79760400
C	-1.72874800	-4.75194900	2.28442900
H	-2.78953700	-5.02958800	2.26303200
H	-1.18593600	-5.44717400	1.63393100
H	-1.36618900	-4.89024300	3.30966500
C	-0.43960900	-2.32798200	-3.11229800
H	0.54705900	-2.20922200	-2.65554600
C	-0.76237200	-1.00587300	-3.84558300
H	-1.75384700	-1.03257600	-4.31496600
H	-0.72049600	-0.15869900	-3.15049900
H	-0.02507200	-0.82490600	-4.63643700
C	-0.36183000	-3.51265100	-4.10502800
H	-0.09446500	-4.44427200	-3.59339800
H	-1.31956700	-3.67138300	-4.61533400
H	0.39675200	-3.31381600	-4.87097800
C	3.84274900	-0.46874200	-1.90756200
H	2.93763300	-1.08102300	-1.97019100
C	3.60660900	0.78057500	-2.78640800
H	2.76615400	1.37214000	-2.40981100
H	4.49175400	1.42746500	-2.81688400
H	3.38212600	0.47803300	-3.81654900
C	5.02139600	-1.31169500	-2.45025100
H	5.96099500	-0.74704300	-2.41245600
H	5.15777900	-2.22964300	-1.86685000
H	4.84037500	-1.59431400	-3.49442900
Ni	0.16900400	0.37258000	-0.00690200
C	-0.31908600	4.40109500	-0.55200000
C	0.41175600	3.23569300	-0.24597700
C	1.80384600	3.29960200	-0.11333600
C	2.42446600	4.53439800	-0.29829900
C	1.68298000	5.69002900	-0.60836100
C	0.29532600	5.64157500	-0.73878800
C	-1.73678200	2.64247600	-0.33544300
H	2.37692900	2.41057400	0.12969400
H	3.50434000	4.60659400	-0.19831200
H	2.19933300	6.63667700	-0.74479200
H	-0.27877800	6.53371300	-0.97381100
H	-3.09149700	1.95947800	-0.11371900
N	-0.48437700	2.16581800	-0.12557800
N	-1.64287000	3.99451200	-0.60263100
C	-2.75863700	4.86273000	-0.91524000
H	-2.89662300	5.62886300	-0.14163500
H	-2.59800600	5.36609200	-1.87636000
H	-3.66176300	4.25529700	-0.98313100
H	3.45626400	-3.40409200	0.28773800
H	1.06269000	-4.60049300	-0.41378100
O	-3.97893700	1.25382300	-0.03669900
C	-4.89292000	1.50079600	1.02437600
C	-5.74448800	0.23330400	1.20096100
C	-4.13229700	1.81031400	2.32868300
C	-5.80989300	2.68357200	0.65625800
H	-6.26628300	-0.00437800	0.26644800
H	-5.10798100	-0.62064400	1.46409500
H	-6.49356400	0.35641200	1.99288100
H	-3.50615300	2.70146600	2.21097600
H	-4.82193200	1.98539400	3.16385700
H	-3.47506600	0.97461300	2.59692500
H	-6.57637300	2.85572500	1.42251300
H	-5.22806500	3.60625300	0.55291300
H	-6.31117400	2.48684700	-0.29800500
Na	-2.38669700	-0.15676500	-0.51945100

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C	-1.04797500	-1.19952200	0.03410900
C	-1.60718100	-3.45076300	0.34072900
C	-2.73616200	-2.80879500	-0.05023800
N	-2.40321600	-1.45600700	-0.23653600

N	-0.58548400	-2.48359400	0.39118300
C	-3.35504800	-0.45100600	-0.64248900
C	-4.12509700	0.20276800	0.34759100
C	-3.51092300	-0.16569100	-2.01820300
C	-5.07269400	1.14915600	-0.07386100
C	-4.46680200	0.79418200	-2.38748800
C	-5.24382900	1.44403000	-1.42753900
H	-5.67777700	1.66305300	0.66598600
H	-4.60006400	1.03571300	-3.43704700
H	-5.97961200	2.18159800	-1.73331400
C	0.77312900	-2.75620000	0.76590400
C	1.68775100	-3.19076900	-0.22564100
C	1.16915500	-2.57060200	2.11495400
C	3.02686200	-3.39588000	0.15336400
C	2.52020700	-2.78669600	2.44178000
C	3.44400900	-3.18735700	1.47106500
H	3.74704500	-3.72233200	-0.58958300
H	2.84901500	-2.64837400	3.46653100
H	4.48230500	-3.34759500	1.74358200
C	-2.66564400	-0.84706300	-3.09354200
H	-2.03559000	-1.59295500	-2.59915700
C	-3.54040300	-1.58765900	-4.13109000
H	-4.19091100	-2.32676900	-3.64917100
H	-4.17817700	-0.89208200	-4.68941000
H	-2.90567900	-2.11101300	-4.85632400
C	-1.71934000	0.16648000	-3.77914000
H	-2.28419300	0.95959200	-4.28429000
H	-1.05674700	0.63099100	-3.04050100
H	-1.10052200	-0.33907000	-4.53109400
C	1.26081300	-3.43248400	-1.67348000
H	0.19026600	-3.21977000	-1.74360800
C	1.97877200	-2.47373500	-2.65084200
H	1.64023400	-2.65692800	-3.67749000
H	1.75376700	-1.42999500	-2.40273900
H	3.06663600	-2.61401000	-2.62763500
C	1.47433200	-4.90889200	-2.08217900
H	2.53580800	-5.18341400	-2.05792600
H	0.93583400	-5.58907000	-1.41246800
H	1.10952600	-5.07467100	-3.10254300
C	0.17825500	-2.16540200	3.20587700
H	-0.78954900	-1.99459300	2.72623100
C	0.58155700	-0.84356400	3.89832700
H	1.55477700	-0.92726300	4.39841300
H	0.62434700	-0.02374100	3.17152700
H	-0.16073000	-0.57675500	4.65977900
C	0.00064500	-3.30432300	4.23880400
H	-0.32357200	-4.23330400	3.75601200
H	0.93672200	-3.51033700	4.77205800
H	-0.75447900	-3.02446400	4.98257400
C	-3.95606600	-0.09500800	1.83726000
H	-3.08587400	-0.74967300	1.94734100
C	-3.66530300	1.18456200	2.65345600
H	-2.78785100	1.70830000	2.26075900
H	-4.51420200	1.87883800	2.63562700
H	-3.47187400	0.92527700	3.70151700
C	-5.18627900	-0.84512500	2.40203900
H	-6.09439000	-0.23601600	2.31485900
H	-5.36091600	-1.78582800	1.86690500
H	-5.03789300	-1.07873500	3.46340300
Ni	-0.20130300	0.38661800	0.01843600
C	0.77155000	4.32808800	0.57150300
C	-0.09537500	3.27462900	0.21787000
C	-1.45425200	3.53078100	-0.00150700
C	-1.90672700	4.84173300	0.14475000
C	-1.03130100	5.88463700	0.50180700
C	0.32525000	5.64343600	0.72015400
C	1.94799600	2.38010700	0.44364000
H	-2.12871100	2.72654100	-0.28011500
H	-2.95741300	5.06440200	-0.02275400
H	-1.41746400	6.89531700	0.60633500
H	1.00147100	6.44901200	0.99358500
H	3.58575800	1.55037900	0.01764500
N	0.64878900	2.09130800	0.15347700
N	2.01941200	3.73947100	0.70480000
C	3.22014500	4.44998600	1.08758900
H	3.48481800	5.21533900	0.34632300
H	3.08973800	4.94252400	2.05933800
H	4.03685100	3.73042600	1.16563200
H	-3.73415500	-3.17757600	-0.21442400
H	-1.43168400	-4.48471700	0.58397700

O	4.27116200	0.80585100	-0.10381600
C	5.11774800	1.02821100	-1.24345300
C	5.94820200	-0.24879900	-1.40849600
C	4.25959500	1.28447000	-2.49340500
C	6.03700700	2.22898900	-0.96544100
H	6.53781300	-0.44006400	-0.50490300
H	5.29323500	-1.11090600	-1.57979400
H	6.63456800	-0.16459500	-2.25868000
H	3.62514200	2.16681600	-2.35451800
H	4.88757900	1.45035100	-3.37703900
H	3.60578000	0.42837400	-2.69402100
H	6.74143300	2.39044600	-1.79033600
H	5.44976100	3.14621300	-0.84232900
H	6.61058300	2.06224700	-0.04719600
Na	2.34004000	-0.18645400	0.53191700

TS₂₅₋₂₆

C	0.74788900	-1.28939300	-0.00307000
C	1.00221500	-3.60331600	0.24189700
C	2.14929800	-3.12965000	-0.30724000
N	1.99790200	-1.74019600	-0.45955200
N	0.15091200	-2.49759300	0.42321500
C	3.00717700	-0.87802300	-1.02215800
C	3.01384900	-0.64823800	-2.41713600
C	3.96576800	-0.29189300	-0.16505300
C	4.01070400	0.18967000	-2.94172800
C	4.94390600	0.53607000	-0.73858700
C	4.96828000	0.77658400	-2.11294000
H	4.03399300	0.38642200	-4.00883300
H	5.68816900	1.00093100	-0.09977900
H	5.73136100	1.42210200	-2.53749100
C	-1.16670800	-2.54411200	0.99187400
C	-1.32619300	-2.32292300	2.38257500
C	-2.27801700	-2.77524800	0.14107700
C	-2.63302300	-2.29971300	2.90332500
C	-3.56357700	-2.74790500	0.71078000
C	-3.74337800	-2.50165900	2.07657400
H	-2.77993600	-2.13517100	3.96588200
H	-4.42910200	-2.91963300	0.08082300
H	-4.74401500	-2.49072200	2.49844800
C	3.95925600	-0.52349500	1.34506500
H	3.11808400	-1.18389700	1.57736700
C	5.25288600	-1.22804200	1.81698800
H	5.39849600	-2.18319200	1.29873100
H	6.13735700	-0.60697300	1.63017700
H	5.20644500	-1.42739000	2.89454200
C	3.72741300	0.79638500	2.11607400
H	4.53373500	1.51643300	1.93035000
H	2.77997600	1.25719000	1.81771000
H	3.69235200	0.60350900	3.19556000
C	-0.13211900	-2.12465500	3.31495700
H	0.76743400	-2.08736300	2.69436000
C	-0.20771200	-0.78597700	4.08323900
H	0.68129600	-0.66473900	4.71338000
H	-0.24292000	0.05631800	3.38369200
H	-1.08663600	-0.74251400	4.73931700
C	0.00994800	-3.31968400	4.28837500
H	-0.86219600	-3.40237000	4.94862700
H	0.11180500	-4.26623800	3.74532100
H	0.89763100	-3.19064700	4.91868900
C	-2.09449100	-3.06590000	-1.34788300
H	-1.10016800	-2.70338600	-1.62673500
C	-3.11727700	-2.32953300	-2.23978200
H	-4.13508700	-2.71521100	-2.09796900
H	-3.12177600	-1.25373100	-2.03656300
H	-2.85886900	-2.47968000	-3.29465300
C	-2.13746100	-4.59205300	-1.61200800
H	-1.36877600	-5.12126100	-1.03823400
H	-3.11412800	-5.00861300	-1.33550600
H	-1.96962500	-4.79765900	-2.67584500
C	1.96453200	-1.25674600	-3.34685200
H	1.35346000	-1.94597400	-2.75539500
C	1.01546900	-0.16686600	-3.89911900
H	0.51058000	0.35221700	-3.07711100
H	1.56699900	0.57238400	-4.49368200
H	0.25204100	-0.61871900	-4.54510700
C	2.60654400	-2.07217200	-4.49249900
H	3.19830000	-1.43413200	-5.15981300

H	3.26761200	-2.85528200	-4.10331100
H	1.82789700	-2.55174100	-5.09784600
Ni	0.04389000	0.36698000	0.09053900
C	0.35805200	3.93305200	0.47050300
C	-0.10743600	3.08596400	1.50285100
C	0.16288300	3.39506500	2.83861200
C	0.90080800	4.54760900	3.11497400
C	1.36171900	5.38084200	2.07997300
C	1.09772900	5.08798600	0.74071100
C	-0.80852300	2.19805900	-0.43567500
H	-0.19257400	2.74952000	3.63782300
H	1.12312100	4.80802400	4.14659500
H	1.93553700	6.27040600	2.32709500
H	1.46059500	5.73279700	-0.05511100
H	-2.41693800	1.55293900	-1.10679300
N	-0.83161100	2.03712400	0.92618400
N	-0.08416200	3.36039300	-0.70930600
C	0.22268600	3.85076400	-2.03468100
H	-0.13489800	4.87997900	-2.16996500
H	1.30305700	3.82975000	-2.22557700
H	-0.27416700	3.20046400	-2.75701400
H	3.05017000	-3.64031600	-0.60178900
O	0.71674400	-4.60322000	0.52059700
H	-3.34199200	1.12483000	-1.02332200
C	-4.35780100	2.00345800	-1.53616100
C	-5.68172600	1.24339800	-1.40684000
C	-4.39494500	3.29948200	-0.70868500
C	-4.05606600	2.31218800	-3.01153300
H	-5.64111600	0.30495700	-1.97022100
H	-5.88688000	1.00450400	-0.35585200
H	-6.51698900	1.84160300	-1.78833200
H	-3.43044700	3.81561000	-0.75453600
H	-5.17005000	3.98273400	-1.07630900
H	-4.60848900	3.07674700	0.34385500
H	-4.83330400	2.94863100	-3.45131300
H	-3.09662600	2.83345500	-3.10558100
H	-3.99738500	1.38402400	-3.58968800
Na	-2.48279900	0.31069700	0.91690500

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C	1.56827700	-0.68740600	0.19311300
C	2.82699800	-2.46983700	1.03287300
C	3.70404400	-1.56427700	0.52992600
N	2.94830800	-0.49383500	0.02209300
N	1.53793600	-1.94576900	0.82556600
C	3.52910700	0.68000200	-0.58212200
C	3.69196000	0.72117100	-1.98553500
C	3.93149000	1.75155600	0.24788200
C	4.26619700	1.87183600	-2.54876000
C	4.50189100	2.87932900	-0.36383600
C	4.66816400	2.94213500	-1.74814300
H	4.39610300	1.93035200	-3.62472100
H	4.81314800	3.71763600	0.25105200
H	5.10968800	3.82402500	-2.20239200
C	0.31842400	-2.59748300	1.21832700
C	-0.28865400	-2.24679200	2.45094700
C	-0.24994200	-3.56614700	0.35616300
C	-1.50975500	-2.86193600	2.78124200
C	-1.47030700	-4.15372100	0.73291900
C	-2.10112200	-3.80073200	1.92855600
H	-1.99414900	-2.61177900	3.71910100
H	-1.93149500	-4.88944600	0.08275700
H	-3.04224500	-4.26685000	2.20390400
C	3.73964200	1.72685000	1.76420300
H	3.35969100	0.73779800	2.03871800
C	5.07314500	1.93794500	2.51768000
H	5.82030100	1.19152100	2.22358200
H	5.49477100	2.93077400	2.32001300
H	4.91378700	1.85464500	3.59942500
C	2.67681400	2.76002900	2.20683600
H	2.98356800	3.78115700	1.94834100
H	1.71545300	2.55252000	1.72368000
H	2.53285100	2.71612100	3.29359700
C	0.36169900	-1.26478600	3.42542600
H	1.19016900	-0.78060500	2.90066600
C	-0.60141100	-0.14369100	3.87482700
H	-0.07441200	0.55430800	4.53594900
H	-0.97103200	0.42459200	3.01406600

H	-1.45936700	-0.53856400	4.43340600
C	0.94544700	-2.02124300	4.64419900
H	0.15480100	-2.52385000	5.21494300
H	1.67127700	-2.78118000	4.33214900
H	1.45357400	-1.32028700	5.31692100
C	0.40793500	-3.95610400	-0.96826400
H	1.39796400	-3.49155500	-0.99724100
C	-0.38725900	-3.40266100	-2.17494200
H	-1.40655600	-3.80950000	-2.19478300
H	-0.43685200	-2.30791000	-2.12414300
H	0.10540900	-3.67789500	-3.11523300
C	0.60795200	-5.48392400	-1.08802100
H	1.18637000	-5.87665500	-0.24416000
H	-0.34908500	-6.01818400	-1.11732500
H	1.14782100	-5.72148300	-2.01209700
C	3.24354800	-0.42524700	-2.89049700
H	2.89244000	-1.23892300	-2.24805900
C	2.05056800	0.00371600	-3.77645300
H	1.21326500	0.33721800	-3.15285500
H	2.33086600	0.82367600	-4.44936700
H	1.71204700	-0.83813500	-4.39362200
C	4.40765200	-0.97518300	-3.74628200
H	4.79092600	-0.21777000	-4.44059300
H	5.24213400	-1.30683500	-3.11755200
H	4.06834200	-1.83057100	-4.34310100
Ni	0.18977600	0.47945700	-0.08395900
C	-2.39574500	3.69144800	0.01196300
C	-3.19326200	2.66317600	0.57312300
C	-4.47968600	2.96294500	1.04062900
C	-4.93808400	4.27634200	0.93186100
C	-4.13491700	5.28538500	0.36922400
C	-2.84853000	5.00789100	-0.09895100
C	-1.26493600	1.71802900	-0.00086800
H	-5.09848100	2.18783500	1.48753400
H	-5.93276300	4.52819900	1.29156500
H	-4.52065700	6.29934300	0.30017000
H	-2.22922000	5.79029300	-0.52978500
H	-2.80205700	-1.68227900	-2.12602100
N	-2.48740200	1.47425500	0.54779000
N	-1.20951300	3.07559600	-0.33637400
C	-0.08121600	3.74505100	-0.94757800
H	-0.35909400	4.18138700	-1.91605200
H	0.29994000	4.54634900	-0.30156100
H	0.70767800	3.00502900	-1.10085500
H	4.77961600	-1.57664900	0.48416400
H	2.99137300	-3.42038700	1.51109000
O	-3.42357300	-1.63770700	-1.37978100
C	-4.68818800	-1.10932300	-1.88221900
C	-5.56371200	-0.92457200	-0.64186100
C	-4.43040600	0.22895800	-2.58407700
C	-5.29362600	-2.14177600	-2.84102000
H	-5.67688100	-1.87379700	-0.10529000
H	-5.12407100	-0.18204500	0.03285500
H	-6.56001700	-0.57205300	-0.92801900
H	-3.77047800	0.09286900	-3.45119100
H	-5.36816500	0.66351000	-2.94830600
H	-3.95912800	0.93861300	-1.89771700
H	-6.26232700	-1.80005500	-3.22261000
H	-4.63610300	-2.30564800	-3.70425800
H	-5.43912400	-3.10082100	-2.33263100
Na	-2.19302100	-0.77133200	0.38932200

TS₂₆₋₂₇

C	0.44923200	2.56856400	0.39617700
C	-1.00826800	4.21661300	1.19172900
C	-1.61416200	3.02638200	1.39829300
N	-0.75526700	2.02931200	0.90222800
N	0.23633900	3.95376500	0.58064000
C	-1.19984900	0.66822100	0.71556600
C	-2.11042000	0.39987600	-0.33563200
C	-0.75886000	-0.34554000	1.59943200
C	-2.55410500	-0.92293400	-0.50227800
C	-1.22471300	-1.65195600	1.38143700
C	-2.10950000	-1.94123400	0.33956400
H	-3.25321600	-1.15346400	-1.29997700

H	-0.89920500	-2.45163700	2.03583800
H	-2.45809400	-2.95904400	0.19267000
C	1.09775800	5.02511700	0.14296200
C	1.85078700	5.74770200	1.10277300
C	1.08669100	5.39750200	-1.22786400
C	2.61443300	6.84261500	0.65735500
C	1.87737600	6.48940600	-1.62057300
C	2.63229800	7.20968800	-0.69010600
H	3.18378800	7.42174900	1.37601700
H	1.88482700	6.79350800	-2.66023500
H	3.20573500	8.07547900	-1.01049100
C	0.13575800	-0.01596400	2.79555800
H	0.80185700	0.79928200	2.49000700
C	-0.72036900	0.47929100	3.98947100
H	-0.07439100	0.74363400	4.83567000
H	-1.30867800	1.36375500	3.72409200
H	-1.41249000	-0.30487100	4.32168300
C	1.02914700	-1.19111400	3.23606800
H	0.44419700	-2.02784500	3.63756400
H	1.64257000	-1.55841900	2.40696500
H	1.70503200	-0.86043900	4.03200300
C	1.81243300	5.41542600	2.59608200
H	1.47594900	4.37721900	2.69381900
C	3.19697400	5.53235200	3.27143100
H	3.15376700	5.10859700	4.28103300
H	3.96680000	4.99602800	2.71240400
H	3.50985800	6.57879900	3.37256700
C	0.80779500	6.32494100	3.35030800
H	0.78776800	6.06196500	4.41464000
H	1.10546400	7.37753000	3.26657700
H	-0.20959500	6.23005800	2.96189400
C	0.17124800	4.70667600	-2.24088300
H	0.07657600	3.65888500	-1.93839500
C	0.71954700	4.71964800	-3.68102300
H	0.70687500	5.72719400	-4.11630000
H	1.73745700	4.32556300	-3.72839600
H	0.09257900	4.08534300	-4.31703000
C	-1.24048400	5.35024300	-2.21215500
H	-1.69896500	5.28814900	-1.22033900
H	-1.18700000	6.40788400	-2.49971200
H	-1.89973800	4.83941400	-2.92438700
C	-2.65599600	1.49468400	-1.25750100
H	-2.14847700	2.43106600	-1.01122500
C	-2.37706500	1.21466800	-2.75121000
H	-1.30199300	1.17663100	-2.94853100
H	-2.82417700	0.26824600	-3.07836500
H	-2.80664600	2.01378300	-3.36760400
C	-4.17035800	1.70996100	-1.01687800
H	-4.74385300	0.81041400	-1.27101100
H	-4.37796200	1.95289400	0.03144500
H	-4.54197900	2.53335600	-1.63845300
Ni	1.91857700	1.56648900	-0.09242400
C	2.92996800	1.81734500	-3.91845300
C	1.96076900	0.80810600	-4.15889300
C	1.58706800	0.42511900	-5.44426700
C	2.20400000	1.07981200	-6.51854300
C	3.16199700	2.08111700	-6.29972000
C	3.53444200	2.46034400	-5.00647600
C	2.26867600	1.10701000	-1.93631000
H	0.85113900	-0.35599200	-5.61627300
H	1.93900100	0.80183100	-7.53512300
H	3.62714400	2.56825800	-7.15318800
H	4.28263800	3.23247400	-4.84164300
N	1.54446900	0.39048600	-2.90147100
N	3.11355100	1.97664300	-2.56166600
C	0.72382100	-0.77234400	-2.64515800
H	0.28769500	-0.69363200	-1.64809100
H	-0.09148900	-0.82305700	-3.37301600
H	1.30632100	-1.70267100	-2.71296500
H	-2.57284200	2.78974700	1.82628300
H	-1.33939100	5.21805500	1.39986900
C	3.61588600	0.73292900	0.49936900
C	3.11698100	0.03772200	-0.72766400
C	4.78901200	0.40051400	1.08577600
C	5.28139900	1.05031100	2.39677100
C	4.76990100	2.47993900	2.57606200
H	3.68686200	2.51607900	2.44171600
H	5.02807500	2.86499500	3.56829800
H	5.23879200	3.13705900	1.83264300
C	4.80266100	0.17887500	3.57535500

H	5.14857500	0.57346100	4.53934400
H	3.70962500	0.15987600	3.58961100
H	5.16052900	-0.85090400	3.47524000
C	5.65120400	-0.76318900	0.58828900
H	6.24005500	-1.18188300	1.41310900
H	4.99986300	-1.57163300	0.22779700
C	6.62736000	-0.37724600	-0.54177000
H	7.26268300	0.44399200	-0.18729500
H	6.05995300	0.01660800	-1.39788700
C	7.50373400	-1.54274800	-1.01948400
H	8.08805400	-1.92715000	-0.17101200
H	6.85871700	-2.37201300	-1.34465100
C	8.45228800	-1.15870900	-2.16056400
H	9.13541500	-0.35642100	-1.85381300
H	9.06350500	-2.01050900	-2.48198400
H	7.89370500	-0.80111000	-3.03489700
H	3.86635600	-0.24356500	-1.47173800
H	2.46512700	-0.82251600	-0.52989500
Na	4.23859900	2.93366200	-0.75646100
H	4.62757200	5.70830400	-0.69344600
O	5.24491100	4.96963800	-0.84472500
C	6.39379300	5.45507400	-1.59364300
C	7.22428200	4.21044000	-1.91077900
C	5.90561600	6.13332400	-2.87968400
C	7.17843200	6.43238200	-0.70910000
H	7.52595300	3.69986400	-0.98982000
H	6.65502100	3.50948900	-2.53258200
H	8.13169200	4.48510500	-2.45882500
H	5.28697000	7.00979100	-2.65097100
H	6.75214800	6.47321800	-3.48667100
H	5.30680600	5.43874500	-3.47802200
H	8.06975000	6.80169300	-1.22866300
H	6.56237000	7.30093300	-0.44465700
H	7.49497800	5.94098900	0.21649300
O	6.73299700	1.09546800	2.34816300
Si	7.89708100	1.20380900	3.59875100
C	7.47347600	2.52049700	4.92192200
H	7.35101300	3.51751200	4.48519800
H	6.55217400	2.27695400	5.46172100
H	8.28048100	2.57544700	5.66243500
C	8.14216000	-0.47345400	4.48203900
H	9.03489200	-0.44455800	5.11878900
H	7.28879200	-0.72536200	5.12015000
H	8.27214700	-1.28829800	3.76164800
C	9.53141300	1.70593200	2.67828700
C	9.27933800	2.96628000	1.82768900
H	8.48926600	2.79090600	1.08950700
H	8.97791900	3.82183800	2.44589100
H	10.19395700	3.25559800	1.28918100
C	10.64343000	2.00227000	3.70577400
H	10.85585800	1.13697100	4.34664300
H	11.57900800	2.25834800	3.18766200
H	10.39045100	2.84802400	4.35675900
C	9.99295600	0.55817600	1.75832000
H	10.22068900	-0.35247400	2.32569200
H	9.23185000	0.30696900	1.01213400
H	10.90821800	0.84552100	1.21981600

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C	-2.36817100	-1.44051700	-0.59862200
C	-4.50467400	-2.15646200	-1.23534100
C	-4.04478500	-3.04960100	-0.32545200
N	-2.75994600	-2.62301000	0.06302400
N	-3.50296500	-1.18574300	-1.39941600
C	-1.99452300	-3.31003100	1.07346100
C	-1.02254200	-4.26209700	0.68284200
C	-2.28473400	-3.05737700	2.43494100
C	-0.33875400	-4.95584900	1.69358300
C	-1.57911800	-3.78460400	3.40821200
C	-0.61345300	-4.72343300	3.04311900
H	0.41358600	-5.68825900	1.42404900
H	-1.79388400	-3.61907900	4.45918500
H	-0.07888500	-5.27901500	3.80800000
C	-3.65891800	-0.03717400	-2.25551300
C	-4.34258100	1.09709100	-1.75757800
C	-3.17764600	-0.09007500	-3.58393800
C	-4.53635600	2.18594000	-2.62340100
C	-3.39088700	1.02606400	-4.40898400

C	-4.06485000	2.15422200	-3.93783100
H	-5.07062100	3.06100500	-2.26539800
H	-3.02811600	1.00718200	-5.43173000
H	-4.22985500	3.00259500	-4.59567900
C	-3.36239400	-2.05776500	2.85777500
H	-3.59936800	-1.44110900	1.98489200
C	-4.65763700	-2.78710200	3.29218500
H	-5.05080500	-3.41723200	2.48751100
H	-4.47088800	-3.42840900	4.16257700
H	-5.43336800	-2.06121800	3.56525400
C	-2.88796300	-1.10387500	3.97567400
H	-2.71977700	-1.63794000	4.91950900
H	-1.95716600	-0.59671400	3.70243700
H	-3.65318300	-0.34082000	4.16431600
C	-4.88055300	1.15898500	-0.32802400
H	-4.54926500	0.25439500	0.19057400
C	-4.30790900	2.36282400	0.45325200
H	-4.68899900	2.36167600	1.48193400
H	-3.21497600	2.31240300	0.49379000
H	-4.59502900	3.31750900	-0.00463800
C	-6.42788400	1.17381300	-0.30988900
H	-6.82252400	2.06433300	-0.81454700
H	-6.83980200	0.29238900	-0.81457200
H	-6.79777300	1.18019800	0.72263500
C	-2.45289600	-1.31580500	-4.13750200
H	-2.35270300	-2.03768300	-3.32150900
C	-1.02430700	-0.96429700	-4.61090000
H	-1.03929800	-0.23977700	-5.43474100
H	-0.44200700	-0.54105600	-3.78542000
H	-0.51152400	-1.86600600	-4.96781800
C	-3.26739600	-1.98890900	-5.26746100
H	-4.26499200	-2.28108200	-4.91933200
H	-3.39393500	-1.31541100	-6.12408000
H	-2.75206700	-2.88963600	-5.62225800
C	-0.75624900	-4.56390400	-0.79262200
H	-0.97280500	-3.64679700	-1.35207500
C	0.71015900	-4.94342700	-1.08362400
H	1.40170000	-4.19816100	-0.67921600
H	0.97154100	-5.92261900	-0.66344700
H	0.86828900	-5.00181800	-2.16670500
C	-1.70252200	-5.67830400	-1.30787500
H	-1.53380000	-6.61306300	-0.75817200
H	-2.75456100	-5.39915700	-1.19261000
H	-1.51843100	-5.87154700	-2.37186300
Ni	-0.84536200	-0.43712700	-0.62521200
C	-1.07638300	5.01043400	0.89745900
C	-0.51559400	4.11835900	1.84070700
C	-0.47765300	4.47437500	3.19378500
C	-1.01623200	5.70165900	3.57310400
C	-1.58227500	6.57162000	2.62257000
C	-1.62008100	6.24157700	1.26826700
C	-0.31951900	3.15698900	-0.09106600
H	-0.01446600	3.81747400	3.92655200
H	-0.99505400	5.99760300	4.61825700
H	-1.99602400	7.52148600	2.94919500
H	-2.05725200	6.92080200	0.54202500
N	-0.06451300	2.97497800	1.19726900
N	-0.92985700	4.37554300	-0.32690200
C	-1.38440100	4.86819800	-1.61623200
H	-0.60381900	4.72890300	-2.36892300
H	-2.28753900	4.34260400	-1.94554400
H	-1.59900100	5.93546800	-1.53314800
H	-4.49907900	-3.93695500	0.08025000
H	-5.43416700	-2.11678700	-1.77707900
C	0.60235000	0.84816800	-0.85066400
C	-0.02522100	2.21180900	-1.22219600
C	1.96695500	0.77404100	-0.91006400
C	2.69520400	-0.59446600	-0.74360400
C	2.39932700	-1.47499200	-1.97220300
H	2.72082700	-0.97633600	-2.89222500
H	2.90596300	-2.44727500	-1.90576700
H	1.32005700	-1.64568600	-2.03374900
C	2.26236600	-1.32909400	0.53541900
H	2.54711700	-0.73339900	1.41404200
H	1.17652600	-1.49684300	0.52657000
H	2.76080200	-2.30087000	0.62225200
C	2.87654800	1.95658600	-1.23873100
H	2.38714100	2.89215000	-0.94278800
H	3.78609500	1.88740000	-0.63465900
C	3.29389900	2.07179200	-2.72081400

H	2.39477200	2.09124400	-3.35468500
H	3.85101700	1.17145900	-3.01001700
C	4.15010700	3.31106300	-3.01473900
H	3.59636800	4.21430700	-2.71805400
H	5.04939800	3.28767700	-2.38267500
C	4.56502400	3.42886400	-4.48562100
H	3.68738100	3.49071300	-5.14163100
H	5.17689300	4.32161400	-4.66282200
H	5.15005700	2.55630300	-4.80247700
H	-0.98446700	2.02028600	-1.72544200
H	0.57215000	2.77405900	-1.95951500
Na	0.24988100	0.64645800	1.63495700
H	0.01588600	1.63126100	4.17772200
O	0.38489400	0.76259300	3.94665200
C	1.20423300	0.30431600	5.06146400
C	2.40169600	1.25030500	5.21550200
C	0.34098700	0.28526200	6.32869900
C	1.65398800	-1.10579900	4.67907700
H	2.98407200	1.28859200	4.28900500
H	2.07036300	2.26917600	5.45385000
H	3.06150300	0.91828900	6.02497300
H	-0.53046600	-0.36191900	6.18939800
H	0.91511700	-0.08321300	7.18593700
H	-0.01380300	1.29398000	6.57776500
H	2.26415100	-1.53870100	5.47886100
H	0.79021200	-1.75647700	4.50875900
H	2.25625500	-1.08804600	3.76476400
O	4.11596500	-0.34031700	-0.63050000
Si	5.48443400	-1.33463800	-0.86858400
H	5.32446300	-3.07325000	-0.08525200
C	4.50653300	-3.64912600	-0.53151200
H	6.24927700	-3.64041800	-0.24717300
H	5.14807400	-3.02319100	0.99457800
C	5.87526300	-1.55522000	-2.72522600
H	5.12407900	-2.17857800	-3.22144800
H	5.90346300	-0.59148200	-3.24497100
H	6.85035600	-2.03887300	-2.86104800
C	6.90860800	-0.35060300	0.00980000
C	8.22011900	-1.16130700	-0.03599800
H	9.03160000	-0.59645300	0.44550700
H	8.13338900	-2.11878100	0.49239100
H	8.53943700	-1.37328200	-1.06426300
C	6.52285900	-0.09014300	1.47958100
H	5.58975200	0.47953000	1.54797500
H	6.38967000	-1.02486000	2.03943200
H	7.31168200	0.48544500	1.98628900
C	7.12998600	1.00190600	-0.69699800
H	7.43825400	0.87212800	-1.74183600
H	6.22209100	1.61483400	-0.68808900
H	7.92360900	1.57090100	-0.19020200

TS₂₇-TP1

C	-1.97395800	-0.13320000	0.62934500
C	-3.49810300	-0.48715700	2.37138000
C	-4.04146600	-1.03596600	1.25880500
N	-3.13451400	-0.82369800	0.20511100
N	-2.25665900	0.05784000	2.00231100
C	-3.41766400	-1.26127600	-1.14083500
C	-4.15387500	-0.41167500	-2.00154000
C	-3.02489900	-2.55969800	-1.53928500
C	-4.47878000	-0.89130900	-3.28033900
C	-3.37376900	-2.99285000	-2.82775100
C	-4.09252600	-2.16736000	-3.69266200
H	-5.04111500	-0.26081900	-3.96017100
H	-3.08242900	-3.98504900	-3.15596100
H	-4.35382100	-2.51894500	-4.68603400
C	-1.42877000	0.79303800	2.92687700
C	-0.51004000	0.09122200	3.74330800
C	-1.60927000	2.19183000	3.03956200
C	0.26892400	0.83357000	4.64517600
C	-0.80712300	2.88795100	3.95807700
C	0.13084700	2.21898600	4.74557900
H	0.98556800	0.32324200	5.27902900
H	-0.92335300	3.96132200	4.06274100
H	0.74371400	2.77449600	5.44906700
C	-2.28019700	-3.50087100	-0.59375200
H	-1.91318700	-2.89466500	0.23423000
C	-3.23068700	-4.57138800	-0.00502500

H	-4.06069200	-4.10885900	0.53992100
H	-3.65388500	-5.19544100	-0.80138600
H	-2.69084100	-5.22720400	0.68954700
C	-1.06154400	-4.16968400	-1.27113300
H	-1.37227600	-4.90539800	-2.02224000
H	-0.42967900	-3.43237700	-1.78105000
H	-0.46292600	-4.71462000	-0.52703400
C	-0.41686400	-1.43524900	3.71698800
H	-0.81918900	-1.76958800	2.75264900
C	1.02767500	-1.96680400	3.83502400
H	1.02922200	-3.05939200	3.72679100
H	1.67973700	-1.54682900	3.06340600
H	1.46232400	-1.74343400	4.81658600
C	-1.29897100	-2.05270300	4.83258300
H	-0.94452100	-1.73676900	5.82141700
H	-2.34595500	-1.74820000	4.73574900
H	-1.25829400	-3.14818100	4.79079300
C	-2.69774300	2.92647700	2.25624600
H	-3.01053500	2.27522700	1.43415000
C	-2.20919000	4.24745500	1.62820700
H	-1.93701700	4.98852500	2.38955500
H	-1.33821900	4.07713300	0.98966000
H	-3.00570100	4.68589000	1.01496000
C	-3.93356700	3.17919000	3.15621400
H	-4.33410400	2.24201000	3.55806500
H	-3.67375400	3.82627000	4.00322600
H	-4.72900500	3.67171100	2.58360200
C	-4.63587400	0.96791800	-1.55057000
H	-3.99976300	1.27972600	-0.71503600
C	-4.50849800	2.04362400	-2.65024300
H	-3.49460900	2.07640300	-3.05865600
H	-5.20688900	1.86740500	-3.47726300
H	-4.74155100	3.03035200	-2.23293600
C	-6.09752200	0.90308900	-1.03979500
H	-6.77314300	0.57840100	-1.84089500
H	-6.20135400	0.20374400	-0.20395900
H	-6.42665400	1.89181300	-0.69734900
Ni	-0.52562000	0.39334600	-0.32136800
C	5.13589400	-1.45539400	0.17504400
C	4.09927900	-2.20438700	0.77473900
C	4.34744000	-3.50740800	1.22229600
C	5.63035200	-4.02386200	1.05675100
C	6.65393000	-3.26379000	0.45844200
C	6.42542200	-1.96425700	0.00854600
C	3.24814300	-0.27490100	0.26997000
H	3.56071200	-4.09024900	1.69389500
H	5.84953300	-5.03176000	1.39794500
H	7.64377700	-3.69736600	0.34750500
H	7.22091900	-1.38110000	-0.44604600
N	2.94039000	-1.44236100	0.81888800
N	4.56164400	-0.23286700	-0.14802300
C	5.26034600	0.87949700	-0.77026500
H	5.76753100	1.50284800	-0.02401400
H	6.00432300	0.48644000	-1.46798200
H	4.55624000	1.49034000	-1.33565100
H	-4.97377800	-1.55326600	1.11233800
H	-3.87130600	-0.42560600	3.37869700
C	1.32069000	0.95697200	-1.00280700
C	2.32087600	0.90582600	0.18823400
C	1.16659800	2.15709800	-1.64840400
C	0.23167500	2.37230400	-2.86629500
C	-0.79213000	3.48578500	-2.55570000
H	-0.29943300	4.43938900	-2.34702000
H	-1.46019200	3.63617900	-3.40996400
H	-1.40195800	3.20892500	-1.68885000
C	-0.52295700	1.12167300	-3.31620400
H	0.15561000	0.31257700	-3.57974400
H	-1.17514700	0.74784700	-2.51471900
H	-1.15462200	1.35896700	-4.18160200
C	1.95590500	3.42076900	-1.29182300
H	3.01870700	3.16560700	-1.17566700
H	1.92467100	4.11142100	-2.13897000
C	1.50212400	4.16834200	-0.02105600
H	1.44116500	3.47488400	0.82716100
H	0.48344300	4.54712800	-0.17018300
C	2.42567000	5.34034700	0.33942700
H	3.44597300	4.96201100	0.50068900
H	2.49023800	6.02871000	-0.51545600
C	1.96658400	6.10980300	1.58284000
H	1.91515000	5.45047900	2.45827500

H	2.65109400	6.93198400	1.82265200
H	0.96805500	6.53965800	1.43525900
H	1.73089200	0.87408600	1.11333600
H	2.94028100	1.80580600	0.26145400
Na	0.80682500	-1.94621100	-0.10208700
H	1.26627600	-0.25645100	-1.72746500
O	1.37430800	-1.44356700	-2.14390300
C	2.15646500	-1.85777700	-3.25027800
C	1.23668000	-2.21286800	-4.43858000
C	3.14529700	-0.75268000	-3.67100300
C	2.94960000	-3.12002200	-2.85127900
H	0.51604900	-2.98213400	-4.13802000
H	0.67066400	-1.33878900	-4.77441800
H	1.80979900	-2.59550900	-5.29343600
H	3.84738400	-0.54381600	-2.85637600
H	3.72867200	-1.05469300	-4.55034600
H	2.61912400	0.17733000	-3.90903300
H	3.56125300	-3.49782200	-3.68113900
H	3.61281000	-2.90727800	-2.00605200
H	2.26012900	-3.92045700	-2.55220500
O	1.11851000	2.83456900	-3.91900200
Si	0.91324400	3.07428700	-5.60209100
C	-0.73400000	3.92901300	-6.06550800
H	-0.86776600	4.88185200	-5.54328000
H	-0.75254700	4.13205300	-7.14342300
H	-1.59892000	3.29563500	-5.83994700
C	1.01161000	1.42707600	-6.55961600
H	0.98914200	1.60828500	-7.64115000
H	1.93189600	0.88126700	-6.32774800
H	0.16917500	0.77140200	-6.31623700
C	2.41211000	4.21602700	-6.06667200
C	2.28564300	5.56924600	-5.33840100
H	1.37862500	6.11139000	-5.63401700
H	2.26154000	5.43975000	-4.25067000
H	3.14423200	6.21321800	-5.57965400
C	2.43797100	4.46364800	-7.58863800
H	3.28413000	5.11459900	-7.85250300
H	2.55509800	3.53214900	-8.15563200
H	1.52514400	4.95984900	-7.94187600
C	3.72951100	3.53842700	-5.63904800
H	3.88992600	2.58798600	-6.16309200
H	4.58569700	4.18915200	-5.87135100
H	3.74064000	3.33384600	-4.56319400

TP1

C	2.20427100	0.38267900	0.77386100
C	3.16414700	-1.17692900	-0.35471200
C	4.20488800	-0.43907300	0.25359900
C	3.47157000	-2.27360500	-1.16798600
C	5.55337000	-0.75531400	0.07680300
C	4.81365400	-2.59839000	-1.34975800
H	2.67814900	-2.84621400	-1.63874700
C	5.83868400	-1.85106100	-0.73697100
H	6.34771600	-0.18086600	0.54508900
H	5.07952500	-3.44482900	-1.97694600
H	6.87477500	-2.13347200	-0.90236500
C	4.23970700	1.57469700	1.76149700
H	4.92939200	1.10979100	2.47472200
H	4.80890600	2.25486400	1.11635200
H	3.50624700	2.15629600	2.32103200
N	1.93352600	-0.63739800	-0.00809800
C	1.18597300	1.29106800	1.41225700
C	-0.23873900	0.87371800	1.14413400
H	1.37260400	2.32152400	1.08684100
H	1.36015000	1.28785900	2.50224800
C	-1.25909200	1.68248200	0.82764800
H	-0.43480600	-0.18495700	1.25917600
N	3.56649800	0.55626400	0.97870300
C	-2.68858700	1.10771500	0.70871700
C	-3.46069200	1.45067700	2.00184900
C	-3.44835600	1.68368600	-0.50290100
H	-3.48825500	2.52983800	2.18909700
H	-4.49072700	1.08508500	1.92717400
H	-2.97910200	0.96058100	2.85286200
H	-4.45603700	1.25755100	-0.53519700
H	-3.54991600	2.77137200	-0.43949400
H	-2.94175200	1.44929600	-1.44464400
C	-1.08764400	3.18711300	0.66171500

C	-0.59339600	3.61941400	-0.73535700
H	-0.38159000	3.56600200	1.41231600
H	-2.03277600	3.70180000	0.87451700
C	-0.40758000	5.13731100	-0.86302200
H	0.35550500	3.11164300	-0.95606800
H	-1.30039800	3.27414900	-1.50060100
C	0.09268800	5.56809100	-2.24603400
H	-1.36117800	5.63941300	-0.64533300
H	0.29837500	5.48313800	-0.09380000
H	0.21784800	6.65536200	-2.30592800
H	1.06062400	5.10716000	-2.47857200
H	-0.61144200	5.26976300	-3.03242800
O	-2.67176300	-0.31819300	0.66658400
Si	-2.57625200	-1.44621200	-0.63346100
C	-2.26649300	-3.12840100	0.28008100
C	-1.18385800	-1.04392800	-1.86879100
H	-1.13065500	-1.82796900	-2.63455900
H	-1.36721700	-0.09622900	-2.38836300
H	-0.20942500	-0.97132500	-1.37436500
C	-4.23988500	-1.52516500	-1.57378900
H	-4.27398200	-2.41732100	-2.21109200
H	-5.08873300	-1.57692600	-0.88343600
H	-4.38468600	-0.65467900	-2.22213800
C	-2.00668200	-4.23923000	-0.75830200
H	-1.10044100	-4.04743500	-1.34525100
H	-1.86946900	-5.20535700	-0.25156800
H	-2.84331900	-4.35724100	-1.45913800
C	-1.04609000	-3.01409000	1.21547100
H	-1.23092800	-2.28801600	2.01459700
H	-0.84102700	-3.98587300	1.68900100
H	-0.13843000	-2.70389100	0.68430000
C	-3.50571200	-3.49782100	1.12115200
H	-3.73997900	-2.71614200	1.85279600
H	-4.39456000	-3.65612600	0.49792900
H	-3.32440000	-4.43103400	1.67456300

R3

C	-3.61974100	3.12730600	-0.65565600
C	-2.77476700	2.21893100	-0.23669400
H	-3.99939200	3.13156000	-1.67674000
C	-1.95474200	1.29493400	0.20378900
C	-0.42010200	1.48875600	0.17054800
C	-0.01093600	2.50506000	-0.90405600
C	0.03030600	1.97407800	1.56169000
H	-0.51224200	3.46564000	-0.75359400
H	1.07047600	2.67198300	-0.87597500
H	-0.27939500	2.12594500	-1.89416700
H	1.11867800	2.09604100	1.60317000
H	-0.42686400	2.94433600	1.78073100
H	-0.27003600	1.27355900	2.34677100
C	-2.51112500	0.00396700	0.79663800
C	-2.88772500	-1.03653700	-0.27387200
H	-3.39838400	0.23389100	1.39967700
H	-1.76748400	-0.42942200	1.47595100
C	-3.39910100	-2.35394000	0.32265700
H	-3.65960400	-0.60470000	-0.92609900
H	-2.01350200	-1.22705500	-0.90733400
C	-3.80428700	-3.37799400	-0.74318100
H	-2.62119700	-2.78715700	0.96859200
H	-4.25775200	-2.14941200	0.97862200
H	-4.16162300	-4.30986200	-0.28961500
H	-4.60738100	-2.98825200	-1.38090700
H	-2.95760100	-3.62688100	-1.39486900
O	0.14234200	0.21811000	-0.17508600
Si	1.49393600	-0.73277800	0.28898800
C	1.63903800	-0.94795400	2.18288200
H	2.37014300	-1.73413600	2.40705600
H	1.95600300	-0.03960000	2.70342400
H	0.68000500	-1.26334000	2.60944400
C	1.04956300	-2.42141700	-0.46888500
H	0.09522100	-2.77324400	-0.06179600
H	0.94126000	-2.35727500	-1.55674600
H	1.80870700	-3.17956700	-0.24650000
C	3.18132300	-0.09449500	-0.44773700
C	4.24901300	-1.18880900	-0.22087300
H	3.98906900	-2.12970300	-0.71965400
H	5.21506900	-0.85930700	-0.62947100
H	4.40387200	-1.40268900	0.84411900

C	3.66330800	1.19843100	0.23921500
H	4.63874400	1.50152500	-0.16824200
H	2.97516700	2.03641800	0.08105100
H	3.79038600	1.06694800	1.32084200
C	3.03466100	0.15256000	-1.96228400
H	3.99103500	0.49012300	-2.38748600
H	2.74367200	-0.76005700	-2.49638700
H	2.28252000	0.91791400	-2.18082000
H	-3.97951600	3.92253300	-0.00327400

Cartesian coordinates for the stationary points given in Fig. 6.

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C	-2.60529600	0.07979400	-0.42822700
C	-4.25701300	-0.89842700	0.58460800
C	-4.44386300	-1.12114300	-0.79696100
C	-5.17563300	-1.41304400	1.50664100
C	-5.52990500	-1.84185000	-1.29765300
C	-6.25894800	-2.13706100	1.01638600
H	-5.04544400	-1.24898700	2.57327700
C	-6.43333900	-2.34806900	-0.36533000
H	-5.67364300	-2.00215900	-2.36201400
H	-6.98674800	-2.54685900	1.71077200
H	-7.29201800	-2.91543400	-0.71250500
C	-3.11245200	-0.46672400	-2.84719700
H	-2.03792300	-0.39136200	-3.01996600
H	-3.46784500	-1.39942200	-3.29286900
H	-3.62414400	0.37447600	-3.32886600
N	-3.10380700	-0.14870900	0.78062000
C	-1.32953300	0.82184900	-0.71054600
C	-0.18632600	-0.13791900	-0.95996700
H	-1.07662600	1.44997500	0.16799200
H	-1.48050500	1.50519800	-1.55451500
C	0.78558900	-0.05018200	-1.88017900
H	-0.14572600	-0.97317400	-0.26806200
N	-3.36909200	-0.49726200	-1.41616000
C	1.87171000	-1.15036700	-1.92994700
C	1.46971100	-2.17435100	-3.01440500
C	3.26894300	-0.59298400	-2.26360900
H	1.35017700	-1.69773200	-3.99427500
H	2.23697500	-2.95163300	-3.09921500
H	0.52420300	-2.64886900	-2.73617300
H	3.97803900	-1.42505400	-2.31318600
H	3.28829100	-0.08223600	-3.23135600
H	3.61705900	0.11091900	-1.50278900
C	0.82847200	1.05727900	-2.92039300
C	1.52917200	2.35114500	-2.45283900
H	-0.19530100	1.31991800	-3.22156800
H	1.31692700	0.69789000	-3.83529300
C	1.50687200	3.45696600	-3.51641600
H	1.04672100	2.71014800	-1.53495900
H	2.56912500	2.13127400	-2.18071300
C	2.21444600	4.73831200	-3.06247200
H	1.97611300	3.08567800	-4.43938700
H	0.46372700	3.68770800	-3.77802400
H	2.17229100	5.51367100	-3.83620500
H	1.75341500	5.14443600	-2.15424400
H	3.27127600	4.54802700	-2.83838100
O	-0.39876900	2.10352200	2.05506200
C	-0.05627400	3.38223800	2.45754000
C	0.83152200	3.33193600	3.72625100
C	0.72958500	4.10186000	1.33170400
C	-1.32617700	4.21599300	2.77482200
H	0.28416800	2.84125400	4.54313800
H	1.73223300	2.74082900	3.52463900
H	1.14050600	4.32760600	4.07422800
H	0.11001900	4.16051000	4.42753400
H	1.03082800	5.12218000	1.60669900
H	1.63193100	3.53003200	1.08647000
H	-1.10642200	5.25107800	3.07152700
H	-1.97938100	4.24346200	1.89302000
H	-1.88578200	3.74594000	3.59773500
Na	-1.86521500	0.74196600	2.52751400
O	1.92070600	-1.90843400	-0.72200900
Si	2.42912200	-1.58397400	0.89707100

C	2.60572200	0.25696700	1.34665800
H	3.10439900	0.33263300	2.32224300
H	3.21904400	0.81342300	0.63016200
H	1.63736500	0.76844900	1.43671700
C	1.05018700	-2.36261300	1.96786200
H	1.25213000	-2.21353300	3.03485500
H	0.07987500	-1.90498400	1.74300800
H	0.95539700	-3.43896000	1.78723100
C	4.08812700	-2.55057600	1.23291600
C	5.30165700	-1.80998400	0.63729000
H	5.24260200	-1.73182200	-0.45344900
H	5.40263700	-0.79560600	1.04219200
H	6.22881900	-2.35185400	0.87517700
C	4.29318900	-2.66945200	2.75891600
H	3.49557500	-3.24866200	3.23845700
H	5.24266200	-3.18120400	2.97300800
H	4.33759900	-1.68817800	3.24876100
C	4.00432400	-3.96254500	0.62137500
H	3.84281000	-3.92181800	-0.46112100
H	4.93631600	-4.51674600	0.80645300
H	3.18387900	-4.54761500	1.05555300

TS₂₈₋₂₉

C	-2.39269100	-0.12277100	-0.73585500
C	-3.63271700	-1.85848800	-0.26113600
C	-4.46028100	-0.95663700	-0.96841200
C	-4.15447600	-3.08017700	0.17597500
C	-5.79675000	-1.23163500	-1.24914000
C	-5.49204000	-3.36586000	-0.10391900
H	-3.52768900	-3.78992400	0.71033400
C	-6.30160000	-2.45749600	-0.80594500
H	-6.42793200	-0.52836000	-1.78511000
H	-5.91602000	-4.31062800	0.22551000
H	-7.33889200	-2.70945000	-1.00774600
C	-4.05574400	1.28322600	-2.04745500
H	-3.18682000	1.71487100	-2.54741300
H	-4.77104700	0.96403100	-2.81120100
H	-4.52649700	2.05291700	-1.42340500
N	-2.36672500	-1.31397400	-0.11674400
C	-1.27352100	0.81387000	-0.74922300
C	0.03503400	0.23045700	-1.13257300
H	-1.11079700	1.14043300	0.62276200
H	-1.50421700	1.76030800	-1.24196700
C	1.12504700	0.85171200	-1.63251100
H	0.12135000	-0.84402700	-0.97817100
N	-3.64635000	0.13223900	-1.26682500
C	2.38420400	0.03374300	-1.98771900
C	2.27016300	-0.45519600	-3.44624700
C	3.68978400	0.83616000	-1.83233200
H	2.14285200	0.38930900	-4.13308100
H	3.16974100	-1.00955100	-3.73842100
H	1.40335200	-1.11463800	-3.54460400
H	4.53556600	0.19922700	-2.10999900
H	3.70982100	1.71562500	-2.48295300
H	3.83595900	1.17842700	-0.80364100
C	1.09368700	2.32296700	-2.00795400
C	1.48663300	3.29929200	-0.87898000
H	0.07967500	2.58392900	-2.34232200
H	1.74037600	2.50949000	-2.87650000
C	1.35453600	4.77226700	-1.28854500
H	0.85857100	3.09855900	-0.00230200
C	2.52064100	3.10556500	-0.56414600
C	1.76304100	5.74746500	-0.17898100
H	1.96780200	4.95801500	-2.18256400
H	0.31556900	4.97358600	-1.58790000
H	1.65519900	6.79003900	-0.50075300
H	1.14536000	5.60866500	0.71666600
H	2.80930400	5.59657800	0.11511000
O	-0.83123300	1.10579600	1.83914700
C	-1.51007400	2.02819300	2.67331900
C	-1.12028700	1.71808800	4.12954100
C	-1.07856500	3.46529900	2.32140300
C	-3.03690300	1.88574000	2.50270800
H	-1.43301600	0.70093000	4.40209700
H	-0.03336200	1.78585700	4.25116900
H	-1.59143800	2.41340800	4.83553200
H	-1.34287200	3.70079900	1.28388500
H	-1.56038800	4.20670300	2.97122100

H	0.00718100	3.56640700	2.42585500
H	-3.58629400	2.57790400	3.15299000
H	-3.33085100	2.09049400	1.46667600
H	-3.35775400	0.86484200	2.74612000
Na	-0.81207000	-1.03648600	1.56187600
O	2.48470600	-1.18096700	-1.21684900
Si	2.75131300	-1.50701300	0.44009200
C	2.61185800	-0.01329200	1.62010500
H	2.76497200	-0.35799500	2.65163800
H	3.37786300	0.74254900	1.41870800
H	1.63931900	0.49074300	1.57035900
C	1.39212200	-2.79084800	0.91362900
H	1.14638600	-2.75419000	1.98593000
H	0.48511900	-2.66594000	0.30899700
H	1.73160700	-3.81349800	0.71710300
C	4.47352400	-2.38549900	0.64903300
C	5.63364000	-1.38430100	0.48609900
H	5.64603100	-0.93241900	-0.51110500
H	5.58480700	-0.57391800	1.22361900
H	6.59653700	-1.89628800	0.62650200
C	4.55648500	-3.00935200	2.05900900
H	3.76698500	-3.75040200	2.23378400
H	5.51889500	-3.52548900	2.18560400
H	4.48985600	-2.25236200	2.85077100
C	4.61585100	-3.49684700	-0.41033600
H	4.54522000	-3.09341900	-1.42600800
H	5.58985600	-3.99690700	-0.30835100
H	3.84248500	-4.26825200	-0.30594400

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C	-2.32317800	-0.13855100	-0.99320300
C	-3.55243000	-1.82990000	-0.31911800
C	-4.43990800	-0.91316000	-0.93675700
C	-4.05752500	-3.02092300	0.21145200
C	-5.80661400	-1.14762300	-1.03425500
C	-5.43198000	-3.26698800	0.11308400
H	-3.39024100	-3.74366000	0.67528600
C	-6.29461200	-2.34910300	-0.50036800
H	-6.47849900	-0.43189100	-1.50056500
H	-5.83737800	-4.19065700	0.51833200
C	-7.35730400	-2.56653800	-0.56314300
H	-4.07694200	1.25183200	-2.18379400
H	-3.27198800	1.53544700	-2.86789800
H	-4.94364300	0.94389700	-2.77651000
H	-4.35805000	2.13146100	-1.58828800
N	-2.26235800	-1.33251600	-0.34489500
C	-1.23470800	0.74011400	-1.21369700
C	0.11514900	0.23830600	-1.34708300
H	-1.19308400	1.39591900	0.81881200
H	-1.46126200	1.72919400	-1.60240300
C	1.26549600	0.91708000	-1.62657800
H	0.21638900	-0.84653600	-1.27175800
N	-3.64081100	0.14531500	-1.36148400
C	2.56946600	0.14881900	-1.90623600
C	2.61274600	-0.26482900	-3.39217500
C	3.83554400	0.96462000	-1.58362200
H	2.52858600	0.61410900	-4.04147900
H	3.55043600	-0.78359900	-3.62641200
H	1.77603500	-0.93458800	-3.60932300
H	4.72114900	0.36288000	-1.80994400
H	3.89460200	1.87535700	-2.18667200
H	3.87490800	1.26000400	-0.53072500
C	1.23249700	2.41159000	-1.89241100
C	1.41450700	3.30320200	-0.64474500
H	0.27218600	2.67355500	-2.35954400
H	1.99328800	2.69229400	-2.63354000
C	1.29322700	4.80238800	-0.94886200
H	0.66892100	3.01691900	0.10919000
C	2.39538500	3.10603800	-0.19080800
C	1.48824500	5.69041000	0.28483900
H	2.03113100	5.07738600	-1.71657500
H	0.30735900	5.00377700	-1.39272400
H	1.39342000	6.75369300	0.03476100
H	0.74408700	5.46272700	1.05836700
H	2.48052800	5.54037900	0.72852100
O	-0.97437200	1.21817700	1.77422600
C	-1.89533000	1.91968500	2.64500300
C	-1.51547500	1.49468800	4.06544800

C	-1.69904200	3.43044300	2.45781100
C	-3.33576000	1.50695200	2.31209400
H	-1.64581000	0.41323300	4.19459400
H	-0.46999500	1.74577600	4.27425300
H	-2.14702700	2.00005300	4.80371300
H	-1.93137800	3.72655700	1.42790200
H	-2.35553500	3.99831400	3.12704200
H	-0.66162000	3.71064500	2.66807200
H	-4.04994700	2.00975600	2.97420300
H	-3.58914600	1.77043300	1.27910800
H	-3.46862100	0.42518000	2.42224200
Na	-0.57935900	-0.89534200	1.10751400
O	2.62182600	-1.11297700	-1.19607200
Si	2.83782600	-1.54315700	0.43848800
C	2.65474600	-0.11166100	1.69770600
H	2.60540500	-0.52136100	2.71519900
H	3.50806500	0.57352900	1.66813000
H	1.76047400	0.49929500	1.52878200
C	1.44885300	-2.83188000	0.80108000
H	1.08153400	-2.77927000	1.83729100
H	0.60941400	-2.74842200	0.09926400
H	1.82419600	-3.85299400	0.67390100
C	4.54564100	-2.43858300	0.67769000
C	5.72304600	-1.45189700	0.55890000
H	5.77217700	-0.99280000	-0.43363900
H	5.66500800	-0.64681100	1.30156300
H	6.67345900	-1.97935600	0.72401300
C	4.58273600	-3.08267400	2.08041300
H	3.77295600	-3.80728000	2.22816900
H	5.53018200	-3.62200500	2.22106300
H	4.51528600	-2.33391100	2.87986100
C	4.70120400	-3.53497000	-0.39576300
H	4.66098500	-3.11447700	-1.40632100
H	5.66713700	-4.04672300	-0.27784700
H	3.91800600	-4.29974200	-0.32284300

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C	-2.13342200	-0.09178200	-1.56074700
C	-2.93193700	-1.81795200	-0.46268000
C	-4.02722000	-1.25047100	-1.16769900
C	-3.14720200	-2.94958200	0.33230100
C	-5.31404800	-1.77006900	-1.09292000
C	-4.44068400	-3.48192000	0.40839200
H	-2.32002400	-3.41249700	0.86583000
C	-5.50811700	-2.90614400	-0.29164100
H	-6.14426100	-1.31898400	-1.63035400
H	-4.61803600	-4.36231300	1.02138700
H	-6.50117200	-3.34076600	-0.21538400
C	-4.18658300	0.63677300	-2.84052400
H	-4.65771100	1.52576000	-2.39818800
H	-3.46915200	0.96153300	-3.60022800
H	-4.96432900	0.03793300	-3.32577000
N	-1.78509300	-1.08265700	-0.68770300
C	-1.26111300	0.89828100	-2.04789100
C	0.14036600	0.70207200	-1.87570200
H	-0.22431800	2.08016800	1.90552900
H	-1.66574000	1.85190200	-2.37329500
C	1.16781900	1.58412400	-1.66008700
H	0.42199100	-0.35331500	-1.83738000
N	-3.49673700	-0.16830100	-1.86033700
C	2.56946000	1.01452700	-1.42124600
C	3.17346600	0.49294900	-2.73832300
C	3.51830800	2.03355400	-0.77126500
H	3.19175600	1.29973500	-3.47976700
H	4.19862200	0.12556500	-2.61615600
H	2.55134500	-0.31286200	-3.13896500
H	4.48721200	1.57531000	-0.55211300
H	3.71093000	2.87928400	-1.43827700
C	3.10339500	2.42116700	0.16443800
C	0.90993200	3.07990900	-1.69438400
C	0.33668700	3.66779500	-0.38321300
H	0.18910400	3.29787900	-2.49489900
H	1.81298700	3.64331200	-1.96098900
C	0.00584300	5.16361800	-0.46678400
H	-0.57555000	3.10724800	-0.13084700
H	1.05691200	3.50503300	0.43430900
C	-0.57538600	5.73171200	0.83251700
H	0.91462600	5.72092600	-0.73530600

H	-0.70547400	5.32808800	-1.28825200
H	-0.80096300	6.80043100	0.74067600
H	-1.50786300	5.22069900	1.10592800
H	0.12716100	5.61342300	1.66780100
O	-0.35673900	1.16067200	2.19314100
C	-1.52838400	1.11862100	3.06451200
C	-1.21945300	1.93418600	4.32508400
C	-2.73428100	1.68552900	2.30622300
C	-1.73283700	-0.36074500	3.39425800
H	-0.33576200	1.53527500	4.83401600
H	-1.02711600	2.98493600	4.07369900
H	-2.06353700	1.90887500	5.02311200
H	-2.91049800	1.11886300	1.38641800
H	-3.63894600	1.63541100	2.92229700
H	-2.57079900	2.73841800	2.04183300
H	-2.56612200	-0.48124700	4.09416200
H	-1.97159700	-0.93521800	2.49212200
H	-0.83348800	-0.77935100	3.86078700
Na	0.10693500	-0.21536700	0.43268400
O	2.41297400	-0.13810200	-0.49260600
Si	3.60442100	-1.12661700	0.28235600
C	2.87323900	-2.92741300	0.31689600
C	3.81958700	-0.44933900	2.05416300
C	4.18660900	0.58272500	2.02670800
H	2.87376300	-0.44486900	2.60872000
H	4.54040400	-1.04489400	2.62588300
C	5.32316700	-1.17795900	-0.55169400
H	5.97607200	-1.83102200	0.04049300
H	5.28886600	-1.57991900	-1.56825300
H	5.80430800	-0.19598800	-0.59380600
C	3.75209900	-3.80373000	1.23627200
H	3.73261800	-3.45984200	2.27766800
H	3.38547600	-4.83985200	1.22791200
H	4.79912100	-3.82926100	0.90990900
C	1.42750300	-2.94106800	0.85562400
H	0.71976900	-2.53019900	0.12592500
H	1.10152800	-3.97427100	1.04155300
H	1.32705600	-2.40428100	1.81030700
C	2.86838400	-3.52789200	-1.10439600
H	2.27779000	-2.91869300	-1.79863600
H	3.88094700	-3.62395300	-1.51361400
H	2.42567000	-4.53396100	-1.08971400

TS₃₀-TP₂

C	-2.71359200	0.14406700	-0.52657500
C	-3.92066400	-1.22446200	0.66911300
C	-4.76560800	-0.72921700	-0.35236900
C	-4.42393300	-2.13688000	1.60281500
C	-6.09943300	-1.11529500	-0.47269800
C	-5.75744300	-2.53027900	1.48806800
H	-3.78610800	-2.53152000	2.38951700
C	-6.58298900	-2.02968800	0.46617500
H	-6.74119200	-0.72456100	-1.25723700
H	-6.16764700	-3.23953300	2.20175100
H	-7.61690100	-2.35742900	0.40526700
C	-4.37598900	0.81091200	-2.31658500
H	-4.93105200	1.73306800	-2.10504400
H	-3.48455000	1.05539500	-2.89754800
H	-5.01054000	0.14692900	-2.91208600
N	-2.66396400	-0.65400300	0.55391700
C	-1.61620000	0.94481700	-1.00771400
C	-0.30586100	0.54002900	-0.85955200
H	1.07229700	1.48760500	0.48807700
H	-1.85393800	1.90994500	-1.44548100
C	0.90933900	1.30233200	-0.95739800
H	-0.15793900	-0.49770000	-0.55568700
N	-3.97453800	0.13441100	-1.09880600
C	2.12774400	0.45778600	-1.45083600
C	2.00576200	0.19081100	-2.96550100
C	3.46882300	1.14607200	-1.14894200
H	1.93688300	1.13200300	-3.52174300
H	2.86990800	-0.35882400	-3.35355000
H	1.10051500	-0.39078500	-3.16852600
H	4.30408500	0.55433100	-1.54331300
H	3.53236600	2.13545000	-1.61205000
H	3.60691200	1.26333800	-0.07101100
C	0.76077400	2.67863200	-1.63476600
C	0.21056300	3.81313600	-0.74911700

H	0.10945500	2.58782000	-2.52193700
H	1.72795800	3.01505100	-2.02777500
C	-0.07431000	5.09879700	-1.53697800
H	-0.70573200	3.48744300	-0.24057000
H	0.93022700	4.02824600	0.04782100
C	-0.58667500	6.24497600	-0.65776000
H	0.84169300	5.41854300	-2.05535400
H	-0.80901400	4.88835700	-2.32837600
H	-0.78259000	7.14922200	-1.24623000
H	-1.51993900	5.96855700	-0.15080600
H	0.14402900	6.50434300	0.11836000
O	0.83834200	1.53622700	1.70671800
C	1.75973200	1.95918300	2.69440600
C	2.80718200	0.86001700	2.96130100
C	2.46725900	3.26211100	2.27496400
C	0.95762400	2.22051800	3.98547800
H	2.30969200	-0.07281000	3.25565500
H	3.38929300	0.65598000	2.05774900
H	3.50355100	1.14282400	3.76107200
H	1.73638400	4.06523000	2.13386700
H	3.18882500	3.58601200	3.03529100
H	3.00896300	3.12480400	1.33284400
H	1.59623300	2.58344200	4.80058100
H	0.17761100	2.96766600	3.79871800
H	0.47459100	1.29562300	4.33259600
Na	-0.85546600	0.20783400	1.72162500
O	2.06798100	-0.80171400	-0.74434000
Si	3.11926800	-2.15092700	-0.65477600
C	1.97774100	-3.56141100	0.03692800
C	4.57872500	-1.83555700	0.53523700
H	5.24414200	-1.05279200	0.15602700
H	4.23583400	-1.52715600	1.52786500
H	5.17779000	-2.74660500	0.65341600
C	3.85198200	-2.67833000	-2.33984900
H	4.40048000	-3.62106300	-2.22246300
H	3.07882500	-2.83273700	-3.09887800
H	4.56029900	-1.93718200	-2.72608300
C	2.81012600	-4.83598500	0.28700800
H	3.60147100	-4.67312700	1.02880500
H	2.16553000	-5.64078700	0.66886800
H	3.28163600	-5.20752500	-0.63119600
C	1.33361400	-3.11796100	1.36565700
H	0.71130900	-2.22715900	1.22154000
H	0.69054400	-3.91669300	1.76381100
H	2.08442600	-2.88475400	-2.13073300
C	0.86418000	-3.87454300	-0.98236200
H	0.25338300	-2.99064000	-1.19726400
H	1.27269900	-4.23962000	-1.93265900
H	0.19576200	-4.65590700	-0.59205100

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C	-3.44843600	0.84059700	-0.57919500
C	-4.85122100	-0.84631000	-0.47375300
C	-5.64013400	0.33343500	-0.46711100
C	-5.48455600	-2.09190100	-0.41725800
C	-7.02837000	0.30376100	-0.39893100
C	-6.88241200	-2.13044800	-0.35394100
H	-4.89848300	-3.00775700	-0.43638200
C	-7.64489500	-0.95502200	-0.34701000
H	-7.61937400	1.21579400	-0.38420000
H	-7.38670700	-3.09272500	-0.31175600
H	-8.72876700	-1.01551600	-0.29859500
C	-5.06387800	2.78147000	-0.70863000
H	-4.26771100	3.26834000	-1.27935400
H	-6.00185500	2.87222400	-1.26627100
H	-5.17820000	3.30211400	0.25207900
N	-3.50881000	-0.52054800	-0.51332100
C	-2.25763800	1.59495000	-0.61730300
C	-1.03491000	1.01540700	-1.09177700
H	1.21195300	-1.22391400	0.57202300
H	-2.27525800	2.62150200	-0.26482200
C	0.25711500	1.39686400	-0.83497100
H	-1.18497700	0.14226000	-1.73059500
N	-4.73314800	1.38512800	-0.54183600
C	1.45213900	0.75047700	-1.52413500
C	1.10610100	-0.47897200	-2.37825800
C	2.16183500	1.77237700	-2.43445400
H	0.44599600	-0.22059000	-3.21150100

H	2.02596400	-0.90190300	-2.79513600
H	0.62055400	-1.25514700	-1.78044500
H	3.07542000	1.36102100	-2.87942300
H	1.48378000	2.03918300	-3.25184500
H	2.41662200	2.69351000	-1.90694900
C	0.53475100	2.54727100	0.11938500
C	0.24527000	2.21927200	1.60015600
H	-0.06167900	3.43030900	-0.15953200
H	1.58089000	2.86522200	0.04583300
C	0.52298000	3.38583500	2.55669500
H	-0.81061500	1.92582200	1.69706800
H	0.84907800	1.34986000	1.89488200
C	0.22369200	3.05142300	4.02214300
H	1.57483600	3.69319300	2.45970700
H	-0.07554700	4.25557800	2.25034000
H	0.43515100	3.90128000	4.68158900
H	-0.83100300	2.78024200	4.15843300
H	0.83005800	2.20407600	4.36702700
O	0.45027200	-1.67048000	1.00497300
C	0.70561100	-3.07225300	1.27416800
C	1.91593400	-3.20636200	2.20560500
C	-0.56351700	-3.57782900	1.96877800
C	0.93470800	-3.82044000	-0.04551800
H	2.82707900	-2.85079100	1.71295200
H	1.76448000	-2.62127600	3.11867400
H	2.07702300	-4.25330200	2.48631400
H	-1.43652400	-3.48722400	1.30929100
H	-0.46483600	-4.63495100	2.23504700
H	-0.75327700	-3.01297800	2.88912800
H	1.09721900	-4.88902100	0.13511900
H	0.06810200	-3.71210400	-0.70701000
H	1.81524500	-3.43024000	-0.56691200
O	2.35474700	0.24270200	-0.46070200
Si	4.00380500	0.54558100	-0.04071300
C	4.59355100	2.34687800	-0.28641100
H	5.54153400	2.47671100	0.24970000
H	4.76052000	2.62129300	-1.33133400
H	3.87924900	3.05799800	0.14159000
C	4.02553600	0.22276800	1.83776400
H	5.01697100	0.41823400	2.26162000
H	3.31311900	0.89209400	2.33297700
H	3.74784400	-0.80327300	2.09618600
C	5.23243300	-0.66873100	-0.94738100
C	6.64001200	-0.48378500	-0.33753700
H	6.66113900	-0.71391000	0.73445500
H	7.35372000	-1.15997800	-0.82965900
H	7.01708500	0.53747900	-0.47062000
C	5.31364400	-0.38108400	-2.45946100
H	6.05065600	-1.04696900	-2.93141900
H	4.35505500	-0.55158800	-2.96237000
H	5.62642500	0.64910300	-2.66930000
C	4.78899200	-2.12992900	-0.74362600
H	5.48895800	-2.81592000	-1.24226200
H	4.76487000	-2.40647800	0.31772300
H	3.79310100	-2.31095700	-1.16450100
Na	-1.53823700	-0.70383800	0.65510500

TS_{31-P3'}

C	-3.42022400	0.74710500	-0.42132900
C	-4.75745600	-0.91863400	0.04167900
C	-5.57988900	0.22035400	-0.13633300
C	-5.34214100	-2.15133500	0.35132800
C	-6.96627000	0.16822600	-0.01267400
C	-6.73161000	-2.21272300	0.47364500
H	-4.72583600	-3.03691100	0.48274000
C	-7.53274400	-1.07319900	0.29305500
H	-7.58738800	1.04982500	-0.14417200
H	-7.20431000	-3.16184400	0.71161700
H	-8.61127700	-1.15484000	0.39446700
C	-5.09582400	2.60830400	-0.80244300
H	-4.31739000	3.04421800	-1.43268400
H	-6.02947000	2.57665800	-1.37257900
H	-5.24306200	3.24725900	0.07755400
N	-3.42826400	-0.56728600	-0.11516700
C	-2.24143200	1.52606100	-0.64427600
C	-1.06353900	0.95519700	-1.14191700
H	1.30950700	-1.33740900	0.15378300
H	-2.28262200	2.58389600	-0.40604900

C	0.21430000	1.52065200	-1.25076800
H	-1.18939900	-0.05727700	-1.52587400
N	-4.70904700	1.26163600	-0.43490500
C	1.28536200	0.78691400	-1.87370600
C	0.95856500	-0.47118600	-2.66241700
C	2.38607700	1.56907900	-2.56560400
H	0.40378200	-0.20851200	-3.57289200
H	1.88237000	-0.97394600	-2.95591900
H	0.36371300	-1.18474700	-2.09253100
H	3.21887200	0.91619300	-2.83450300
H	1.97556200	1.98922600	-3.49542100
H	2.77431300	2.39747200	-1.97711300
C	0.41494200	2.91327200	-0.67142300
C	0.41289600	2.96851800	0.87260100
H	-0.38050000	3.58076700	-1.03959800
H	1.34738400	3.36122200	-1.02578900
C	0.58909900	4.38593600	1.43262500
H	-0.52969400	2.54885400	1.25070200
H	1.21310600	2.32138700	1.25354500
C	0.57152700	4.43741700	2.96419400
H	1.53607700	4.80688700	1.06465700
H	-0.20467900	5.03503000	1.03486900
H	0.70424500	5.46077100	3.33426500
H	-0.37910300	4.06066400	3.36295600
H	1.37482700	3.82312500	3.38962200
O	0.54966000	-1.87446200	0.55703400
C	0.75554500	-3.30108700	0.56741500
C	1.76133100	-3.67219500	1.66729500
C	-0.61420600	-3.91648400	0.88518000
C	1.24347100	-3.77314900	-0.80917900
H	2.74427000	-3.24071400	1.46053000
H	1.41835200	-3.29593400	2.63753100
H	1.87885900	-4.75978700	1.74173900
H	-1.35163700	-3.64833600	0.11833000
H	-0.55466800	-5.00928200	0.92462600
H	-0.97714500	-3.57202000	1.86313500
H	1.43972800	-4.85137100	-0.80528100
H	0.49243800	-3.56400100	-1.57854200
H	2.16758300	-3.25751900	-1.08862400
O	2.27592400	-0.12884300	-0.51400800
Si	3.66333800	0.31143000	0.35517000
C	4.15772600	2.16543800	0.24266800
H	4.86069100	2.39392400	1.05280200
H	4.64955900	2.43015700	-0.69904100
H	3.29422200	2.82580000	0.36920800
C	3.33198000	0.00403600	2.22021900
H	4.23664500	0.16396700	2.81947800
H	2.56975500	0.70446500	2.58368700
H	2.96918600	-1.00878300	2.42115400
C	5.24460600	-0.71337300	-0.19279800
C	6.49543400	-0.15937700	0.52041200
H	6.40392200	-0.20720600	1.61288000
H	7.38327100	-0.74750800	0.24320600
H	6.69750000	0.88289400	0.24766900
C	5.44839500	-0.60083200	-1.71539700
H	6.34560200	-1.15644000	-2.02775900
H	4.59468200	-1.01532300	-2.26440700
H	5.58312400	0.43979700	-2.03655400
C	5.09172500	-2.20063400	0.17225400
H	5.98179900	-2.76884200	-0.13791900
H	4.97299100	-2.34684800	1.25305100
H	4.22683100	-2.65139300	-0.32777300
Na	-1.31660800	-0.77231900	0.78993700

TBSONa

O	1.65180700	-0.06796600	-0.01602200
Si	0.18711200	0.67322600	-0.00103400
C	-0.03519500	1.79569200	1.54397400
H	-1.00921500	2.30048800	1.55307300
H	0.05392200	1.22575100	2.47674300
H	0.73793600	2.57438100	1.55987500
C	-0.05561000	1.81608200	-1.52765700
H	-1.02997600	2.32017600	-1.51760800
H	0.71687500	2.59539300	-1.54296800
H	0.02219900	1.25859900	-2.46887600
C	-1.25435500	-0.65512400	0.00009100
C	-2.64194400	0.01197300	0.01384400
H	-2.79959300	0.64714800	-0.86692800

H	-3.44005700	-0.74738100	0.01484000
H	-2.78717200	0.63638900	0.90441600
C	-1.11436200	-1.55171400	1.24501900
H	-1.87892500	-2.34471800	1.24740400
H	-0.12940800	-2.03461700	1.27604300
H	-1.23340100	-0.98022700	2.17441700
C	-1.13087800	-1.53535500	-1.25819100
H	-1.89575100	-2.32806800	-1.26111700
H	-1.26176500	-0.95157700	-2.17828100
H	-0.14655700	-2.01782700	-1.30846000
Na	3.42190200	-0.93860600	-0.00203700

TP2

C	2.38495700	-0.02442600	0.10021400
C	3.30020300	-1.94426300	-0.21916700
C	4.33397800	-1.09113900	0.24090300
C	3.58735700	-3.28363600	-0.51839200
C	5.64750200	-1.53202600	0.41762600
C	4.89452300	-3.72901700	-0.34837000
H	2.80078500	-3.94351400	-0.87158500
C	5.91006400	-2.86659800	0.11273100
H	6.43393600	-0.87592200	0.78027500
H	5.14178500	-4.76301900	-0.57313500
H	6.91895200	-3.25051000	0.23677700
C	4.39908400	1.33528800	0.90561100
H	4.41567500	1.38575800	2.00156700
H	5.42967800	1.33754100	0.53977600
H	3.90284400	2.22594100	0.51584300
N	2.10794400	-1.25527000	-0.29221800
C	1.41585900	1.06225300	0.19841700
C	0.16564700	0.94658200	-0.28089400
H	-1.37390400	2.04027500	-1.20580200
H	1.74250600	1.97086600	0.69579700
C	-0.95829000	1.95139400	-0.18935100
H	-0.09368700	0.01037900	-0.76398600
N	3.72819000	0.14027500	0.42997000
C	-2.14741800	1.33651300	0.64907000
C	-1.75272300	1.15510200	2.12264100
C	-3.40709100	2.21025400	0.53306900
H	-1.49950100	2.11617400	2.58474600
H	-2.57963800	0.72047200	2.69248300
H	-0.88777900	0.49127500	2.20790900
H	-4.24513500	1.73399900	1.05413000
H	-3.26968800	3.19570400	0.98818400
H	-3.68967400	2.34806400	-0.51628500
C	-0.51786600	3.35882000	0.26250200
C	0.26359900	4.13197200	-0.81284900
H	0.08430600	3.29038900	1.17861500
H	-1.39789300	3.95375300	0.53212600
C	0.74293000	5.51086500	-0.34001800
H	1.12586000	3.54062900	-1.14707200
H	-0.37743800	4.25670400	-1.69792900
C	1.50157900	6.28788400	-1.42143500
H	-0.12127500	6.10108100	-0.00300400
H	1.38744300	5.38860500	0.54282700
H	1.83525800	7.26504800	-1.05379400
H	2.38880500	5.73648800	-1.75674300
H	0.86980200	6.46073000	-2.30135500
O	-2.37922700	0.05902200	0.04429700
Si	-3.65225900	-1.08967100	0.13042500
C	-4.27031400	-1.37570600	1.91556500
H	-5.03865300	-2.15823000	1.92212900
H	-3.46233400	-1.69603800	2.58158200
H	-4.72281900	-0.47406200	2.34344100
C	-5.12991200	-0.52738200	-0.94155100
H	-5.64678200	0.33524900	-0.50772600
H	-4.80454300	-0.24943600	-1.94984600
H	-5.86425500	-1.33602900	-1.03864700
C	-2.86237700	-2.70089400	-0.59470800
C	-3.89129900	-3.84984600	-0.53610200
H	-4.80318000	-3.62194800	-1.10271400
H	-3.45961800	-4.76304400	-0.96995000
H	-4.18475300	-4.08811400	0.49379900
C	-1.61402000	-3.09814700	0.22006800
H	-1.19838700	-4.03938400	-0.16821400
H	-0.82369600	-2.34275700	0.16123700
H	-1.85135600	-3.26201800	1.27921300
C	-2.45256600	-2.46517400	-2.06297000

H	-1.97515200	-3.36736300	-2.47159400
H	-3.31753700	-2.23647400	-2.69823200
H	-1.73688300	-1.64111800	-2.15508500

P3

C	-1.24091500	-0.02823900	-0.19172100
C	-3.22518500	-0.75231100	0.21441800
C	-3.37026400	0.61999200	-0.11292600
C	-4.35907700	-1.51359200	0.53387900
C	-4.61378100	1.25567000	-0.13956200
C	-5.59998200	-0.88528800	0.51314400
H	-4.25548100	-2.56431400	0.78721400
C	-5.72611000	0.47922300	0.18104600
H	-4.72203000	2.30433000	-0.40245100
H	-6.49328100	-1.45446600	0.75572300
H	-6.71203100	0.93580900	0.17107100
C	-1.72737700	2.41773500	-0.75905600
H	-1.68366000	2.52259800	-1.85032400
H	-2.47524000	3.11357800	-0.37047800
H	-0.75963100	2.69632100	-0.33594600
N	-1.89987900	-1.12187700	0.15660400
C	0.19453700	0.05542500	-0.39090100
C	1.00629700	-1.01225800	-0.19784000
H	0.59393900	1.01269500	-0.70869300
C	2.45562100	-1.05600000	-0.35699300
H	0.50217500	-1.91661000	0.12510200
N	-2.08342400	1.06989300	-0.35803000
C	3.15584100	-2.20030000	-0.10609400
C	2.54001200	-3.52473300	0.28420800
C	4.66292900	-2.28617800	-0.18192400
H	1.45859000	-3.57890800	0.15980700
H	2.98234600	-4.33061300	-0.31722300
H	2.77049300	-3.76278100	1.33273800
H	5.05448700	-2.79281500	0.71073800
H	4.97441400	-2.89923500	-1.04085700
H	5.16442200	-1.32056500	-0.25836100
C	3.14981900	0.23473900	-0.77052700
C	3.48199900	1.16791200	0.41170000
H	2.51132500	0.77313600	-1.48217100
H	4.06881000	0.01774000	-1.32393600
C	4.11125700	2.49670100	-0.02625600
H	2.56799900	1.36433600	0.98833400
H	4.16469700	0.64777300	1.09831200
C	4.45409000	3.41820500	1.14932100
H	5.02096700	2.29330700	-0.60951600
H	3.42424100	3.01580600	-0.71050600
H	4.90000200	4.35827100	0.80457200
H	3.55875900	3.66745500	1.73219100
H	5.16854700	2.94082700	1.83115300

Cartesian coordinates for the stationary points given in Fig. S1.

Z14

C	1.08175900	1.15886700	-0.53087400
C	1.72769600	2.23173200	-2.47546000
C	1.41840200	3.19566600	-1.57187600
N	1.02690400	2.54042900	-0.39280400
N	1.52381700	0.99666800	-1.83801200
C	0.73132300	3.25589800	0.83313000
C	-0.59388000	3.67650100	1.09058100
C	1.79975100	3.55701800	1.70884500
C	-0.82599900	4.41375000	2.26296400
C	1.51063300	4.29423300	2.86830200
C	0.21192300	4.71956600	3.14434400
H	-1.83111400	4.74977600	2.48907100
H	2.31227400	4.53773400	3.55801300
H	0.00743400	5.29046900	4.04490600
C	1.87764600	-0.26605100	-2.45476700
C	3.20383700	-0.73471300	-2.30505400
C	0.91695700	-0.95842400	-3.22900000
C	3.55461700	-1.93018500	-2.95260100
C	1.32328200	-2.14694900	-3.85751500

C	2.62606000	-2.62956700	-3.72313200
H	4.56566500	-2.31134200	-2.85389200
H	0.61049000	-2.69994300	-4.45767400
H	2.91647300	-3.55040200	-4.21917900
C	3.24298400	3.13804800	1.42647800
H	3.24549000	2.51555000	0.52683200
C	4.13519600	4.37036800	1.14306900
H	3.75140400	4.95383600	0.29835800
H	4.18262100	5.03368600	2.01492200
H	5.15777300	4.05450400	0.90414100
C	3.83116600	2.28143600	2.57031300
H	3.88028600	2.84279800	3.51082900
H	3.22457200	1.38574600	2.73678100
H	4.85020600	1.96391500	2.31844900
C	4.25782500	0.01244800	-1.48716100
H	3.79453600	0.91634800	-1.08073100
C	4.74495400	-0.82805200	-0.28430700
H	5.47594600	-0.25988300	0.30378200
H	3.90838000	-1.09200700	0.37126700
H	5.22820300	-1.75585500	-0.61325700
C	5.44681900	0.45998200	-2.36975500
H	5.97798800	-0.40129900	-2.79193700
H	5.11063800	1.08839200	-3.20238400
H	6.16488100	1.03616500	-1.77421200
C	-0.50503800	-0.43218200	-3.42483100
H	-0.75158200	0.21062400	-2.57291400
C	-1.56183000	-1.55650700	-3.46738200
H	-1.48846500	-2.15113300	-4.38615400
H	-1.45897400	-2.23493100	-2.61295900
H	-2.56056900	-1.11342500	-3.42808800
C	-0.60619800	0.43484700	-4.70533200
H	0.08311000	1.28538600	-4.67467700
H	-0.37179100	-0.16099500	-5.59634900
H	-1.62399300	0.82687400	-4.81119600
C	-1.74193900	3.38633200	0.12383000
H	-1.47508100	2.50131500	-0.46341200
C	-3.06988700	3.06976600	0.84354800
H	-2.94110200	2.27470000	1.58614500
H	-3.47919300	3.95046000	1.35318600
H	-3.80928400	2.73379600	0.11091100
C	-1.94578900	4.56139300	-0.86595700
H	-2.21719100	5.47875300	-0.32869100
H	-1.03931800	4.76416000	-1.44632000
H	-2.75206500	4.32339100	-1.56902200
Ni	0.65191700	-0.16067200	0.79852200
C	-5.25872900	-0.66313600	-0.23589200
C	-4.97403000	0.17019500	-1.34681200
C	-6.02117200	0.62994900	-2.15606400
C	-7.31854900	0.24449000	-1.83162900
C	-7.58326900	-0.58508400	-0.72247000
C	-6.55839000	-1.05434500	0.09617800
C	-3.09607000	-0.27125000	-0.42856200
H	-5.81325300	1.26835800	-3.00969700
H	-8.14820100	0.58795500	-2.44357700
H	-8.60970900	-0.86449700	-0.50105900
H	-6.76664800	-1.69325000	0.94969100
H	-2.04122400	-0.31719800	-0.17430800
N	-3.60598400	0.39683300	-1.43732800
N	-4.02646100	-0.93186300	0.33662100
C	-3.75969300	-1.74778800	1.50655900
H	-4.25862600	-1.33241900	2.38961700
H	-4.11349400	-2.77294500	1.35074400
H	-2.68181300	-1.77051600	1.68433900
H	1.44482900	4.26861100	-1.64476100
H	2.07727600	2.29781600	-3.49064200
C	0.23036200	-1.40408500	2.17242100
C	0.23045000	-0.09858200	2.67002000
C	0.11522600	-2.72241500	2.36844200
C	-0.18314400	-3.35544200	3.75305300
C	-1.58745200	-4.00874000	3.74501300
H	-1.69698700	-4.74458100	2.94079500
H	-1.77553900	-4.52753500	4.69413800
H	-2.37000500	-3.25153300	3.62017900
C	-0.15011900	-2.31668200	4.88787000
H	0.83242400	-1.83943700	4.96435200
H	-0.89183000	-1.52670000	4.73594900
H	-0.36615800	-2.80437300	5.84694400
C	0.86214600	-4.44819500	4.08229300
H	0.64920100	-4.89114500	5.06381900
H	0.85706000	-5.26084500	3.34829400

H	1.87343700	-4.02703800	4.11550000
C	0.29216200	-3.67481900	1.18449100
H	-0.21680800	-4.62795500	1.38190300
H	-0.20112600	-3.24485300	0.30254500
C	1.75706400	-3.97464300	0.80609700
H	2.30014300	-4.35179200	1.68252800
H	2.24439200	-3.03165900	0.52443500
C	1.88524600	-4.98593300	-0.34104300
H	1.35906500	-5.91258500	-0.06805500
H	1.37286800	-4.59293900	-1.23058200
C	3.33938700	-5.31533700	-0.69527300
H	3.87167800	-5.73636400	0.16699200
H	3.39946300	-6.04483200	-1.51202900
H	3.87948300	-4.41478400	-1.01135400
H	-0.70396300	0.43976000	2.85740100
H	1.08161600	0.29618100	3.23284200

ZTS₁₄₋₁₅

C	-1.17338700	1.05477900	0.28702200
C	-2.70914300	2.21765200	1.56411900
C	-2.10106300	3.11948400	0.75720400
N	-1.16010000	2.41056200	-0.01081800
N	-2.15297700	0.96173400	1.26768400
C	-0.31673000	3.07290100	-0.98345300
C	0.76766700	3.85673500	-0.52073000
C	-0.65006000	2.98678000	-2.35559300
C	1.53130800	4.54440200	-1.47830900
C	0.14981800	3.69197000	-3.26949500
C	1.23069000	4.46195900	-2.83853400
H	2.36764100	5.15246300	-1.15221400
H	-0.08543600	3.64682500	-4.32733500
H	1.83265200	5.00470000	-3.56094600
C	-2.64601300	-0.25685100	1.88140700
C	-3.89931400	-0.75999100	1.45620400
C	-1.89721300	-0.87026400	2.91413300
C	-4.39287700	-1.91136500	2.09090500
C	-2.43570400	-2.02540100	3.50465500
C	-3.66767700	-2.54168300	3.10091800
H	-5.35135400	-2.31808700	1.78687500
H	-1.88376400	-2.52465000	4.29135900
H	-4.06262900	-3.43415900	3.57652600
C	-1.87909500	2.22676200	-2.85737300
H	-2.23904600	1.59054500	-2.04400000
C	-3.01592300	3.21429600	-3.21984200
H	-3.29058700	3.83706600	-2.36092600
H	-2.71177100	3.88116700	-4.03579800
H	-3.90896200	2.66663900	-3.54429900
C	-1.55907800	1.29879800	-4.04962500
H	-1.24734900	1.86394000	-4.93582500
H	-0.76161700	0.59215700	-3.79674500
H	-2.45005000	0.72235400	-4.32523300
C	-4.74153200	-0.08318200	0.37002500
H	-4.11054200	0.65256300	-0.13964900
C	-5.24549900	-1.07335300	-0.70509900
H	-5.77702200	-0.52648800	-1.49307100
H	-4.41836700	-1.62027000	-1.16657600
H	-5.94533200	-1.80540700	-0.28595500
C	-5.94279500	0.67228100	0.99230900
H	-6.61426300	-0.02496100	1.50777400
H	-5.61825600	1.42207800	1.72170700
H	-6.51915800	1.18389500	0.21221500
C	-0.58006700	-0.27994300	3.42189400
H	-0.05411200	0.16950900	2.57410600
C	0.38055700	-1.33376600	4.00590000
H	0.01739900	-1.74410500	4.95703800
H	0.54079400	-2.15649100	3.30267400
H	1.35371000	-0.86891200	4.18777500
C	-0.85237200	0.83119000	4.46890200
H	-1.46879700	1.63800900	4.05751900
H	-1.37061900	0.42044100	5.34481200
H	0.09477500	1.26778500	4.80719600
C	1.09166400	4.02211400	0.96604000
H	0.56238400	3.23727600	1.51622400
C	2.59602600	3.86254900	1.27515900
H	2.98773200	2.91480700	0.90014100
H	3.18831300	4.67628900	0.83940700
H	2.75471400	3.88717800	2.35924000
C	0.59283300	5.39435800	1.48716100

H	1.10770200	6.21410600	0.97128500
H	-0.48340000	5.52744800	1.33404100
H	0.79695800	5.48843600	2.56013000
Ni	-0.14338300	-0.38238900	-0.42201100
C	3.87936900	0.60375300	-0.07309400
C	3.55252100	0.18594500	1.24237200
C	4.53211200	0.22927900	2.24413200
C	5.80433100	0.68585700	1.90594700
C	6.11067000	1.09940100	0.59430600
C	5.15140500	1.06818000	-0.41821100
C	1.73241000	-0.04358700	0.07566100
H	4.29502200	-0.08988300	3.25527000
H	6.57927900	0.72522000	2.66716700
H	7.11384900	1.45010000	0.36639200
H	5.39026200	1.39153300	-1.42791200
H	1.05513500	-1.23062400	-0.59992800
N	2.23028900	-0.21864600	1.29619200
N	2.71476600	0.43984200	-0.79810700
C	2.55162000	0.72885500	-2.20754100
H	2.61604200	1.80496000	-2.40416200
H	3.31867100	0.21141800	-2.79660000
H	1.56651300	0.37684600	-2.52099600
H	-2.23776600	4.18059000	0.65166400
H	-3.47491200	2.33750400	2.30938200
C	-0.25277100	-2.13611000	-1.36340100
C	-1.51059300	-1.52241200	-1.27884300
C	0.42911700	-3.22878200	-1.73156600
C	-0.33794000	-4.40102300	-2.42072900
C	0.60776700	-5.50151300	-2.94827000
H	1.21216600	-5.95155600	-2.15390400
H	0.01182000	-6.30365300	-3.39989800
H	1.28637500	-5.12348800	-3.72159000
C	-1.14827300	-3.87816100	-3.62740000
H	-1.88270100	-3.12768700	-3.32415400
H	-0.48752700	-3.42319800	-4.37525700
H	-1.68709100	-4.70369100	-4.11026800
C	-1.30550300	-5.04609300	-1.40106200
H	-1.87063400	-5.86268200	-1.86970600
H	-0.76058000	-5.46030200	-0.54524100
H	-2.02213200	-4.31228000	-1.02006200
C	1.90955300	-3.38831300	-1.41709100
H	2.41795100	-3.93716300	-2.21759400
H	2.38410400	-2.40049300	-1.38680600
C	2.19049500	-4.08873800	-0.06988300
H	1.72059700	-5.08255400	-0.05869600
H	1.71171000	-3.50904900	0.73025500
C	3.68869900	-4.22990200	0.22872500
H	4.17200600	-4.79223400	-0.58381200
H	4.14967500	-3.23260300	0.23191500
C	3.96949400	-4.92230000	1.56673100
H	3.54585500	-5.93450300	1.58759600
H	5.04617400	-5.00740800	1.75459600
H	3.52944800	-4.36023500	2.39931100
H	-1.94490800	-1.03450100	-2.15292900
H	-2.24073500	-1.89435000	-0.56060200

Z₁₅

C	-1.33193600	0.64411100	-0.22012300
C	-3.37519000	1.59066100	0.30351200
C	-2.65490600	2.53814200	-0.33831700
N	-1.40807600	1.96514800	-0.64476800
N	-2.57427800	0.43732000	0.37048800
C	-0.37912300	2.74881700	-1.29903800
C	0.31757600	3.71797900	-0.53731500
C	-0.18261000	2.60370300	-2.69266900
C	1.24827100	4.52834800	-1.20898200
C	0.76886000	3.43168800	-3.30948400
C	1.47947100	4.38363400	-2.57690700
H	1.79388400	5.28181700	-0.65175500
H	0.94162300	3.34243700	-4.37607400
H	2.20454800	5.02003600	-3.07480500
C	-3.08908100	-0.78007200	0.97608600
C	-3.95488100	-1.60043600	0.21122800
C	-2.79968200	-1.04938500	2.33617200
C	-4.49740500	-2.73717300	0.83262500
C	-3.37207800	-2.20044000	2.90301500
C	-4.20461700	-3.03882400	2.16193300
H	-5.15906000	-3.38714500	0.27132200

H	-3.16229500	-2.44230600	3.93763600
H	-4.63241000	-3.92323600	2.62404200
C	-1.03543900	1.65677900	-3.53816000
H	-1.45074500	0.89585400	-2.87170200
C	-2.22084800	2.42491000	-4.17562200
H	-2.84505200	2.90152300	-3.41180300
H	-1.85800000	3.20744600	-4.85315200
H	-2.85332300	1.74035300	-4.75376200
C	-0.22778000	0.91590200	-4.62490900
H	0.14015600	1.59762100	-5.40068400
H	0.63385200	0.39457800	-4.19486800
H	-0.86372900	0.17304300	-5.12011100
C	-4.37114300	-1.25536800	-1.22246600
H	-3.63550900	-0.55103500	-1.62568500
C	-4.40689300	-2.48189100	-2.16253600
H	-4.59304100	-2.15318800	-3.19179600
H	-3.46431300	-3.03549200	-2.14755900
H	-5.21336600	-3.17339500	-1.89273500
C	-5.75822700	-0.56160700	-1.24013800
H	-6.52762900	-1.23377600	-0.84153500
H	-5.76792800	0.35314300	-0.63982300
H	-6.03806200	-0.29558500	-2.26663400
C	-1.95321900	-0.10603400	3.19510600
H	-1.18632700	0.34271800	2.55634700
C	-1.19324700	-0.82243600	4.32898600
H	-1.86862900	-1.19172500	5.11143100
H	-0.60024200	-1.65575800	3.94472900
H	-0.50036700	-0.11532400	4.79603700
C	-2.83114800	1.02484700	3.79233700
H	-3.32337400	1.61987800	3.01635700
H	-3.60828800	0.60768900	4.44544800
H	-2.21139200	1.70164800	4.39261300
C	0.04690100	3.95180300	0.95147800
H	-0.51353600	3.09201600	1.33281200
C	1.33797500	4.06002000	1.79113600
H	1.97711800	3.18424600	1.66350300
H	1.91845800	4.95413800	1.53267000
H	1.08085800	4.13419800	2.85380200
C	-0.81825100	5.22191100	1.15782000
H	-0.28518800	6.11382100	0.80636000
H	-1.76958900	5.16737700	0.61801000
H	-1.04029900	5.35853700	2.22264200
N	0.10075200	-0.60095200	-0.47865200
C	3.28299700	0.93761400	1.67272300
C	2.46059200	0.36392500	2.67259300
C	2.89060300	0.36980300	4.00546200
C	4.12502100	0.94796200	4.30264100
C	4.92780600	1.51726900	3.29663200
C	4.51787000	1.52281600	1.96142700
C	1.37850300	0.10207100	0.78738200
H	2.27314100	-0.07239700	4.78279700
H	4.47733400	0.95948500	5.33115400
H	5.88538400	1.95805100	3.56202500
H	5.14129400	1.96165500	1.18639300
H	0.97005900	-1.51783000	-2.75843700
N	1.29972200	-0.12999300	2.09682500
N	2.57735400	0.76991800	0.49278800
C	3.02530000	1.25475900	-0.79359100
H	3.19065000	2.33786900	-0.76655400
H	3.95944300	0.76679800	-1.09904400
H	2.25267000	1.04428100	-1.53461500
H	-2.89202000	3.55268300	-0.60239900
H	-4.36541300	1.61527000	0.72081300
C	0.49809900	-1.99804400	-1.89787500
C	-0.90021200	-1.81912500	-1.79785100
C	1.38214000	-2.38748800	-0.87208100
C	1.06306000	-3.48188400	0.20175600
C	2.25428400	-3.67565200	1.16905100
H	2.46377600	-2.75394400	1.72117400
H	1.99963400	-4.45192700	1.90017900
H	3.16949300	-3.99771000	0.66366800
C	0.78205300	-4.82013200	-0.52977500
H	-0.08552200	-4.73061100	-1.19267400
H	1.63317800	-5.14735000	-1.13495200
H	0.56850400	-5.60974600	0.20234900
C	-0.15351300	-3.16643800	1.10216200
H	-0.22955900	-3.94027000	1.87755400
H	-0.02910400	-2.20305300	1.60384900
H	-1.10367000	-3.17032500	0.56547200
C	2.85686400	-2.15626600	-1.21746600

H	2.92162000	-1.24088600	-1.81423800
H	3.43531100	-1.95856900	-0.30937300
C	3.54973900	-3.27154100	-2.03039200
H	2.95355400	-3.48858900	-2.92898700
H	3.58858300	-4.20576800	-1.45694200
C	4.97715000	-2.88913500	-2.44788200
H	4.94695600	-1.95820100	-3.03273800
H	5.56819600	-2.66402600	-1.54872400
C	5.68109900	-3.98009300	-3.26188500
H	5.13071800	-4.20422000	-4.18425500
H	6.69599400	-3.67717000	-3.54469400
H	5.75949900	-4.91276900	-2.68965600
H	-1.41194800	-1.40514800	-2.66265100
H	-1.51551200	-2.46186600	-1.17962800

ZTS₁₅₋₁₆

C	1.13601200	-0.91073500	0.15636200
C	2.76068000	-1.69590700	1.57169200
C	2.05562800	-2.76935300	1.13437900
N	1.05313400	-2.28460200	0.27805200
N	2.19638300	-0.56130100	0.97049500
C	0.13676700	-3.16535600	-0.42283900
C	-0.98963700	-3.67638900	0.26690100
C	0.44359200	-3.53919600	-1.75210900
C	-1.82715300	-4.56275100	-0.42994700
C	-0.43262800	-4.42522500	-2.40009300
C	-1.55806700	-4.92964500	-1.74950300
H	-2.70001200	-4.96768300	0.06805300
H	-0.22249100	-4.72897800	-3.41984600
H	-2.22135600	-5.61613200	-2.26653200
C	2.76696300	0.76757400	1.11990800
C	3.84892900	1.12481400	0.28087800
C	2.27509700	1.62236000	2.13320700
C	4.42841400	2.38915800	0.46964400
C	2.89462900	2.87475600	2.27534100
C	3.95529700	3.25698200	1.45342500
H	5.25798400	2.69368800	-0.15898600
H	2.53960900	3.55811300	3.03737900
H	4.41524500	4.23179300	1.58202600
C	1.71169900	-3.07744200	-2.47309300
H	2.17908500	-2.28936700	-1.87484900
C	2.72719300	-4.24189700	-2.58289500
H	2.98231700	-4.64416200	-1.59581700
H	2.32027000	-5.06270800	-3.18543600
H	3.65147800	-3.89696400	-3.06130200
C	1.41858300	-2.47273000	-3.86391600
H	0.98139200	-3.21184900	-4.54529800
H	0.73302400	-1.62316300	-3.78699700
H	2.34937900	-2.11410800	-4.31844500
C	4.43353300	0.17599800	-0.76828800
H	3.74762800	-0.66995200	-0.88456000
C	4.57553200	0.83701600	-2.15763900
H	4.94001600	0.10107200	-2.88439300
H	3.61600900	1.22366500	-2.51205100
H	5.29389300	1.66480300	-2.14045500
C	5.79558700	-0.39056600	-0.29519900
H	6.52935200	0.41435500	-0.16893800
H	5.70422900	-0.91373300	0.66345400
H	6.19233500	-1.09770300	-1.03339900
C	1.15893000	1.19663300	3.08765700
H	0.54192000	0.44989100	2.57993100
C	0.20490300	2.35122000	3.45425800
H	0.69403900	3.11733000	4.06876900
H	-0.20141800	2.82226300	2.55518500
H	-0.63724400	1.95460600	4.03178400
C	1.75578000	0.56112800	4.36904700
H	2.37394100	-0.31453200	4.13991500
H	2.38119200	1.28348600	4.90850600
H	0.95130900	0.23943700	5.04121700
C	-1.28510000	-3.33710400	1.73028200
H	-0.81357700	-2.37365500	1.95286000
C	-2.79424100	-3.18691800	2.02390300
H	-3.28092500	-2.50729400	1.32072900
H	-3.31143800	-4.15388100	1.98874300
H	-2.93363000	-2.77898200	3.03063200
C	-0.68640900	-4.40769100	2.67957200
H	-1.13390300	-5.38925200	2.48079800
H	0.39798200	-4.50378300	2.56907600

H	-0.89616900	-4.14412100	3.72284500
Ni	0.30888100	0.27863800	-1.00770800
C	-3.50472600	-0.11214900	0.09543500
C	-2.91500700	0.36378400	1.29170200
C	-3.72727700	0.67820600	2.38779100
C	-5.10423700	0.50525500	2.25906100
C	-5.67481800	0.02710600	1.06339500
C	-4.88358300	-0.29138000	-0.04190400
C	-1.28242400	0.03130000	-0.08872800
H	-3.28628300	1.04800500	3.30918600
H	-5.75462400	0.74447500	3.09628500
H	-6.75255500	-0.09621300	0.99877900
H	-5.32658800	-0.66102000	-0.96260000
H	-1.24351300	1.52046000	-3.49020700
N	-1.53548200	0.41853400	1.14681700
N	-2.44432300	-0.32914000	-0.76975700
C	-2.56226200	-0.85486200	-2.11551100
H	-2.94767200	-1.88113200	-2.09779900
H	-3.23250300	-0.22940700	-2.71561300
H	-1.57506500	-0.85806600	-2.57977100
H	2.17009500	-3.81943600	1.33292700
H	3.60394900	-1.62310400	2.23502900
C	-0.54806700	2.16573400	-2.94469700
C	0.71643500	1.46106400	-2.60431900
C	-1.03312300	3.41311000	-2.70305500
C	-0.22835100	4.54259500	-2.01032600
C	-1.01896800	5.86626600	-1.89126000
H	-1.94680000	5.75014600	-1.32228000
H	-0.40445900	6.60859200	-1.36679600
H	-1.27016100	6.28764800	-2.87103200
C	1.03785800	4.87264200	-2.84189300
H	1.69158400	4.00643800	-2.96455700
H	0.75788000	5.22039100	-3.84350800
H	1.61843700	5.67012800	-2.35823700
C	0.17389600	4.12807700	-0.57530300
H	0.78050800	4.91205700	-0.10140900
H	-0.71764300	3.96973200	0.04305400
H	0.75154600	3.20080800	-0.55811200
C	-2.45880500	3.68892500	-3.17157400
H	-2.55563400	4.70368300	-3.57843800
H	-2.69116600	3.01422600	-4.00763800
C	-3.55020600	3.48752800	-2.09646600
H	-3.35168400	4.13241200	-1.22971900
H	-3.48891500	2.45740200	-1.71957700
C	-4.96866500	3.76349400	-2.61380700
H	-5.01822100	4.78831700	-3.01006500
H	-5.17828200	3.10062200	-3.46665100
C	-6.04996400	3.57709300	-1.54333700
H	-5.89636700	4.26725700	-0.70441200
H	-7.05268000	3.76239800	-1.94759700
H	-6.03246600	2.55957800	-1.13465900
H	1.04530200	0.84636800	-3.45356900
H	1.53448300	2.13001200	-2.32361300

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C	-1.89212200	0.52488400	0.41702000
C	-3.96147200	0.27382000	1.39864400
C	-4.08783400	1.23055600	0.44203200
N	-2.82576500	1.37626300	-0.14893300
N	-2.62413400	-0.15171900	1.37455500
C	-2.54349600	2.31725700	-1.21534300
C	-2.76855300	1.91971600	-2.55265900
C	-2.08581100	3.61215200	-0.87464100
C	-2.50179500	2.86030100	-3.56099400
C	-1.83651600	4.51128400	-1.92298200
C	-2.03701000	4.13875100	-3.25305700
H	-2.66030500	2.58437800	-4.59748500
H	-1.48484400	5.51163200	-1.69610000
H	-1.83513100	4.84799500	-4.04964300
C	-2.10509900	-1.15205100	2.28565200
C	-1.47228800	-0.72398700	3.47399800
C	-2.29443900	-2.51981800	1.97844800
C	-1.01240000	-1.71006500	4.36180700
C	-1.82135300	-3.46313000	2.90467700
C	-1.18494000	-3.06565700	4.08227800
H	-0.52040000	-1.40968800	5.28109400
H	-1.95004000	-4.51934400	2.69857600
H	-0.82650500	-3.81374000	4.78259500
C	-1.91911000	4.06710000	0.57723500

H	-1.91233700	3.17462300	1.21306700
C	-3.12031300	4.94140300	1.01656700
H	-4.06778400	4.40052300	0.91480300
H	-3.18332100	5.84925400	0.40474000
H	-3.01123900	5.24424800	2.06483700
C	-0.58933200	4.81347800	0.82410400
H	-0.55573400	5.77063100	0.29150200
H	0.27033500	4.21713800	0.50033600
H	-0.47453600	5.02896500	1.89285700
C	-1.30037300	0.75249600	3.83367700
H	-1.69679700	1.35191900	3.00785900
C	0.18828700	1.13397400	4.00097900
H	0.28367100	2.20371300	4.22268000
H	0.75262400	0.92224600	3.08601300
H	0.65447500	0.57942200	4.82383500
C	-2.11091500	1.11779900	5.10029500
H	-1.75186000	0.56452400	5.97615000
H	-3.17465000	0.88784300	4.97123900
H	-2.01611000	2.18831300	5.31741700
C	-3.02449900	-2.98007100	0.71468300
H	-2.98682100	-2.15915800	-0.00984700
C	-2.36375000	-4.20508500	0.04702900
H	-2.47145400	-5.10912400	0.65891900
H	-1.30063700	-4.03963400	-0.14239000
H	-2.84658300	-4.40402300	-0.91599800
C	-4.51325100	-3.28654300	1.02018100
H	-5.03784200	-2.41660300	1.42951700
H	-4.59683700	-4.10345100	1.74746800
H	-5.03118000	-3.59395800	0.10412900
C	-3.33930600	0.54972800	-2.92180400
H	-3.31197700	-0.08181200	-2.02795100
C	-2.50582000	-0.17393900	-4.00178500
H	-1.49830700	-0.38488400	-3.63188600
H	-2.44534500	0.40765000	-4.92965200
H	-2.97891100	-1.13337200	-4.24479900
C	-4.81967800	0.68658200	-3.35942900
H	-4.90567700	1.29414000	-4.26859600
H	-5.43128700	1.15985600	-2.58170800
H	-5.24351300	-0.30161400	-3.57296100
Ni	0.00766500	0.51523400	-0.07084000
C	1.16057200	-3.25352800	-0.98093600
C	0.42724200	-2.84624200	-2.12343500
C	0.28459300	-3.72693700	-3.20191900
C	0.87572700	-4.98754200	-3.11066500
C	1.59832100	-5.37699600	-1.96774000
C	1.75115100	-4.51453600	-0.87938000
C	0.36340000	-1.17312900	-0.74139500
H	-0.27264200	-3.42626800	-4.08496000
H	0.77873900	-5.68506100	-3.93894400
H	2.04771400	-6.36603800	-1.93053800
H	2.31024500	-4.81746700	0.00215000
H	2.92989500	0.98255000	1.25939500
N	-0.05110800	-1.55649300	-1.93877200
N	1.10770900	-2.17155900	-0.11638700
C	1.69527600	-2.13938800	1.20449100
H	2.77612800	-2.31432400	1.15277300
H	1.23937300	-2.89640500	1.85456800
H	1.52235900	-1.15329600	1.63601000
H	-4.93748700	1.81032600	0.12690100
H	-4.67754000	-0.13692300	2.08787500
C	2.99523400	0.89256600	0.17143900
C	1.72207600	1.20986900	-0.50220100
C	4.21306600	0.51197800	-0.29061900
C	4.57721200	0.34051900	-1.78743000
C	6.00011500	-0.23033100	-1.99243700
H	6.77938400	0.40000700	-1.55125600
H	6.20697300	-0.30114400	-3.06673700
H	6.09983800	-1.23938400	-1.57643000
C	3.61316000	-0.64930500	-2.48524000
H	2.57118400	-0.32911700	-2.45769800
H	3.66235200	-1.63657200	-2.01236800
H	3.89934400	-0.76982800	-3.53836500
C	4.53027400	1.71662900	-2.49960400
H	4.76839100	1.60402300	-3.56558500
H	5.26104100	2.40809500	-2.06321800
H	3.54489100	2.18390000	-2.42269400
C	5.29783700	0.31567500	0.76387800
H	5.95452500	-0.52426800	0.50793800
H	4.82265300	0.04501100	1.71600800
C	6.16977700	1.56585300	1.01737100

H	6.64345800	1.89365000	0.08195100
H	5.51405300	2.39120100	1.32908600
C	7.25353600	1.33817900	2.07937100
H	7.90956200	0.51653000	1.75770800
H	6.78005800	1.00012800	3.01259400
C	8.09874300	2.58585000	2.35857900
H	8.61038800	2.92888100	1.45068300
H	8.86464200	2.39070800	3.11844900
H	7.47572500	3.41424000	2.71825000
H	1.78577500	1.36072600	-1.58163200
H	1.28956600	2.14479300	-0.04467300

C	-1.90727800	3.87136000	-1.83505200
H	-3.21558300	3.59466700	-0.15168000
H	-0.65577800	3.86779800	3.58060500
H	-1.83697800	4.94569400	-1.69525400
C	-1.30826500	-3.75749800	-1.81312000
C	-0.22182000	-4.31575000	-2.52559600
C	-1.94472900	-4.45401700	-0.75853600
C	0.21891000	-5.59673200	-2.15725500
C	-1.46821900	-5.73344900	-0.43116400
C	-0.39572900	-6.30020600	-1.12022000
H	1.04768900	-6.04973900	-2.69098300
H	-1.94042900	-6.28947500	0.37179400
H	-0.04068400	-7.29056200	-0.85142000
C	-0.62195200	1.22938100	-4.30002900
H	-0.63727900	0.14643600	-4.14603900
C	-1.39760600	1.53708200	-5.60486800
H	-2.43476100	1.18785300	-5.54540600
H	-1.41532500	2.61535100	-5.80688300
H	-0.91966600	1.04075300	-6.45795200
C	0.85670600	1.65120200	-4.42836300
H	0.96434800	2.72449600	-4.62474600
H	1.40668800	1.41407600	-3.51373700
H	1.32520700	1.11480400	-5.26247400
C	0.42773200	-3.58570700	-3.70086500
H	0.13637300	-2.53365300	-3.63447800
C	1.96978700	-3.62753500	-3.64682100
H	2.38728000	-3.01322000	-4.45418000
H	2.33198400	-3.23477800	-2.69100000
H	2.35976200	-4.64476500	-3.77350200
C	-0.08870600	-4.14652800	-5.04863200
H	0.17252500	-5.20649600	-5.15870700
H	-1.17838500	-4.05817100	-5.12457800
H	0.35616300	-3.59795000	-5.88817300
C	-3.14737900	-3.87232900	-0.01341500
H	-3.19833700	-2.80440900	-0.25019800
C	-3.01697700	-3.99482300	1.52036800
H	-3.03192300	-5.04125200	1.84855600
H	-2.08882700	-3.53896700	1.87620400
H	-3.85820300	-3.48713200	2.00795100
C	-4.46530300	-4.52853200	-0.49505800
H	-4.61193500	-4.39280500	-1.57218400
H	-4.46132300	-5.60603200	-0.28919000
H	-5.32533200	-4.08724800	0.02346800
C	-3.71915600	0.89424300	-0.21617300
H	-3.38963400	-0.14882200	-0.26685200
C	-3.67389000	1.32060600	1.26637500
H	-2.65826200	1.27182200	1.67383900
H	-4.05692600	2.33722100	1.41545700
H	-4.29775000	0.64594500	1.86367800
C	-5.17708900	0.96086400	-0.73913000
H	-5.55027100	1.99233100	-0.71816600
H	-5.25020400	0.59427300	-1.76797200
H	-5.83514800	0.34699900	-0.11249600
Ni	0.21843400	-0.88477800	-0.78823500
C	3.98672400	2.31818700	-2.02586900
C	2.95768700	2.97461600	-1.31159700
C	2.84567300	4.36884700	-1.37703200
C	3.77456600	5.07018100	-2.14629200
C	4.79901600	4.40378900	-2.84091200
C	4.92242000	3.01346900	-2.79113700
C	2.71400000	0.84701400	-0.91685100
H	2.04932400	4.88333900	-0.84698900
H	3.70587600	6.15276400	-2.21110100
H	5.50907400	4.97886900	-3.42859400
H	5.71860600	2.50547400	-3.32788700
N	2.19186700	2.04392400	-0.62328100
N	3.80089200	0.96627900	-1.76772000
C	4.57412700	-0.12718300	-2.32747500
H	5.15308900	0.24699800	-3.17440800
H	5.26384600	-0.55369700	-1.58978900
H	3.90457000	-0.91394800	-2.68639800
H	-3.90841600	-0.41460400	-3.68461200
H	-3.45753600	-3.13060000	-3.45893700
C	1.33478600	-0.53844700	0.73821400
C	2.20778400	-0.45791100	-0.47520100
C	1.80972600	-0.72430000	1.99180000
C	0.85412200	-1.04134000	3.17855100
C	0.50663900	-2.55110100	3.15154400
H	1.39789600	-3.17432500	3.28342500
H	-0.19993400	-2.80638700	3.95446600

ZP1

C	1.59673600	0.28953900	-0.25440500
C	3.17916400	-1.03825100	0.33500400
C	3.81089100	0.08618700	-0.24441400
C	3.95403500	-2.09635000	0.82356200
C	5.19844200	0.19529600	-0.35528800
C	5.33938500	-1.99792100	0.71716300
H	3.47648700	-2.96337700	1.26986900
C	5.95213200	-0.86993400	0.13685400
H	5.67610300	1.06287800	-0.80203000
H	5.96384100	-2.80599600	1.08828300
H	7.03593100	-0.82805400	0.07093800
C	2.94595900	2.21402400	-1.26833700
H	3.52490500	2.89569200	-0.63411700
H	3.46987500	2.09626500	-2.22417300
H	1.97151800	2.66384600	-1.46170600
N	1.80185500	-0.87637700	0.31104600
C	0.24588600	0.90281900	-0.52340600
C	-0.88702100	0.04392200	-0.01018100
H	0.14320400	1.04040500	-1.61319300
H	0.22141900	1.91246800	-0.09992100
C	-2.13449300	0.36974500	0.37615200
H	-0.61699300	-1.00876300	0.02968500
N	2.77508400	0.92958100	-0.61804200
C	-2.70560800	1.81198900	0.44193700
C	-1.96551200	2.61608600	1.54042200
C	-2.57065800	2.52525400	-0.92485500
C	-4.20709200	1.84932500	0.81264900
H	-2.08757300	2.13658900	2.51824400
H	-0.89205400	2.70314400	1.35145200
H	-2.37468600	3.63226000	1.60985100
H	-3.10332600	1.97071000	-1.70614100
H	-3.00448900	3.53204500	-0.87212700
H	-1.53196400	2.63417300	-1.24613600
H	-4.55565600	2.88854200	0.79635300
H	-4.82527000	1.28528600	0.10702600
H	-4.39670700	1.46169000	1.81886300
C	-3.02834200	-0.80715100	0.76474500
C	-3.82729200	-1.40312200	-0.41423000
H	-3.72494200	-0.52989000	1.56367200
H	-2.39783200	-1.60316700	1.17910600
C	-4.71881900	-2.58125400	-0.00032200
H	-4.44797400	-0.62872100	-0.88623000
H	-3.11614400	-1.73151500	-1.18493100
C	-5.48756000	-3.19728700	-1.17426000
H	-4.09807800	-3.35290600	0.47683800
H	-5.43044200	-2.24608400	0.76792300
H	-6.11419800	-4.03512300	-0.84718400
H	-6.14316400	-2.45785000	-1.65111200
H	-4.80176000	-3.57446000	-1.94289000

Cartesian coordinates for the stationary points given in Fig. S2.

TS₁₉₋₃₃

C	-1.28551600	-1.23164500	-1.76404800
C	-2.93613100	-2.29273400	-3.02948300
C	-3.15911800	-0.96124900	-3.13866300
N	-2.17261100	-0.31532200	-2.36814800
N	-1.81421000	-2.46309300	-2.19595600
C	-2.08672400	1.10824100	-2.19350800
C	-2.79313500	1.71185000	-1.11991200
C	-1.31651700	1.87192500	-3.10056900
C	-2.68009800	3.10366000	-0.95702300
C	-1.24237300	3.26132100	-2.89920700

H	0.05798100	-2.81082000	2.18803200
C	-0.46776300	-0.25596100	3.06355100
H	-0.28574500	0.82667700	3.12800600
H	-0.96021000	-0.47417600	2.11229400
H	-1.14974000	-0.52481400	3.88144300
C	1.46945700	-0.70688300	4.55515800
H	0.74520300	-0.92274400	5.35085400
H	2.36856400	-1.29508900	4.76788000
H	1.73748400	0.35454300	4.63266700
C	3.31517100	-0.72499400	2.27341700
H	3.81520400	-0.17262900	1.46781400
H	3.54496800	-0.17308100	3.19492100
C	3.97926400	-2.11661400	2.36876600
H	3.72121300	-2.70069400	1.47368200
H	3.56722500	-2.67358700	3.22084400
C	5.50612400	-2.04729600	2.51294700
H	5.92594100	-1.49634200	1.65811900
H	5.76002500	-1.45730500	3.40557800
C	6.16968200	-3.42572700	2.60710600
H	5.96049600	-4.02740400	1.71363700
H	7.25865100	-3.34359000	2.70664000
H	5.79730200	-3.98538200	3.47417100
H	1.42821100	-0.85041000	-1.72827800
H	2.96737500	-1.23907600	-0.57156200
Na	-0.00100400	1.60966900	0.41872600
H	1.63082400	3.21243900	1.09673600
O	0.80376100	3.43666300	1.56997000
C	1.08949600	4.27422900	2.71430100
C	2.19123700	3.62184300	3.55958500
C	1.52666000	5.66111900	2.22030900
C	-0.22418900	4.36156100	3.49399200
H	1.88982700	2.61816200	3.87501800
H	3.12235500	3.53423600	2.98589500
H	2.40537700	4.21809800	4.45393000
H	0.74299200	6.10981100	1.60018400
H	1.72906500	6.33318100	3.06228100
H	2.44097300	5.58890500	1.61952500
H	-0.10764000	4.99985200	4.37625800
H	-1.01523900	4.78521600	2.86514100
H	-0.54114600	3.36739100	3.82714600

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C	-1.81464100	-1.14560900	-0.00788300
C	-3.73778400	-2.43797000	-0.16923200
C	-2.71049100	-3.21310300	-0.58967600
N	-1.54837500	-2.42232700	-0.51907200
N	-3.20365700	-1.17556000	0.15346900
C	-0.24068600	-2.89042700	-0.90785300
C	0.19164100	-2.67726100	-2.24523100
C	0.55856700	-3.57801900	0.03474200
C	1.47766600	-3.12358500	-2.59803100
C	1.83234100	-4.01054400	-0.37439500
C	2.29385500	-3.77644300	-1.66873700
H	1.83780300	-2.97680000	-3.60968900
H	2.47006600	-4.52702400	0.33349700
H	3.28396900	-4.11155500	-1.96084100
C	-4.04781000	-0.05648300	0.51561200
C	-4.20162300	0.29565000	1.87570000
C	-4.75397700	0.61381000	-0.51454700
C	-5.04523300	1.37631800	2.18200800
C	-5.58927300	1.68216300	-0.15178700
C	-5.72590500	2.06945000	1.18150700
H	-5.17640100	1.66934700	3.21791200
H	-6.13864700	2.21451900	-0.92078600
H	-6.37209800	2.90250000	1.44091800
C	0.04862200	-3.91188100	1.43592000
H	-0.81502600	-3.27142300	1.63339000
C	-0.41095800	-5.39035900	1.50134200
H	-1.19581700	-5.60391000	0.76658000
H	0.42705300	-6.07126800	1.30660900
H	-0.80816900	-5.61850400	2.49751800
C	1.08556800	-3.61484300	2.53834300
H	1.97669400	-4.24797600	2.45308900
H	1.39708300	-2.56826100	2.50135200
H	0.63959000	-3.80473800	3.52200800
C	-3.55787100	-0.51017300	3.00332000
H	-2.76813300	-1.12677200	2.56713600
C	-2.87776300	0.38230700	4.06194500

H	-2.37387700	-0.24667100	4.80550800
H	-2.12467800	1.02394900	3.59417000
H	-3.59706800	1.01445500	4.59698600
C	-4.60322000	-1.44650100	3.65924700
H	-5.42058000	-0.87159300	4.11261500
H	-5.04210000	-2.13215400	2.92478500
H	-4.13303600	-2.04777100	4.44695800
C	-4.69276300	0.16693400	-1.97791600
H	-3.83893200	-0.50999800	-2.08780700
C	-4.48043900	1.33690400	-2.96278400
H	-5.33633000	2.02215000	-2.97086900
H	-3.58757200	1.91254000	-2.70898500
H	-4.36344400	0.94912900	-3.98211200
C	-5.97106100	-0.62032100	-2.36317800
H	-6.11990700	-1.49301900	-1.71862700
H	-6.85901200	0.01713200	-2.27408900
H	-5.90687200	-0.97010400	-3.40073900
C	-0.73314100	-2.06216600	-3.30115500
H	-1.41979900	-1.38123700	-2.78497200
C	0.00965600	-1.24914300	-4.38329300
H	0.67852600	-0.49383700	-3.95667000
H	0.60583300	-1.89478200	-5.03874600
H	-0.71704300	-0.72538500	-5.01379900
C	-1.58483000	-3.16285400	-3.98633200
H	-0.93749600	-3.88086100	-4.50454100
H	-2.19398800	-3.71190900	-3.26303500
H	-2.25895700	-2.71510200	-4.72624000
Ni	-0.55560800	0.01737600	0.76440400
C	3.64843600	-0.62355700	2.77684100
C	3.87262100	-0.68513100	1.38096400
C	4.97895400	-1.38459600	0.88672800
C	5.83613900	-2.00227300	1.80104700
C	5.60276500	-1.92782800	3.18328600
C	4.50169100	-1.23258400	3.69409500
C	2.04487700	0.48462300	1.66299400
H	5.15929700	-1.44541400	-0.18302000
H	6.70138100	-2.54940000	1.43573000
H	6.28859300	-2.41529000	3.87075100
H	4.32945800	-1.17239900	4.76513200
N	2.88278100	0.02008400	0.71143200
N	2.48562500	0.12175000	2.92676300
C	1.74556500	0.33150900	4.15563900
H	2.14499800	-0.32925600	4.92829800
H	1.82495000	1.36806600	4.50448100
H	0.69231700	0.08572700	3.98450600
H	-2.68655600	-4.23631100	-0.92107300
H	-4.78775600	-2.65004000	-0.07139000
C	0.31250100	1.62630200	0.15955100
C	0.82857600	1.23189000	1.46916300
C	0.42788700	2.82829000	-0.44899000
C	-0.40366900	3.21708000	-1.69831700
C	-1.82645000	3.62782800	-1.24356000
H	-1.79507200	4.47401600	-0.54903000
H	-2.44121000	3.92838100	-2.10372000
H	-2.31904400	2.79620300	-0.73105800
C	-0.52636700	2.02849200	-2.67127700
H	0.46061200	1.75713600	-3.07268400
H	-0.95694400	1.15813800	-2.16881700
H	-1.16329700	2.28714700	-3.52760200
C	0.21159400	4.39319600	-2.48850800
H	-0.39729600	4.60357600	-3.37695500
H	0.25613800	5.31523800	-1.89959100
H	1.22800100	4.16396900	-2.83293700
C	1.33496200	3.89447400	0.17195700
H	2.07767500	3.38094100	0.79238600
H	1.90069600	4.43245000	-0.60035600
C	0.62057400	4.93683800	1.05991000
H	0.02263100	4.41094100	1.81752600
H	-0.09142600	5.52316800	0.46279200
C	1.59600400	5.89784000	1.75335900
H	2.30730300	5.31645900	2.35754600
H	2.19777800	6.41543400	0.99198500
C	0.89871300	6.93358800	2.64229200
H	0.31886700	6.44721800	3.43673500
H	1.62140400	7.60504300	3.12110100
H	0.20416600	7.55241000	2.06020700
H	-0.68456300	-0.90760800	1.97714600
H	0.50517900	1.79509300	2.34618000
Na	1.47443400	-0.15467900	-1.24069900
H	3.65638500	0.58049700	-1.05769800

O	3.52852100	0.49122500	-2.03088100
C	4.50517900	1.27275900	-2.75160300
C	4.50275700	2.71239500	-2.21955700
C	5.88849100	0.62827900	-2.57614900
C	4.06677400	1.22944700	-4.21731100
H	3.50822100	3.15854100	-2.31972800
H	4.77912300	2.73522900	-1.15850300
H	5.22037100	3.33456400	-2.76686000
H	5.87486400	-0.40657200	-2.93514100
H	6.65451500	1.17870800	-3.13482100
H	6.18176900	0.62058100	-1.51980300
H	4.76506600	1.79001200	-4.84804000
H	4.03332300	0.19478800	-4.57691400
H	3.06978600	1.66881200	-4.33323500

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C	-1.83230800	-1.05598700	-0.13994600
C	-3.79176200	-2.26752900	-0.43885200
C	-2.79370100	-3.00136400	-0.98437300
N	-1.60937100	-2.25585500	-0.82889900
N	-3.21838700	-1.07685700	0.04656800
C	-0.32072300	-2.71041900	-1.28886900
C	0.11147700	-2.34302300	-2.59254000
C	0.45865900	-3.54060800	-0.44883900
C	1.37796600	-2.78926200	-3.01278900
C	1.71272900	-3.96525100	-0.92281100
C	2.17391900	-3.58705400	-2.18303100
H	1.73522100	-2.53167300	-4.00341200
H	2.33469700	-4.59025200	-0.29270000
H	3.14610300	-3.92446300	-2.52886400
C	-4.02280200	-0.01691100	0.61764100
C	-4.16713100	0.07194600	2.02093000
C	-4.70578600	0.86088600	-0.26117900
C	-4.97609100	1.09987900	2.53349100
C	-5.50566500	1.86611900	0.30442600
C	-5.63179500	1.99392200	1.68808300
H	-5.09926400	1.19160300	3.60707700
H	-6.03677500	2.55342000	-0.34463500
H	-6.25141200	2.78180300	2.10552200
C	-0.05223700	-4.02788100	0.90626200
H	-0.90277700	-3.39994100	1.18417200
C	-0.54195300	-5.49418500	0.79797700
H	-1.32961300	-5.60368900	0.04347600
H	0.28203100	-6.16532200	0.52517300
H	-0.94579300	-5.82870200	1.76083900
C	0.99471400	-3.88268200	2.02950600
H	1.87519800	-4.51422100	1.86223900
H	1.32215700	-2.84432900	2.11850400
H	0.55020400	-4.18333500	2.98569900
C	-3.55044500	-0.95382000	2.97090000
H	-2.78094400	-1.50045100	2.42000900
C	-2.84165600	-0.30022300	4.17538500
H	-2.35819600	-1.07385200	4.78377600
H	-2.06765500	0.39293600	3.83195700
H	-3.54045800	0.24250700	4.82405000
C	-4.62517000	-1.96355000	3.44464600
H	-5.41664800	-1.46084700	4.01485500
H	-5.09530600	-2.47498600	2.59640200
H	-4.17233500	-2.72484600	4.09168800
C	-4.65611000	0.69668000	-1.78265200
H	-3.77713600	0.08924800	-2.02498900
C	-4.51553800	2.03648800	-2.53693700
H	-5.41588400	2.65427300	-2.43708700
H	-3.66348100	2.61306700	-2.17072200
H	-4.36894500	1.84637500	-3.60695700
C	-5.91084300	-0.05690800	-2.29415100
H	-6.01159200	-1.04351200	-1.83111400
H	-6.81957400	0.51484000	-2.06975700
H	-5.85652100	-0.19591300	-3.38084500
C	-0.79181000	-1.56012900	-3.55115600
H	-1.44054400	-0.91748100	-2.94495700
C	-0.01916500	-0.65315600	-4.53362500
H	0.69791500	0.00136600	-4.02764300
H	0.52572700	-1.23999400	-5.28303000
H	-0.72601400	-0.01412000	-5.07398900
C	-1.69994200	-2.52848900	-4.35302100
H	-1.09190400	-3.20824400	-4.96251000
H	-2.33091000	-3.13101300	-3.69382700

H	-2.35575200	-1.96222600	-5.02517700
Ni	-0.52418800	-0.03692200	0.74426700
C	3.64408900	-1.09099100	2.75946700
C	3.82726000	-1.14704700	1.35557100
C	4.87958200	-1.90227500	0.82613800
C	5.72147400	-2.58242800	1.70925700
C	5.52605700	-2.51582500	3.09811200
C	4.48153800	-1.76383000	3.64607600
C	2.09524600	0.13575800	1.69712900
H	5.03486700	-1.95168000	-0.24889300
H	6.54588000	-3.17138900	1.31542600
H	6.19903200	-3.05258400	3.76118000
H	4.34095300	-1.70885800	4.72211600
N	2.86554800	-0.38022800	0.72294300
N	2.53684600	-0.27403200	2.94846800
C	1.86220400	-0.00910500	4.20364000
H	2.23150300	-0.70612500	4.95941300
H	2.04173300	1.01469400	4.55379200
H	0.78607200	-0.16318800	4.07557800
H	-2.80345800	-3.96889100	-1.45459500
H	-4.84400500	-2.46893200	-0.34398900
C	0.46127000	1.54097400	0.27242400
C	0.95063100	1.00021600	1.54205600
C	0.62263000	2.80551000	-0.19396900
C	-0.28311000	3.41120000	-1.30051800
C	-1.60683600	3.88690100	-0.64863200
H	-1.42976200	4.62706000	0.13815500
H	-2.26256200	4.35230200	-1.39810400
H	-2.13420200	3.04062700	-0.19754600
C	-0.63039000	2.37002100	-2.38202000
H	0.26360900	2.07540200	-2.94425300
H	-1.06568900	1.47434200	-1.93188200
H	-1.34604300	2.78891100	-3.10140000
C	0.36613200	4.62000000	-2.01118600
H	-0.29610900	4.98521700	-2.80597400
H	0.55179400	5.45805600	-1.33099400
H	1.32148700	4.35249700	-2.48233600
C	1.62648500	3.73279900	0.50417800
H	2.36403000	3.09880000	1.00900300
H	2.18652200	4.33532200	-0.22583100
C	1.03981800	4.69762700	1.55846500
H	0.41601300	4.12623200	2.25976000
H	0.37233900	5.42493800	1.07738000
C	2.12234000	5.45729600	2.33778500
H	2.78376100	4.73337800	2.83516000
H	2.75697600	6.01177400	1.63097000
C	1.55112300	6.42669100	3.37853700
H	0.93686700	5.89697600	4.11737000
H	2.34757600	6.94976900	3.92106900
H	0.91558600	7.18615600	2.90611700
H	-0.72303500	-1.04267800	1.87873200
H	0.68726600	1.54773700	2.44889900
Na	1.64667600	-0.23520400	-1.23117400
H	2.36509600	2.08259700	-1.96538300
O	2.72367600	1.36186300	-2.51868600
C	4.11354500	1.65705100	-2.83130700
C	4.67662200	0.36378000	-3.42371900
C	4.14957700	2.79327500	-3.86192900
C	4.85150200	2.04386800	-1.54407700
H	4.64908000	-0.44394000	-2.68376400
H	4.09422400	0.05733300	-4.29993500
H	5.71686300	0.50524600	-3.73522200
H	3.69373500	3.70318800	-3.45350000
H	5.18079800	3.03366400	-4.14519100
H	3.59773200	2.51056800	-4.76466200
H	5.91613200	2.21320300	-1.74219200
H	4.44055100	2.96981000	-1.12251200
H	4.75125000	1.25566000	-0.79153300

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C	-1.74876900	-1.13538800	0.05326000
C	-3.54289300	-2.56299500	-0.27028000
C	-2.42873300	-3.25243900	-0.60915200
N	-1.34231300	-2.37836700	-0.42875700
N	-3.13498900	-1.27359100	0.11366400
C	0.02248400	-2.78773000	-0.66555200
C	0.59679000	-2.56662600	-1.94502400
C	0.71575100	-3.45876500	0.36684000

C	1.92695100	-2.98202800	-2.13973900
C	2.03957300	-3.85878300	0.11572900
C	2.64408600	-3.61307400	-1.11601900
H	2.39551200	-2.83570100	-3.10637100
H	2.60028900	-4.35992900	0.89646100
H	3.66807100	-3.92849000	-1.29084000
C	-4.09938900	-0.26381500	0.50833800
C	-4.40154600	-0.09659300	1.87994100
C	-4.77985900	0.45777300	-0.50423300
C	-5.35655300	0.87356500	2.22501300
C	-5.72812600	1.41131800	-0.10120700
C	-6.00391300	1.62975300	1.24860100
H	-5.60228700	1.02853100	3.26951900
H	-6.25760000	1.98605400	-0.85214500
H	-6.73650400	2.37696700	1.53777300
C	0.05133900	-3.81860100	1.69653900
H	-0.93304500	-3.34236800	1.72126200
C	-0.16338600	-5.34980200	1.79295900
H	-0.76074500	-5.72749500	0.95481500
H	0.79429900	-5.88402300	1.79051800
H	-0.68578400	-5.59954000	2.72379500
C	0.83537700	-3.29498400	2.91784100
H	1.84875800	-3.70861700	2.96669000
H	0.91019500	-2.20571100	2.88780100
H	0.31407200	-3.57788200	3.84043700
C	-3.80710200	-0.99609500	2.96410100
H	-2.90525000	-1.45983800	2.55649900
C	-3.37332600	-0.21795700	4.22330100
H	-2.87231100	-0.89714000	4.92336000
H	-2.67121700	0.57863600	3.95964100
H	-4.22693300	0.22471000	4.75075800
C	-4.80724900	-2.12047700	3.33469800
H	-5.73278900	-1.70229800	3.74926300
H	-5.07401100	-2.72520300	2.46017000
H	-4.36883000	-2.78714700	4.08728900
C	-4.58078200	0.16738700	-1.99534600
H	-3.59315300	-0.29082100	-2.12071100
C	-4.62355200	1.43168100	-2.87980600
H	-5.63166400	1.86083900	-2.92283800
H	-3.93808900	2.19919800	-2.51660600
H	-4.33655600	1.17446800	-3.90587500
C	-5.64525700	-0.84023300	-2.50464700
H	-5.61201500	-1.78836500	-1.96045000
H	-6.65230500	-0.42103000	-2.39069100
H	-5.48490800	-1.05508400	-3.56802100
C	-0.21604300	-1.99085700	-3.10998500
H	-0.99096500	-1.34215200	-2.68673500
C	0.61470500	-1.14127500	-4.09589700
H	1.14982000	-0.31927000	-3.60754700
H	1.34151700	-1.75307900	-4.64430100
H	-0.05546400	-0.69554100	-4.83944600
C	-0.92356600	-3.13596700	-3.88205300
H	-0.18449200	-3.82069600	-4.31548000
H	-1.58743200	-3.71635000	-3.23411800
H	-1.52456600	-2.72216600	-4.70016500
Ni	-0.62440400	0.20164400	0.79625400
C	3.18334200	-0.50752200	3.39460300
C	3.52203900	-0.89491900	2.07593000
C	4.58580700	-1.78016100	1.86518300
C	5.27685200	-2.26031900	2.97778000
C	4.92345300	-1.86987100	4.28184200
C	3.87028900	-0.98197800	4.51136500
C	1.85468000	0.48928100	1.89865600
H	4.86461700	-2.07633100	0.85780600
H	6.10970900	-2.94383500	2.83580400
H	5.48452400	-2.25839600	5.12717900
H	3.61011600	-0.67299600	5.51979500
N	2.68589800	-0.26434400	1.17112900
N	2.11333100	0.36432400	3.25474000
C	1.33707900	0.96070500	4.32512200
H	1.48464700	0.37753000	5.23731900
H	1.63795100	1.99761600	4.51790000
H	0.27697700	0.93135900	4.05716500
H	-2.29567600	-4.26548300	-0.94488600
H	-4.57737800	-2.85484300	-0.25791100
C	0.39414400	1.59488800	0.07065400
C	0.85397500	1.42534400	1.41393900
C	0.54123400	2.78627000	-0.70796000
C	-0.60938800	3.16394300	-1.70835100
C	-1.92248000	3.43108000	-0.93844000

H	-1.81157800	4.22349100	-0.19260000
H	-2.71423700	3.74727000	-1.63076400
H	-2.25915900	2.52729400	-0.41882600
C	-0.84630000	2.01867600	-2.71195700
H	0.06826300	1.81543000	-3.27530900
H	-1.14189500	1.10110900	-2.19473800
H	-1.64186500	2.28928100	-3.41776700
C	-0.25090500	4.42583200	-2.52092100
H	-1.03174500	4.62100800	-3.26685000
H	-0.17082400	5.32034400	-1.89402600
H	0.69527000	4.30033800	-3.05761300
C	1.30129800	3.96389900	-0.03998400
H	2.16081400	3.52756200	0.48464100
H	1.72933000	4.60348800	-0.82117500
C	0.54422400	4.87146400	0.95032700
H	-0.03298500	4.26754900	1.66432900
H	-0.19162400	5.48549700	0.41511000
C	1.48680200	5.80411200	1.72604600
H	2.20764000	5.19855200	2.29435600
H	2.08279500	6.39091100	1.01242400
C	0.75190600	6.75336400	2.67874200
H	0.16585800	6.19584300	3.42050800
H	1.45162900	7.39820300	3.22340700
H	0.05677700	7.40306400	2.13230300
H	-1.12456300	-0.30018300	2.12904400
H	0.71018200	2.26673800	2.09521800
Na	2.08799700	-0.19920800	-1.06069900
H	1.45744500	2.30114700	-1.46819100
O	2.39240900	1.54957700	-2.29371000
C	3.54145900	2.03880100	-2.93845000
C	4.45842300	0.83987700	-3.27852800
C	3.16077900	2.75607600	-4.25194600
C	4.32069100	3.01114300	-2.02710500
H	4.76728500	0.32509900	-2.35796200
H	3.92353800	0.12396900	-3.91534400
H	5.36915400	1.15046400	-3.80701400
H	2.52145300	3.62081600	-4.04290000
H	4.04329700	3.11341100	-4.79887900
H	2.60217800	2.07526300	-4.90496200
H	5.24550700	3.36533500	-2.50130700
H	3.70865900	3.88698100	-1.78647500
H	4.58545900	2.51575200	-1.08497100

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C	1.26037400	-0.95051200	-1.18417100
C	2.66057700	-1.76306200	-2.82854800
C	1.47908500	-2.41857700	-2.94964500
N	0.63498200	-1.91966200	-1.94663800
N	2.52507000	-0.87969700	-1.74534000
C	-0.73932700	-2.34978300	-1.79148000
C	-1.04770800	-3.32147600	-0.80739900
C	-1.71058600	-1.81120100	-2.66443000
C	-2.39444800	-3.70263800	-0.67995900
C	-3.03634100	-2.24861300	-2.50987400
C	-3.37790400	-3.17113800	-1.52046200
H	-2.67145400	-4.42507500	0.07739700
H	-3.80504300	-1.85231200	-3.16415900
H	-4.40984100	-3.48920900	-1.40774300
C	3.60720500	-0.02440400	-1.30371500
C	3.61573200	1.33158400	-1.70263400
C	4.65094400	-0.59562700	-0.53734100
C	4.68934000	2.12840800	-1.27217800
C	5.70464600	0.24466700	-0.14498200
C	5.71968900	1.59480500	-0.49732700
H	4.72272600	3.17402500	-1.55811900
H	6.52011200	-0.16256500	0.44267300
H	6.54083300	2.22851300	-0.17734500
C	-1.36215400	-0.81536200	-3.77277700
H	-0.29964700	-0.56745500	-3.68510500
C	-1.57813000	-1.44689600	-5.16952200
H	-0.99183400	-2.36531100	-5.29174900
H	-2.63287500	-1.69964000	-5.33019100
H	-1.27845200	-0.74295200	-5.95482100
C	-2.14355800	0.51010400	-3.64038200
H	-3.22408700	0.35906200	-3.73717700
H	-1.95461700	0.97455000	-2.66876100
H	-1.83073800	1.20694300	-4.42771300
C	2.55622100	1.92222400	-2.63403300

H	1.73965900	1.19978500	-2.72056700
C	1.94166600	3.22656500	-2.08387700
H	1.15816400	3.58341200	-2.76308400
H	1.49048800	3.05743600	-1.10216700
H	2.68849500	4.02421400	-1.99229700
C	3.14543800	2.14125600	-4.04978300
H	3.96223700	2.87283700	-4.02758400
H	3.54102700	1.20826800	-4.46776600
H	2.37167100	2.51874700	-4.72872400
C	4.69321400	-2.08501900	-0.18494100
H	3.71016800	-2.51453800	-0.40574100
C	4.97778600	-2.34621300	1.31074800
H	5.96962100	-1.98477000	1.60570500
H	4.23505600	-1.85928900	1.94883100
H	4.94660000	-3.42320500	1.51234900
C	5.73629500	-2.82323100	-1.06167100
H	5.52965100	-2.69810400	-2.13031600
H	6.74577900	-2.44032200	-0.86990200
H	5.73198200	-3.89628400	-0.83727000
C	0.04033900	-4.00925000	0.02228300
H	0.85673800	-3.29074200	0.16267000
C	-0.42826400	-4.45240600	1.42360400
H	-0.89502500	-3.63154800	1.98993500
H	-1.14071900	-5.28581900	1.36174000
H	0.43704900	-4.81711700	1.99103600
C	0.61269800	-5.22103100	-0.76113400
H	-0.17212400	-5.96704200	-0.93576300
H	1.02691300	-4.92949600	-1.73276800
H	1.41044100	-5.69907600	-0.18047400
Ni	0.45047300	0.15281400	0.20181200
C	-4.27254500	2.71471000	-0.88260800
C	-4.29140700	1.30383400	-0.79338100
C	-5.29920700	0.57996100	-1.44240700
C	-6.24960800	1.28887700	-2.17428600
C	-6.20757800	2.69381500	-2.26485900
C	-5.21781600	3.43254500	-1.61753300
C	-2.59931000	1.96949300	0.39310900
H	-5.33261200	-0.50263300	-1.36831200
H	-7.04425600	0.74958300	-2.68267500
H	-6.96607700	3.21358600	-2.84349100
H	-5.19494400	4.51681400	-1.67874300
N	-3.24181900	0.87283500	0.00144400
N	-3.18605900	3.11366400	-0.12148100
C	-2.75405000	4.48439300	0.07404700
H	-3.44455800	5.02799900	0.73010400
H	-1.76013000	4.48146400	0.52268900
H	-2.70351000	5.00045900	-0.89058300
H	1.15420900	-3.17433200	-3.64262800
H	3.57251400	-1.83396900	-3.39409400
C	-0.35986100	1.34377100	1.45918500
C	-1.53079500	2.03129500	1.39435700
C	0.39942700	1.55759000	2.80153400
C	1.57101500	0.55408900	3.08292600
C	2.92378800	1.00823100	2.50529700
H	3.27581500	1.93510900	2.97078600
H	3.68923600	0.24499800	2.68889700
H	2.87139800	1.16911200	1.42252900
C	1.20908900	-0.82624400	2.50601400
H	0.19416000	-1.16651900	2.76609200
H	1.35671500	-0.87741000	1.39527100
H	1.91859100	-1.59013400	2.85393200
C	1.72424100	0.38212800	4.61164100
H	2.55753900	-0.29284900	4.84348900
H	1.92797500	1.33745700	5.10929700
H	0.81541700	-0.04283600	5.05295700
C	0.76235700	3.05168900	3.07246300
H	-0.14982300	3.56693000	3.40301700
H	1.43974800	3.09729500	3.93606000
C	1.36226300	3.87995700	1.92437600
H	0.66330700	3.88098900	1.07849400
H	2.28499700	3.42239600	1.55006300
C	1.65692900	5.32822800	2.34162900
H	0.73539200	5.79286500	2.72227700
H	2.36338400	5.32832800	3.18423500
C	2.22483700	6.18359600	1.20372800
H	1.52671700	6.23403500	0.35850200
H	2.42408200	7.21030600	1.53262900
H	3.16699500	5.76601900	0.82686100
H	-0.20945500	0.90653600	-0.82813400
H	-1.80085500	2.69697600	2.22285500

Na	-2.25684300	-0.89456200	1.18298300
H	-0.34563900	1.30193900	3.56867900
O	-1.85775900	-1.92999400	2.95776800
C	-2.48076700	-2.21531700	4.15654600
C	-1.50389100	-2.94619200	5.11523500
C	-2.96147600	-0.91320000	4.85148800
C	-3.71545200	-3.12865200	3.92846800
H	-1.15369600	-3.87747100	4.65363800
H	-0.62565600	-2.31561300	5.30249000
H	-1.96026200	-3.19385500	6.08415700
H	-3.66842300	-0.38232800	4.19881900
H	-3.45822700	-1.09400500	5.81573700
H	-2.10484200	-0.24972900	5.02657800
H	-4.24484500	-3.38345000	4.85789600
H	-4.42693200	-2.62604200	3.25827900
H	-3.40156600	-4.06316600	3.44669900

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C	-1.33357200	-0.92825600	1.16499600
C	-2.74135900	-1.74307900	2.81290400
C	-1.58119300	-2.43904800	2.90251800
N	-0.73281200	-1.94158200	1.90178000
N	-2.59140300	-0.83622200	1.75162900
C	0.62844600	-2.40239900	1.73683100
C	0.92389100	-3.33617800	0.71122200
C	1.60413600	-1.93952700	2.64898100
C	2.26130500	-3.75136600	0.58283600
C	2.91621700	-2.41817700	2.49783100
C	3.24646600	-3.29852800	1.46689800
H	2.52860700	-4.44028200	-0.20829600
H	3.68362100	-2.08924200	3.19024100
H	4.26895600	-3.64581700	1.35505200
C	-3.65795800	0.05017100	1.33782400
C	-3.61817700	1.40582500	1.74137900
C	-4.73553200	-0.48847300	0.59728500
C	-4.67511200	2.23493500	1.33445100
C	-5.77099600	0.38466000	0.22485600
C	-5.73652700	1.73337300	0.57746900
H	-4.67355500	3.28038300	1.62032500
H	-6.61065100	0.00204200	-0.34533200
H	-6.54350600	2.39318900	0.27433100
C	1.26837300	-0.98432300	3.79643000
H	0.23220600	-0.65582300	3.66982500
C	1.36659500	-1.70819700	5.16184000
H	0.70710800	-2.58268500	5.20466800
H	2.39018500	-2.05275000	5.35190400
H	1.08439600	-1.02747000	5.97364000
C	2.14643100	0.28557000	3.78809200
H	3.20352200	0.05277300	3.95717000
H	2.06789100	0.80984900	2.83198900
H	1.82460800	0.96477400	4.58686400
C	-2.51879600	1.93572100	2.66412800
H	-1.62946200	1.31725600	2.50954900
C	-2.10832300	3.39035200	2.36212700
H	-1.24816600	3.66634300	2.98324900
H	-1.82403000	3.50954500	1.31273600
H	-2.91272700	4.10143200	2.58563500
C	-2.95017500	1.79488600	4.14679600
H	-3.84379200	2.39789600	4.34987700
H	-3.17857800	0.75458000	4.40340700
H	-2.14854500	2.14041900	4.81070000
C	-4.83905300	-1.97835300	0.25867100
H	-3.87647400	-2.44736000	0.48746200
C	-5.12832600	-2.24459000	-1.23482600
H	-6.09136400	-1.82276800	-1.54474600
H	-4.34915700	-1.81728100	-1.87122800
H	-5.16644000	-3.32466900	-1.41888500
C	-5.91524400	-2.66088100	1.14062500
H	-5.70690500	-2.53095900	2.20857700
H	-6.90754100	-2.23880100	0.94128300
H	-5.95538400	-3.73595700	0.92947600
C	-0.17087500	-3.95463900	-0.16458700
H	-0.94709400	-3.19530900	-0.31664500
C	0.32065200	-4.40335900	-1.55715200
H	0.87582500	-3.61630900	-2.09019000
H	0.96384100	-5.29061800	-1.48381400
H	-0.54556800	-4.68892100	-2.16632900
C	-0.82676100	-5.14981500	0.57810200
H	-0.08433600	-5.93487700	0.76645700

H	-1.26236300	-4.85362700	1.53840800
H	-1.62428000	-5.57962400	-0.03931400
Ni	-0.55695600	0.10906000	-0.27034300
C	4.31911900	2.64427500	0.62218200
C	4.18753400	1.24883900	0.80584200
C	5.12257700	0.56136400	1.59001400
C	6.14830800	1.29392500	2.18240600
C	6.25312900	2.68721300	2.00402700
C	5.34040700	3.38756600	1.21701400
C	2.57387200	1.84786000	-0.51630700
H	5.04356700	-0.51274600	1.72208600
H	6.88765800	0.78179100	2.79201500
H	7.06694600	3.22595300	2.48111400
H	5.43245700	4.45948600	1.06806400
N	3.09338000	0.78390900	0.09124600
N	3.28076300	3.00188000	-0.22098500
C	2.99774100	4.34839400	-0.68170000
H	3.73549900	4.67609000	-1.42372300
H	2.00435800	4.36804900	-1.13156700
H	3.01511900	5.04259900	0.16502500
H	-1.27456900	-3.22263500	3.57256700
H	-3.64903000	-1.80345300	3.38668500
C	0.26872300	1.28102400	-1.49469500
C	1.52064000	1.83949800	-1.52773200
C	-0.50843400	1.51843700	-2.82166400
C	-1.56495500	0.43453200	-3.24161200
C	-2.98017700	0.70952800	-2.70155900
H	-3.38349100	1.65986200	-3.06898600
H	-3.66498200	-0.07861100	-3.03676800
H	-3.00464400	0.72905600	-1.60638100
C	-1.10055100	-0.96153500	-2.78342100
H	-0.05931900	-1.19286900	-3.05034500
H	-1.21281700	-1.08246900	-1.68138600
H	-1.74383300	-1.74109200	-3.21441700
C	-1.63402400	0.40641500	-4.78714800
H	-2.38568600	-0.31778700	-5.12416500
H	-1.90898100	1.38182700	-5.20599200
H	-0.67035700	0.11146500	-5.21878100
C	-0.99647000	2.99245900	-2.96803500
H	-0.12010400	3.60724400	-3.21711300
H	-1.65146600	3.05557400	-3.84719900
C	-1.69997100	3.66148000	-1.77643900
H	-0.99535600	3.74112800	-0.93780700
H	-2.53134700	3.04644100	-1.41455800
C	-2.22305500	5.06188300	-2.12996100
H	-1.39236200	5.67845900	-2.50375900
H	-2.93591500	4.98081800	-2.96321700
C	-2.89846700	5.77585300	-0.95417500
H	-2.19993600	5.91686500	-0.11991100
H	-3.27217200	6.76439100	-1.24593400
H	-3.74912500	5.19473500	-0.57706600
H	-0.29068000	1.55143300	-0.11987700
H	1.83174000	2.33623400	-2.45102900
Na	2.25349800	-1.06394200	-1.10592900
H	0.27565600	1.40837700	-3.58285800
O	2.09719700	-1.99325300	-2.96002300
C	2.81459000	-2.27486400	-4.10338500
C	1.91783000	-3.00024300	-5.14156000
C	3.35132300	-0.96980100	-4.75070700
C	4.02606800	-3.19098600	-3.78040300
H	1.53316000	-3.93437000	-4.71415100
H	1.05652100	-2.36907500	-5.39375300
H	2.44981300	-3.24255600	-6.07262200
H	3.99958700	-0.44254600	-4.03711300
H	3.92793500	-1.14584200	-5.67047000
H	2.51142200	-0.30673800	-4.99440700
H	4.62685500	-3.44630100	-4.66530900
H	4.68287400	-2.69057600	-3.05511400
H	3.67200000	-4.12517600	-3.32626200

Cartesian coordinates for the stationary points given in Fig. S3.

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C	2.69462400	-1.25206900	1.03425800
C	4.28168400	-2.60750600	0.44857000

C	4.06364400	-2.82073700	1.82566100
C	5.25925600	-3.34428600	-0.22899900
C	4.79268500	-3.75420000	2.56466500
C	5.99234500	-4.27756900	0.49963800
H	5.43647000	-3.18846600	-1.28942500
C	5.76269400	-4.47942900	1.87458500
H	4.62051400	-3.91199000	3.62524500
H	6.75948400	-4.86208200	0.00002800
H	6.35579000	-5.21533300	2.41001300
C	2.52826400	-1.78687400	3.52475700
H	1.79724800	-0.97949900	3.55081000
H	2.04633200	-2.71208400	3.86038800
H	3.34298000	-1.54125400	4.21433000
N	3.41388600	-1.62489000	-0.01087500
C	1.62284100	-0.19401600	1.01871900
C	1.07413000	0.11549700	-0.38123400
H	2.03011200	0.71351900	1.48393500
H	0.81076700	-0.52631200	1.67904300
C	0.69671300	1.40463000	-0.83279200
H	1.28986000	-0.66559100	-1.10847900
N	3.04702900	-1.94188600	2.17734500
C	0.65021300	1.75888300	-2.35299800
C	1.74281100	2.79533200	-2.72984900
C	0.84245800	0.52228500	-3.25739000
C	-0.72218400	2.37660900	-2.71353000
H	1.51117100	3.78034400	-2.31209200
H	2.75333300	2.52514000	-2.39308600
H	1.76693400	2.91103400	-3.82194300
H	0.13176300	-0.27750800	-3.02175000
H	0.70002700	0.80924600	-4.30570200
H	1.85567300	0.10099700	-3.19165200
H	-0.73217600	2.68789700	-3.76623000
H	-1.53634700	1.66004200	-2.55454400
H	-0.93162300	3.26441400	-2.10729100
C	0.71644700	2.57628900	0.15718700
C	2.07302500	3.29720700	0.41293700
H	0.34396300	2.20771500	1.12130200
H	-0.02506100	3.32243500	-0.15380700
C	2.16325900	3.85842200	1.83979000
H	2.92822900	2.63971500	0.20873400
H	2.19258400	4.12603300	-0.29356500
C	3.44517600	4.65759700	2.09547100
H	1.28752000	4.49460200	2.03883700
H	2.10032300	3.02967100	2.56301800
H	3.48715400	5.03149700	3.12588500
H	4.33520800	4.04176600	1.92138600
H	3.51107000	5.52190200	1.42349800
O	4.81827000	1.87746000	-1.48476800
C	5.99650900	2.58140100	-1.57860800
C	6.79601000	2.47638900	-0.25277000
C	6.87908100	2.02509500	-2.72828800
C	5.70948100	4.07922900	-1.86476300
H	6.18591300	2.86056100	0.57457400
H	7.02187700	1.42279300	-0.04070900
H	7.74356900	3.03428200	-0.27020300
H	6.32460100	2.07879200	-3.67391300
H	7.82683200	2.56888700	-2.85285400
H	7.11475300	0.96945200	-2.53406600
H	6.62385600	4.68459900	-1.94402400
H	5.15104800	4.17504500	-2.80419700
H	5.08898800	4.49633800	-1.06237600
Na	3.74491300	0.16494300	-1.47423400
C	-2.63650700	-0.35822700	0.08779100
C	-4.51984100	-1.69064300	0.30511000
C	-4.76232900	-0.54423100	0.99089100
N	-3.62054400	0.26064900	0.85645600
N	-3.23451900	-1.57135800	-0.24454600
C	-3.51498400	1.57273300	1.45924900
C	-2.89915200	1.69727800	2.72634100
C	-4.08669500	2.67849400	0.78934400
C	-2.85467400	2.97304200	3.30933900
C	-4.01817200	3.93191300	1.41912600
C	-3.40614000	4.08076300	2.66339300
H	-2.38819600	3.10114200	4.27965800
H	-4.44879000	4.79826400	0.92897800
H	-3.36197100	5.05868200	3.13243700
C	-2.64720900	-2.59099900	-1.08718900
C	-2.89202400	-2.54723000	-2.47910500
C	-1.89532500	-3.62659800	-0.48842400
C	-2.34772900	-3.57093000	-3.27073400

C	-1.37343000	-4.62557800	-1.32524900
C	-1.59317800	-4.59828900	-2.70285500
H	-2.51881600	-3.56402500	-4.34173100
H	-0.79165900	-5.43279200	-0.89336300
H	-1.18054900	-5.37990600	-3.33305200
C	-4.80535300	2.53926000	-0.55364400
H	-4.55415700	1.55717200	-0.96818100
C	-6.34176900	2.59268900	-0.36348500
H	-6.69159900	1.80695100	0.31532400
H	-6.64866000	3.55886600	0.05506200
H	-6.85097700	2.46298900	-1.32587500
C	-4.35317900	3.59860300	-1.58261400
H	-4.63387400	4.61211800	-1.27311900
H	-3.26920800	3.57321800	-1.72627600
H	-4.83139400	3.40698700	-2.55038900
C	-3.75684800	-1.46264200	-3.12277600
H	-3.89313600	-0.66212100	-2.38812600
C	-3.09073100	-0.83052100	-4.36428800
H	-3.70769200	-0.00557400	-4.73948800
H	-2.10041200	-0.43372200	-4.12181500
H	-2.97878100	-1.55433700	-5.18010200
C	-5.15780000	-2.01801400	-3.47974000
H	-5.08126800	-2.82720900	-4.21611700
H	-5.66880100	-2.41522300	-2.59544700
H	-5.78448400	-1.22727700	-3.90924100
C	-1.67778500	-3.70594500	1.02229500
H	-1.97949600	-2.74604100	1.45422800
C	-0.19462900	-3.92497000	1.39169900
H	0.17093400	-4.90243500	1.05614400
H	0.43962700	-3.15506000	0.94161900
H	-0.07200400	-3.88653500	2.48130400
C	-2.56643300	-4.80687700	1.65143500
H	-3.62845600	-4.62803200	1.44893400
H	-2.30940500	-5.79427200	1.24923400
H	-2.42767500	-4.83716400	2.73895100
C	-2.35100900	0.48535800	3.48058600
H	-2.18812600	-0.31324100	2.74918600
C	-0.99251800	0.76335200	4.15863300
H	-0.26347600	1.14925200	3.43834600
H	-1.08074400	1.49056100	4.97409800
H	-0.59868100	-0.16379800	4.59341300
C	-3.38082300	-0.02388200	4.51980700
H	-3.58696200	0.74609800	5.27322900
H	-4.32986000	-0.29212300	4.04292300
H	-2.99736300	-0.91195700	5.03684900
Ni	-0.88983500	0.23769000	-0.32737000
H	-5.62308200	-0.22543000	1.55210400
H	-5.12673300	-2.56612200	0.15390200

TS₃₆₋₃₇

C	2.92674600	-0.38822200	0.92653400
C	4.38179700	-2.02164000	0.97043000
C	4.17560500	-1.63113600	2.31477900
C	5.26574400	-3.06640100	0.68284800
C	4.83047500	-2.24424300	3.37994200
C	5.92407700	-3.69038700	1.74575100
H	5.42657200	-3.38607300	-0.34379700
C	5.71112500	-3.28786900	3.07373900
H	4.67611000	-1.92679500	4.40753900
H	6.61508500	-4.50398000	1.54109500
H	6.24090300	-3.79034500	3.87837100
C	2.72840900	0.11450000	3.40844700
H	2.60219200	-0.58307200	4.24103300
H	3.40123000	0.92421500	3.71889600
H	1.75151800	0.53435700	3.16743500
N	3.61443100	-1.23258200	0.13084500
C	2.10424700	0.69550100	0.41786500
C	1.28536700	0.32565000	-0.79732200
H	3.12432500	1.61636000	-0.02206400
H	1.56103300	1.24211000	1.19026700
C	0.49812400	1.15155300	-1.63236200
H	1.60126200	-0.62771200	-1.22814300
N	3.24496200	-0.59872300	2.25927300
C	0.33422700	0.77075000	-3.13908000
C	1.64136200	1.07893200	-3.92075700
C	0.03667700	-0.73062700	-3.35252600
C	-0.82330100	1.55983400	-3.78873600
H	2.00049100	2.09831900	-3.76200300

H	2.44132500	0.38209800	-3.62081700
H	1.49839500	0.93105100	-4.99946400
H	-0.88520400	-1.02299600	-2.84093500
H	-0.07124700	-0.94156700	-4.42544600
H	0.83772100	-1.37551700	-2.97464800
H	-0.96601800	1.23617600	-4.82767300
H	-1.75999600	1.38810100	-3.24845200
H	-0.63673700	2.63806100	-3.80711700
C	0.23466600	2.60663400	-1.22752700
C	1.15204500	3.71121600	-1.80428400
H	0.30623000	2.66762500	-0.13473000
H	-0.80651200	2.86595600	-1.46468800
C	0.86195300	5.08318500	-1.17882300
H	2.19962500	3.43872100	-1.62824200
H	1.01506600	3.79396600	-2.89105700
C	1.70778200	6.21251700	-1.77790100
H	-0.20470900	5.32381300	-1.30139100
H	1.03842600	5.03015600	-0.09473500
H	1.48690700	7.17697900	-1.30487400
H	2.77923500	6.01497600	-1.64890300
H	1.52062500	6.31881300	-2.85401500
O	4.02730000	2.17140500	-0.66123100
C	4.95209000	2.93725800	0.09306300
C	5.87627400	2.01392800	0.91401600
C	5.79314600	3.75746200	-0.90043500
C	4.19550300	3.88992200	1.04032700
H	5.29448400	1.39638400	1.60765200
H	6.43033200	1.33875000	0.24886700
H	6.60913600	2.58363400	1.49947700
H	5.14434200	4.40425600	-1.50109700
H	6.53163900	4.38584400	-0.38645300
H	6.33251200	3.08962300	-1.58419900
H	4.88575100	4.51405500	1.62141200
H	3.53389500	4.54879200	0.46797500
H	3.57720600	3.32196300	1.74559500
Na	3.93984900	0.24186800	-1.64487200
C	-2.19609200	-0.73081900	0.34164200
C	-4.39295500	-1.39292600	0.71303400
C	-3.60889000	-2.16287600	1.50584400
N	-2.28080800	-1.75605700	1.28818300
N	-3.53887800	-0.52692600	0.00593300
C	-1.17570900	-2.28589900	2.05483500
C	-0.32594400	-3.25864300	1.47670100
C	-1.01114500	-1.84287600	3.38725500
C	0.70878800	-3.77610000	2.27061000
C	0.03158400	-2.40414800	4.14293200
C	0.88656600	-3.35773000	3.59101600
H	1.38726400	-4.50967400	1.85217700
H	0.17375000	-2.08612500	5.17118600
H	1.69647800	-3.77249600	4.18266200
C	-4.03830100	0.47263600	-0.91112300
C	-4.16697700	1.80948100	-0.46201800
C	-4.44803500	0.07454800	-2.20542100
C	-4.70415700	2.75079900	-1.35375300
C	-4.98830900	1.05528900	-3.05368000
C	-5.11082100	2.38043700	-2.63664600
H	-4.81162200	3.78242500	-1.03851700
H	-5.31249400	0.77753600	-4.05066500
H	-5.52714800	3.12429300	-3.30904200
C	-1.91872400	-0.78653300	4.02198600
H	-2.66509400	-0.48919100	3.27982500
C	-2.68011500	-1.34937900	5.24502000
H	-3.27679800	-2.22766900	4.97318700
H	-1.98965400	-1.64858300	6.04252700
H	-3.35706400	-0.59051600	5.65526900
C	-1.13074200	0.48816700	4.40240800
H	-0.35401300	0.27305100	5.14612200
H	-0.65148500	0.92391300	3.51915800
H	-1.80578800	1.23894700	4.83088000
C	-3.80798200	2.21835700	0.96772900
H	-3.09038700	1.48601900	1.35033700
C	-3.12678100	3.60006700	1.05423200
H	-2.79894900	3.78644200	2.08377500
H	-2.24839600	3.64965500	0.40338300
H	-3.80815900	4.41387700	0.77797100
C	-5.06474500	2.17616600	1.87346600
H	-5.82051300	2.89032500	1.52346600
H	-5.51893400	1.17922000	1.88188900
H	-4.80065000	2.43900100	2.90515100
C	-4.35836500	-1.37746800	-2.67981900

H	-3.67951800	-1.90705100	-2.00238600
C	-3.78156200	-1.50729300	-4.10720800
H	-4.46218900	-1.09126200	-4.85947300
H	-2.82005600	-0.99501600	-4.19758600
H	-3.63126800	-2.56543500	-4.35222300
C	-5.74161800	-2.07227300	-2.60711400
H	-6.15307400	-2.05425700	-1.59255800
H	-6.45996100	-1.57400200	-3.26958200
H	-5.66007900	-3.11983900	-2.92118600
C	-0.54857300	-3.77252100	0.05394700
H	-1.03861000	-2.97116200	-0.50938600
C	0.76517500	-4.10493700	-0.68397300
H	1.47181200	-3.26997300	-0.63403600
H	1.25587500	-4.99355700	-0.26832700
H	0.55117000	-4.31606100	-1.73846500
C	-1.49393300	-5.00038100	0.05889500
H	-1.05186300	-5.82805600	0.62753900
H	-2.46374700	-4.75947600	0.50813200
H	-1.67129900	-5.34865000	-0.96606000
Ni	-0.64832400	0.04311100	-0.37996600
H	-3.85773800	-2.94386000	-2.20311600
H	-5.46058500	-1.37063500	0.58392700

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C	2.69428900	-0.90199500	-0.40164600
C	3.89728900	-2.18554800	-1.72320100
C	4.13000100	-2.64692400	-0.40005000
C	4.54232500	-2.81984700	-2.79049500
C	4.98715900	-3.70433800	-0.11929300
C	5.40119500	-3.89191600	-2.51527000
H	4.36463000	-2.49145500	-3.81193700
C	5.62196500	-4.33034600	-1.20418100
H	5.16731700	-4.04014200	0.89873200
H	5.90468800	-4.39420900	-3.33769900
H	6.29436800	-5.16358300	-1.01876900
C	3.25641000	-1.91350600	1.85447400
H	2.24071700	-1.66917100	2.17678600
H	3.48265200	-2.93376300	2.17712500
H	3.95727700	-1.22896900	2.35653800
N	3.03297500	-1.10955700	-1.71084300
C	1.88024900	0.14230200	0.07807800
C	0.94965600	0.84301400	-0.80542700
H	3.95261500	1.43866200	0.10772100
H	1.80436800	0.28201300	1.15095400
C	0.23352900	2.05524800	-0.61155800
H	0.94024700	0.43499500	-1.82199500
N	3.34953700	-1.83429200	0.41657100
C	-0.20289200	2.87493900	-1.86702400
C	1.03659000	3.45586900	-2.60870300
C	-0.98014600	2.02955500	-2.89945400
C	-1.11827100	4.05312900	-1.47080400
H	1.73156600	3.96776700	-1.93618500
H	1.58102600	2.65273200	-3.13340500
H	0.73671000	4.16863100	-3.38862200
H	-1.91525200	1.65472700	-2.47641300
H	-1.21541700	2.63862100	-3.78413300
H	-0.40642500	1.16257400	-3.24476600
H	-1.49659000	4.55846300	-2.36824200
H	-1.97707800	3.68826200	-0.89807900
H	-0.60312200	4.80525100	-0.86435000
C	0.42909200	2.81593100	0.70475400
C	1.58352700	3.84457200	0.79181400
H	0.58896900	2.07801800	1.50000700
H	-0.50178600	3.32821900	0.97952300
C	1.76132100	4.40092300	2.21211200
H	2.52363200	3.38464800	0.45874600
H	1.39623300	4.68666100	0.11183100
C	2.84683300	5.47769300	2.31808500
H	0.80358200	4.81604600	2.55821300
H	1.99697200	3.57386200	2.89795200
H	2.94400000	5.85257600	3.34404900
H	3.82533100	5.08621200	2.01310700
H	2.61895400	6.33422600	1.67119800
O	4.51211400	1.92499800	-0.54010600
C	5.90348200	1.90248500	-0.12304700
C	6.34402700	0.45324000	0.11423800
C	6.67650900	2.53317100	-1.28329900
C	6.04688600	2.74243900	1.15246400

H	5.76849300	-0.00158200	0.92880600
H	6.19320800	-0.15716100	-0.78184700
H	7.40396200	0.40931100	0.38906400
H	6.30355100	3.54235200	-1.48988000
H	7.74292100	2.60187500	-1.04494100
H	6.57295700	1.92831500	-2.19230300
H	7.09067400	2.77510500	1.48502600
H	5.70504400	3.76768900	0.97764400
H	5.44874300	2.31632800	1.96689800
Na	3.19875500	1.11511600	-2.17756600
C	-2.42847700	-0.51113700	0.42539900
C	-4.50774400	-1.55440800	0.50356000
C	-3.89431500	-1.80804200	1.68651500
N	-2.64052800	-1.17902900	1.63843300
N	-3.62560700	-0.77017700	-0.25500500
C	-1.67192900	-1.31604300	2.70068100
C	-0.91750900	-2.50853100	2.77070600
C	-1.55040800	-0.28978200	3.66757000
C	-0.02249900	-2.65712300	3.84382000
C	-0.63762900	-0.48535300	4.71511400
C	0.11866800	-1.65686700	4.80560400
H	0.56487600	-3.56624000	3.92430900
H	-0.51960100	0.28265900	5.47084400
H	0.81350700	-1.78970500	5.62954300
C	-3.94206600	-0.34073800	-1.59707300
C	-4.76839600	0.79415600	-1.77492400
C	-3.47681500	-1.10683300	-2.68959500
C	-5.11046000	1.15792200	-3.08680300
C	-3.84145400	-0.69480400	-3.98170700
C	-4.64864500	0.42525300	-4.18158100
H	-5.74367800	2.02288900	-3.25247500
H	-3.49306900	-1.26354300	-4.83768400
H	-4.92221600	0.72472200	-5.18873900
C	-2.42075400	0.96608600	3.60623900
H	-2.66086200	1.14139300	2.55172100
C	-3.75022600	0.75023300	4.37342400
H	-4.31522800	-0.09634100	3.96949900
H	-3.55735400	0.55568100	5.43596500
H	-4.38152500	1.64430800	4.30070000
C	-1.70882700	2.23224900	4.12469600
H	-1.52664300	2.18934200	5.20561200
H	-0.75117300	2.38691700	3.61821700
H	-2.33747900	3.11047800	3.93666600
C	-5.31996200	1.58833900	-0.58942000
H	-4.73336500	1.31447800	0.29403200
C	-5.18250900	3.11508500	-0.77482400
H	-5.49421400	3.63129300	0.14101800
H	-4.14816900	3.39634800	-0.99195800
H	-5.81477600	3.48523200	-1.59075100
C	-6.79867100	1.21731900	-0.31378600
H	-7.42909100	1.46784000	-1.17591600
H	-6.91590000	0.14719700	-0.11230100
H	-7.17613400	1.76980600	0.55519200
C	-2.63552000	-2.37077500	-2.50966700
H	-2.42077500	-2.48308300	-1.44280200
C	-1.27394200	-2.27056300	-3.23255600
H	-1.39879000	-2.14430000	-4.31508000
H	-0.69528000	-1.42559000	-2.84700100
H	-0.69015000	-3.18350400	-3.06652000
C	-3.41717500	-3.62580900	-2.96719600
H	-4.36182600	-3.72833900	-2.42038600
H	-3.65201700	-3.58079300	-4.03768800
H	-2.82019100	-4.52881300	-2.79221400
C	-1.06021800	-3.63084600	1.74078000
H	-1.75670400	-3.29159900	0.96817200
C	0.27708300	-3.94455000	1.03353700
H	0.68029300	-3.05336100	0.54296200
H	1.02787100	-4.32042900	1.73913000
H	0.12719200	-4.71664000	0.26941900
C	-1.65909000	-4.90559400	2.38201600
H	-0.99894000	-5.30494400	3.16153200
H	-2.63425400	-4.70362700	2.84047600
H	-1.79369900	-5.68612300	1.62373100
Ni	-0.90999600	0.42017800	-0.14942100
H	-4.21743400	-2.37470100	2.54245500
H	-5.47012600	-1.85648500	0.12917300

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C	1.58882200	1.14350900	0.16339700
C	2.61826800	2.47384000	1.56793200
C	2.04997400	3.30291800	0.56905600
C	3.34389900	3.05071900	2.61533300
C	2.19904400	4.68755700	0.58029400
C	3.49446000	4.44142500	2.63493500
H	3.76193600	2.42961600	3.40449600
C	2.93216900	5.24755600	1.63396500
H	1.76823400	5.31407000	-0.19570900
H	4.05231100	4.90664100	3.44364400
H	3.06448400	6.32534800	1.67524800
C	0.61183000	2.81602300	-1.45687800
H	1.20804700	2.80864400	-2.37922100
H	-0.21869000	2.10529800	-1.55001900
H	0.19944000	3.81660100	-1.30669000
N	2.34915300	1.14544300	1.28364600
C	1.09439900	-0.03143100	-0.52492300
C	1.42319700	-1.33677600	0.06425100
H	5.73850500	-1.04114600	-0.79867500
H	1.18090200	0.04238200	-1.61296200
C	1.92768500	-2.45607300	-0.54296100
H	1.24186200	-1.38781600	1.13774600
N	1.40272100	2.43943900	-0.30280200
C	2.09929000	-3.80049300	0.19405600
C	1.95856800	-3.67514000	1.72453000
C	1.02050000	-4.80697900	-0.28381100
C	3.49520700	-4.40658500	-0.09691000
H	2.70597500	-2.99181300	2.15798000
H	0.96609300	-3.32433100	2.02241600
H	2.11927000	-4.65322400	2.19333200
H	1.07434200	-4.97759600	-1.36454100
H	1.15176700	-5.77949100	0.20941100
H	0.01855900	-4.43640700	-0.04906300
H	3.59987900	-5.38485900	0.38896100
H	3.66645800	-4.55442600	-1.16842000
H	4.29952500	-3.76025900	0.28279200
C	2.16908400	-2.45080600	-2.04875800
C	3.48340500	-1.77577500	-2.49849100
H	1.33437900	-1.94062600	-2.54950700
H	2.16535300	-3.47434800	-2.44337000
C	3.65932000	-1.72205200	-4.02207000
H	3.51562000	-0.75197400	-2.09774900
H	4.33392000	-2.32348000	-2.06006500
C	4.97456100	-1.06828300	-4.45933600
H	3.60425100	-2.74164800	-4.42865200
H	2.81431900	-1.17326100	-4.46013500
H	5.06768000	-1.04023600	-5.55098200
H	5.04389300	-0.03446700	-4.09606300
H	5.84134200	-1.61928400	-4.07026200
O	5.74196600	-0.67266500	0.10097700
C	6.85243600	0.27157000	0.20726400
C	8.16220900	-0.50376700	0.02627500
C	6.68461700	1.35429400	-0.86458900
C	6.74420200	0.86261600	1.61325600
H	8.24508500	-1.29935200	0.77399700
H	8.21313500	-0.96087900	-0.97002100
H	9.02633200	0.16151400	0.13019700
H	5.73173500	1.87857400	-0.73846500
H	7.49265800	2.09128600	-0.80240800
H	6.71106500	0.91717800	-1.87099600
H	7.57251900	1.55385800	1.79875300
H	5.81019100	1.42333300	1.73574200
H	6.78957100	0.07000500	2.36951500
Na	3.67791300	-0.67978100	1.00445600
C	-2.69526100	-0.00244000	0.04889700
C	-4.94288200	0.65128200	0.13095700
C	-4.86411100	-0.55959700	0.73437600
N	-3.51576700	-0.95726400	0.68630200
N	-3.64201200	0.99093600	-0.28323700
C	-3.05507500	-2.20723900	1.23066000
C	-3.14797800	-3.37469200	0.43846800
C	-2.57189400	-2.24640800	2.55882000
C	-2.74301900	-4.59353100	1.00612400
C	-2.17080100	-3.48788900	3.07887400
C	-2.25679800	-4.65254000	2.31348900
H	-2.80764700	-5.50292700	0.41671900
H	-1.79602900	-3.54238300	4.09631800
H	-1.94814200	-5.60427300	2.73578900
C	-3.33821700	2.23085800	-0.94830900
C	-3.11012700	3.38921300	-0.16943200

C	-3.32672500	2.27199500	-2.36214000
C	-2.85924800	4.59775000	-0.83988700
C	-3.07012900	3.50363200	-2.98580400
C	-2.83841200	4.65777800	-2.23456400
H	-2.67966600	5.49920600	-0.26219800
H	-3.05805600	3.55893900	-4.06996500
H	-2.64770800	5.60264200	-2.73513200
C	-2.48937300	-0.99413500	3.43037300
H	-2.85640200	-0.15254700	2.83566100
C	-3.39045600	-1.11432900	4.68181700
H	-4.43278600	-1.30898900	4.40342300
H	-3.06075400	-1.92889200	5.33847800
H	-3.35962900	-0.18417200	5.26208600
C	-1.03002200	-0.66754300	3.82125700
H	-0.57769100	-1.48302300	4.40028000
H	-0.42600800	-0.49313100	2.92422100
H	-0.99530200	0.24078300	4.43531600
C	-3.11762800	3.35551900	1.35857800
H	-3.37781200	2.33855900	1.66703500
C	-1.71537700	3.65892700	1.93358500
H	-1.73285300	3.60105500	3.02887400
H	-0.98401100	2.93333700	1.56402700
H	-1.37461900	4.66403700	1.65622800
C	-4.18224900	4.30913500	1.94855900
H	-3.97018700	5.35521700	1.69583500
H	-5.18420900	4.06982400	1.57346300
H	-4.19822000	4.22782500	3.04211400
C	-3.60103500	1.03108900	-3.21076700
H	-3.72963200	0.18676300	-2.52725300
C	-2.40646400	0.68878600	-4.12899900
H	-2.19653300	1.49812600	-4.83960900
H	-1.50800200	0.50660100	-3.52912400
H	-2.62189800	-0.21806200	-4.70756900
C	-4.90676500	1.18452000	-4.02559500
H	-5.76295500	1.37957200	-3.36950900
H	-4.83696400	2.01282800	-4.74150400
H	-5.11225700	0.26792900	-4.59195000
C	-3.66902900	-3.33952900	-0.99812000
H	-3.92156000	-2.30151700	-1.23403400
C	-2.58347100	-3.78093700	-2.00618500
H	-1.69811100	-3.14245900	-1.91935400
H	-2.27865800	-4.82148700	-1.83833900
H	-2.96596000	-3.70465900	-3.03175300
C	-4.95456100	-4.18397200	-1.15899400
H	-4.76534800	-5.24441600	-0.95177100
H	-5.74159100	-3.84402800	-0.47591300
H	-5.33576400	-4.10625000	-2.18450700
Ni	-0.90757900	-0.02908300	-0.23463200
H	-5.62387400	-1.17133100	1.19011500
H	-5.78457400	1.29980800	-0.04237200

TS₃₈₋₃₉

C	-0.82929100	-1.92935400	-1.25776100
C	-0.66762300	-4.09326500	-1.00367000
C	-0.00545900	-3.78059300	-2.21530700
C	-0.72562600	-5.42090900	-0.56701000
C	0.58936200	-4.75795400	-3.01125500
C	-0.12663200	-6.40449200	-1.35631000
H	-1.21943400	-5.67450100	0.36786100
C	0.52036900	-6.07912800	-2.56005200
H	1.08392900	-4.51296600	-3.94684800
H	-0.16095800	-7.44177200	-1.03428000
H	0.97434300	-6.86741800	-3.15405000
C	0.37099400	-1.59899700	-3.45402500
H	0.76555900	-0.65474300	-3.06926000
H	1.17797000	-2.13465000	-3.95801200
H	-0.42217000	-1.38992000	-4.18295800
N	-1.19062900	-2.93877800	-0.44343300
C	-1.17353600	-0.52909200	-1.12526200
C	-1.74763300	0.06819200	0.04184100
H	-3.99032100	0.20419000	0.33961200
H	-1.32481200	-0.02239800	-2.07537000
C	-2.75289400	1.12429200	0.05359500
H	-1.62625600	-0.48634000	0.97768600
N	-0.11972700	-2.40341300	-2.35078500
C	-2.73486800	2.09175500	1.28072400
C	-2.48238200	1.32452000	2.59582800
C	-1.62630500	3.16104300	1.11597200

C	-4.08147000	2.83515000	1.43415600
H	-3.19761900	0.50088000	2.71245800
H	-1.46907900	0.91226600	2.64172300
H	-2.60239300	1.99208900	3.45881200
H	-1.76608700	3.74512900	0.19930900
H	-1.63482300	3.86961200	1.95534900
H	-0.64039100	2.68517900	1.06286500
H	-4.03452300	3.53789300	2.27629000
H	-4.34340800	3.41691400	0.54370800
H	-4.90163000	2.13880100	1.63002300
C	-2.94315400	1.83417900	-1.30044000
C	-3.84583800	1.11927100	-2.32572200
H	-1.96224200	2.02197800	-1.77359400
H	-3.36956700	2.83207600	-1.14458600
C	-3.81884900	1.77601600	-3.71269200
H	-3.55640300	0.06421200	-2.42133200
H	-4.87658400	1.11235900	-1.95218100
C	-4.75261900	1.10089900	-4.72338700
H	-4.09090200	2.83751500	-3.61709800
H	-2.78962800	1.76396700	-4.10152800
H	-4.70718800	1.58814000	-5.70482100
H	-4.48771400	0.04493000	-4.86360600
H	-5.79523200	1.13507700	-4.38312100
O	-4.65578100	-0.74181800	0.54847300
C	-6.04545800	-0.71563400	0.85630400
C	-6.25492700	-0.43161800	2.35642900
C	-6.79091700	0.32483500	0.00218500
C	-6.59550200	-2.11781700	0.52823400
H	-5.71626800	-1.17382100	2.95855400
H	-5.87411900	0.55750600	2.62719700
H	-7.31647500	-0.47445800	2.63085000
H	-6.68768400	0.08903500	-1.06206100
H	-7.85996500	0.33965700	0.24757600
H	-6.39184700	1.32994100	0.16838200
H	-7.67225100	-2.19060700	0.72506600
H	-6.42386800	-2.35477200	-0.52849900
H	-6.09706600	-2.88062800	1.14372900
Na	-3.16122400	-2.26012600	0.45071000
C	2.00877700	0.88319100	0.51105500
C	4.21770900	1.61885300	0.53045200
C	3.89381900	1.30299800	1.80778500
N	2.55857000	0.86187700	1.80136500
N	3.08199100	1.36130200	-0.25308700
C	1.90098100	0.39936200	3.00487900
C	1.51313100	1.34571800	3.98349600
C	1.73977800	-0.99461800	3.20707700
C	0.92537600	0.86589200	5.16611200
C	1.13534200	-1.41622500	4.40158400
C	0.72761900	-0.49813500	5.37109100
H	0.61791900	1.57086300	5.93045400
H	0.99433100	-2.47553500	4.58101800
H	0.26633400	-0.84811900	6.28960100
C	3.08733200	1.47604200	-1.69310200
C	3.74572500	0.47566200	-2.44591000
C	2.48025300	2.59910900	-2.30420400
C	3.76746600	0.61308200	-3.84407900
C	2.52526700	2.68374700	-3.70433000
C	3.15803000	1.70063600	-4.46907700
H	4.26948200	-0.13847800	-4.44515800
H	2.06485900	3.52915500	-4.20225500
H	3.18317400	1.78952300	-5.55097900
C	2.28468500	-2.02234000	2.21255500
H	2.25785400	-1.56568300	1.21788200
C	3.75897300	-2.36510500	2.54972300
H	4.39316200	-1.47190800	2.54833500
H	3.83079800	-2.83099700	3.54071000
H	4.16244400	-3.07073300	1.81317600
C	1.44359800	-3.31193500	2.13270300
H	1.49210900	-3.89415200	3.06133800
H	0.39650100	-3.08825700	1.90786000
H	1.82306000	-3.95121100	1.32785600
C	4.45690200	-0.71211100	-1.79195400
H	4.24692300	-0.68455000	-0.71867700
C	3.94361500	-2.07291500	-2.31240100
H	4.47726500	-2.89085100	-1.81387900
H	2.87598800	-2.19358600	-2.10687500
H	4.10467000	-2.18239000	-3.39184200
C	5.99088900	-0.60378000	-1.97139400
H	6.26873800	-0.64682300	-3.03158100
H	6.37674100	0.33761000	-1.56376500

H	6.49474800	-1.43052600	-1.45665900
C	1.85387700	3.71927500	-1.47272300
H	1.51392100	3.27747600	-0.53064800
C	0.62083500	4.36186200	-2.13922500
H	0.88542600	4.92444000	-3.04299800
H	-0.12422600	3.60559800	-2.40694000
H	0.15191400	5.06607700	-1.44275800
C	2.91293200	4.80053500	-1.13849700
H	3.76472500	4.37415000	-0.59745400
H	3.29254400	5.26962600	-2.05497500
H	2.47118700	5.58532200	-0.51247600
C	1.75599500	2.84856900	3.82216000
H	1.95665600	3.04481200	2.76320300
C	0.53263700	3.69962100	4.22934900
H	-0.37262800	3.36507600	3.71849800
H	0.35248800	3.65686100	5.31020900
H	0.70644700	4.75033500	3.96856400
C	2.99288900	3.30326300	4.63867800
H	2.82966100	3.13223900	5.70979500
H	3.89974000	2.76274000	4.34954600
H	3.17472100	4.37449200	4.49003700
Ni	0.36151400	0.32239700	-0.16882700
H	4.47698700	1.34063100	2.71038800
H	5.13508400	1.98571200	0.10423700

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C	1.12189100	2.19819700	0.30191600
C	1.65189400	3.35611600	2.06494000
C	0.80569700	4.17984800	1.28617400
C	2.16088700	3.83092500	3.27945000
C	0.45951400	5.47367100	1.67646100
C	1.81411800	5.12043800	3.67885200
H	2.80522700	3.20611100	3.89263300
C	0.97714100	5.93024900	2.88940600
H	-0.17953200	6.10692400	1.06783800
H	2.19826200	5.51038400	4.61726300
H	0.73071800	6.93263500	3.22788500
C	-0.30504500	3.85627800	-0.96791000
H	0.33972400	4.24480500	-1.76587000
H	-0.89889800	3.02550800	-1.35406100
H	-0.98745100	4.64756300	-0.65131000
N	1.84580300	2.14218700	1.42398800
C	1.03284800	1.17015400	-0.72932600
C	1.54472900	-0.14498000	-0.57684700
H	3.38915100	-0.73974300	-1.33408800
H	0.91662600	1.56893100	-1.73520200
C	2.34237400	-0.89785200	-1.65164600
H	1.85399000	-0.42104100	0.43341900
N	0.47541400	3.41533200	0.17501300
C	2.17641800	-2.45838200	-1.60986600
C	2.29713700	-2.95072500	-0.15167900
C	0.82979300	-2.90181400	-2.21010500
C	3.32885500	-3.11493100	-2.40281000
H	3.20236500	-2.53786000	0.31262900
H	1.42755400	-2.66125500	0.44994700
H	2.36512200	-4.04615100	-0.12312000
H	0.72447600	-2.58706400	-3.25512700
H	0.73913700	-3.99490200	-2.19011000
H	-0.01138900	-2.47690800	-1.64652500
H	3.24643400	-4.20810300	-2.35265800
H	3.32649800	-2.83963600	-3.46367400
H	4.29840300	-2.83081400	-1.97892200
C	2.18260400	-0.29259800	-3.06824400
C	3.15434900	0.86177400	-3.36627000
H	1.14634900	0.04042400	-3.22633500
H	2.35260800	-1.06637900	-3.82510200
C	2.93822400	1.50031600	-4.74448200
H	3.07287500	1.63717300	-2.59177000
H	4.18316600	0.48166500	-3.29823100
C	3.92965100	2.62827300	-5.05138400
H	3.01643400	0.72429800	-5.51968200
H	1.91052600	1.88887600	-4.80937200
H	3.74973300	3.06545600	-6.04071700
H	3.85333200	3.43472000	-4.31099700
H	4.96305900	2.26145100	-5.03109800
O	4.99946900	-0.67685200	0.54718300
C	6.33724200	-1.00284100	0.53916400
C	6.53214000	-2.49473200	0.91696700

C	6.94157000	-0.76240700	-0.86935500
C	7.12813800	-0.13779700	1.55980200
H	6.10081200	-2.68122400	1.90868200
H	6.00187600	-3.13121000	0.19838400
H	7.58794500	-2.80093400	0.93496600
H	6.80867600	0.29016100	-1.15144600
H	8.01271400	-1.00365500	-0.92830300
H	6.41082700	-1.37522400	-1.60826700
H	8.20261800	-0.36864500	1.59266800
H	7.01956800	0.92624700	1.30395700
H	6.71722900	-0.29167100	2.56746700
Na	3.71619500	0.72858800	1.30813900
C	-2.16524800	-0.78020200	0.12131000
C	-4.46516100	-1.03055400	0.16108300
C	-3.95380800	-1.87891200	1.08861600
N	-2.55894200	-1.72625000	1.06132500
N	-3.37642000	-0.36331600	-0.41844700
C	-1.68779300	-2.42060700	1.99179000
C	-1.39577900	-3.78794900	1.77412700
C	-1.22076400	-1.72251000	3.13124100
C	-0.58377700	-4.43927800	2.71666400
C	-0.40659700	-2.42248700	4.03579500
C	-0.08471600	-3.76406000	3.82990500
H	-0.33607200	-5.48458600	2.57297000
H	-0.02979600	-1.91282700	4.91524800
H	0.54845400	-4.28516700	4.54087500
C	-3.53466100	0.70222600	-1.38506100
C	-3.93067900	1.97679100	-0.91711900
C	-3.33313400	0.42934100	-2.75818700
C	-4.09859600	2.99808300	-1.86708700
C	-3.51005400	1.48781400	-3.66332800
C	-3.88353500	2.76006900	-3.22471100
H	-4.40633400	3.98562200	-1.53892500
H	-3.36100200	1.31330700	-4.72255500
H	-4.01813200	3.56200700	-3.94399600
C	-1.64233100	-0.28613500	3.44756900
H	-2.03084800	0.16377900	2.52893500
C	-2.78422400	-0.28360500	4.49545600
H	-3.64949700	-0.85964100	4.14744800
H	-2.44586900	-0.72271700	5.44181100
H	-3.11490600	0.74244600	4.69696500
C	-0.46930900	0.59973700	3.91709000
H	-0.05786000	0.25951100	4.87491600
H	0.33641200	0.61574800	3.17718900
H	-0.81456800	1.63043400	4.05838500
C	-4.22047600	2.26153000	0.55920600
H	-3.96776200	1.36638700	1.13550300
C	-3.35881600	3.41287300	1.12315000
H	-3.59809900	3.57724200	2.18029800
H	-2.29250500	3.17808200	1.05176400
H	-3.54379700	4.35455600	0.59244200
C	-5.72624200	2.54612100	0.77990200
H	-6.04090500	3.44992100	0.24472500
H	-6.34725400	1.71562800	0.42520500
H	-5.93274200	2.69658000	1.84593600
C	-3.00788000	-0.97739000	-3.26156500
H	-2.54467200	-1.52712200	-2.43620800
C	-2.00211100	-0.99008500	-4.43091400
H	-2.42338600	-0.54908700	-5.34214600
H	-1.08769600	-0.44603000	-4.17410000
H	-1.72500000	-2.02347500	-4.66717600
C	-4.30872100	-1.72249000	-3.65537100
H	-5.00672900	-1.78431400	-2.81300900
H	-4.81794400	-1.20849700	-4.47991400
H	-4.07795700	-2.74348700	-3.98160100
C	-1.97229000	-4.57832900	0.59701500
H	-2.29434200	-3.85997700	-0.16569300
C	-0.93754500	-5.51993700	-0.05753800
H	-0.01286900	-4.99141800	-0.29896300
H	-0.68869500	-6.36338500	0.59714500
H	-1.34856100	-5.93767400	-0.98394100
C	-3.21126000	-5.40097300	1.03590000
H	-2.93113900	-6.13290000	1.80303800
H	-4.00252400	-4.76868900	1.45130000
H	-3.62751300	-5.94717900	0.18111600
Ni	-0.41000300	-0.11344600	-0.34255500
H	-4.43868500	-2.56108500	1.76333600
H	-5.48073300	-0.82933800	-0.13154300

Cartesian coordinates for the stationary points given in Fig. S4.

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C	-1.94244000	-0.67001600	0.41639200
C	-2.79226200	-2.62533700	0.10843400
C	-3.85753100	-1.79541700	0.52892600
C	-3.03332700	-3.97491700	-0.17570900
C	-5.16192200	-2.26976500	0.68395800
C	-4.33150400	-4.45619700	-0.02768600
H	-2.22294500	-4.62035100	-0.50204000
C	-5.38019900	-3.61621800	0.39641300
H	-5.97342500	-1.62801300	1.01531100
H	-4.54371600	-5.50015900	-0.24163200
H	-6.38055300	-4.02651900	0.50363500
C	-3.98741000	0.63395900	1.19688100
H	-4.96592100	0.70570100	0.71166600
H	-4.13629500	0.59080200	2.28287300
H	-3.41242200	1.52569200	0.94324700
N	-1.61614700	-1.89290700	0.04963500
C	-0.98085800	0.48077700	0.50139900
C	-1.24820800	1.55852000	-0.53342400
H	0.02686300	0.06896800	0.36441800
H	-1.00207200	0.89941300	1.51639600
C	-0.99891400	2.87336900	-0.39961600
H	-1.64758400	1.18094100	-1.47010200
N	-3.29055400	-0.54346500	0.71075300
C	-1.32259100	3.88460200	-1.51800700
C	-1.80035000	3.20921900	-3.20921900
C	-2.45054900	4.83070000	-1.03385400
C	-0.07170700	4.72962300	-1.86006100
H	-1.04557800	2.52358200	-3.21858900
H	-2.72946700	2.64713000	-2.67118500
H	-1.99656500	3.97257800	-3.57951800
H	-2.17394100	5.37520800	-0.12471100
H	-2.67983800	5.57534100	-1.80610100
H	-3.36784600	4.26807600	-0.82397500
H	-0.31417700	5.45957600	-2.64208900
H	0.30119100	5.28800400	-0.99536700
H	0.74158700	4.09566300	-2.23116400
C	-0.37375800	3.41843500	0.87930800
C	1.14265700	3.15239800	1.00540100
H	-0.87331500	2.97728900	1.75365500
H	-0.54604900	4.49789700	0.96046300
C	1.72818600	3.68149000	2.32165200
H	1.33963900	2.07625800	0.92132600
H	1.66544700	3.62066400	0.16089600
C	3.23314100	3.42492000	2.45420200
H	1.53164700	4.76068100	2.40217500
H	1.20237400	3.21339100	3.16649200
H	3.62441700	3.81164300	3.40248000
H	3.45500500	2.35146800	2.41464200
H	3.78980300	3.90967900	1.64228400
C	3.90939600	-2.39076900	-0.41263500
C	3.60303600	-1.05568400	-0.04973500
C	4.63956900	-0.13131700	0.13080800
C	5.94855200	-0.56820300	-0.05332700
C	6.23482600	-1.90079100	-0.41270900
C	5.21990700	-2.83724300	-0.59937200
C	1.72911700	-2.07838200	-0.21293900
H	4.41594100	0.89550800	0.40459500
H	6.77003700	0.13020200	0.08155400
H	7.26931900	-2.20475300	-0.54753000
H	5.44512700	-3.86316900	-0.87723100
H	0.66718800	-2.31328500	-0.21849300
N	2.22804200	-0.89719500	0.06729200
N	2.68178200	-3.02626800	-0.51119600
C	2.44687800	-4.41256400	-0.86048600
H	2.92354300	-5.08379300	-0.13685300
H	1.37070800	-4.59876600	-0.85665800
H	2.83958000	-4.63486400	-1.85932600

TS₄₀₋₄₁

C	0.98522900	1.69315600	-0.90838400
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C	3.02394700	2.04198400	-0.17685600
C	3.10595800	2.06577400	-1.59478300
C	4.18616400	2.23301700	0.57909700
C	4.30623700	2.26316400	-2.26687900
C	5.39861800	2.43810100	-0.09205600
H	4.13697700	2.24415800	1.66584400
C	5.46107200	2.45393400	-1.49076000
H	4.36106500	2.26728700	-3.35258900
H	6.30762000	2.59402300	0.48418000
H	6.41418200	2.61640500	-1.98700100
C	1.35488200	1.91610000	-3.40754700
H	2.08871100	2.46359500	-4.00556500
H	1.21909500	0.91902800	-3.84992300
H	0.39994600	2.44978900	-3.45791700
N	1.72854400	1.79767700	0.22792600
C	-0.39123200	1.42144900	-1.00042700
C	-1.28976900	1.58547800	0.11145100
H	-0.52545600	-0.47129800	0.20761300
H	-0.80011400	1.24188800	-1.98968900
C	-2.64016100	1.36995200	0.15275900
H	-0.79800600	1.92964900	1.01952300
N	1.80610700	1.85298000	-2.03742800
C	-3.48825600	1.65898300	1.40298800
C	-2.63292000	1.96159200	2.64904500
C	-4.39785600	2.89044900	1.15234200
C	-4.38735400	0.44417500	1.74513000
H	-1.95633700	1.13123900	2.88455700
H	-2.02781500	2.86529200	2.52036100
H	-3.28234200	2.12051500	3.51869000
H	-5.06201300	2.74064200	0.29377600
H	-5.03119500	3.09577900	2.02616800
H	-3.79079100	3.78066900	0.95302100
H	-5.01757900	0.66062800	2.61775700
H	-5.05537700	0.18021800	0.91792000
H	-3.77866000	-0.43793600	1.98034900
C	-3.36858400	0.91849800	-1.10453800
C	-3.21845800	-0.57992100	-1.44967500
H	-3.01047200	1.50002300	-1.96818600
H	-4.44104400	1.13951300	-1.03046600
C	-3.95257200	-0.99123100	-2.73296100
H	-2.14957600	-0.81580700	-1.55966500
H	-3.59204100	-1.18440800	-0.61012800
C	-3.80355900	-2.47901200	-3.06948700
H	-5.01923300	-0.74396700	-2.63338500
H	-3.57906000	-0.38754300	-3.57215600
H	-4.33815500	-2.74062800	-3.99022800
H	-2.74939100	-2.75040900	-3.21102500
H	-4.20439900	-3.10959000	-2.26501300
C	1.00501900	-2.90819400	1.72021600
C	-0.09144000	-2.50711700	0.93173800
C	-1.03181700	-3.42800500	0.46852900
C	-0.83318500	-4.76047300	0.82165900
C	0.26272800	-5.16113800	1.61037600
C	1.20213400	-4.24363200	2.07538100
C	1.11341700	-0.70079500	1.42944700
H	-1.87445200	-3.11423700	-0.13790800
H	-1.54187700	-5.50921000	0.48154900
H	0.37820600	-6.21066500	1.86311100
H	2.04529500	-4.55600400	2.68284200
H	1.45835200	0.35110000	1.33612500
N	0.02434000	-1.12921400	0.78459000
N	1.73346900	-1.74941500	2.00243500
C	2.97219100	-1.67477200	2.76775300
H	3.70958000	-2.36211600	2.34390100
H	3.35903200	-0.65680000	2.70514500
H	2.78925900	-1.93518900	3.81467300

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C	1.96512500	-1.28364500	0.06935900
C	3.65107500	-0.06346900	-0.61801000
C	4.11470400	-0.77046300	0.52471900
C	4.51769400	0.81939000	-1.27382900
C	5.40122400	-0.61359800	1.02588700
C	5.81773200	0.97940000	-0.77486500
H	4.19048800	1.34504600	-2.16814400
C	6.25532600	0.27627100	0.35391700
H	5.74156400	-1.15130800	1.90726700
H	6.50194000	1.65796400	-1.27884300

H	7.26911200	0.41806000	0.71873300
C	3.05096200	-2.52827200	1.99267300
H	4.07130000	-2.89737600	2.13463300
H	2.69211400	-2.11968100	2.94793900
H	2.41250900	-3.37184300	1.71293100
N	2.33425900	-0.37961800	-0.87637500
C	0.68596500	-1.84712200	0.22252500
C	-0.28932800	-1.77643600	-0.80765000
H	-1.44055700	0.09672500	-0.54642700
H	0.45488600	-2.34611200	1.15802500
C	-1.64135100	-2.06435900	-0.74684200
H	0.10878100	-1.42659400	-1.76005200
N	3.03777400	-1.54721900	0.93310200
C	-2.51183300	-2.19348100	-2.01431000
C	-1.85746400	-1.56135500	-3.25974500
C	-2.75666600	-3.69247100	-2.33364800
C	-3.88581900	-1.50632700	-1.81472300
H	-1.62748600	-0.49927200	-3.10769200
H	-0.92849000	-2.06997500	-3.53691500
H	-2.53914000	-1.63111700	-4.11621700
H	-3.26587300	-4.20755300	-1.51161300
H	-3.38001200	-3.80794200	-3.23092400
H	-1.80438900	-4.20480300	-2.51041700
H	-4.53778700	-1.67555000	-2.68155300
H	-4.41112600	-1.88432300	-0.93092700
H	-3.77058200	-0.42006800	-1.69836300
C	-2.21761200	-2.60198400	0.56036100
C	-2.46494500	-1.54028400	1.65203400
H	-1.54044100	-3.36464400	0.97773000
H	-3.16406000	-3.12742900	0.38094900
C	-2.93914400	-2.13008600	2.98673300
H	-1.53871500	-0.97224500	1.81494500
H	-3.21650300	-0.81963500	1.29298900
C	-3.19009900	-1.07024300	4.06496600
H	-3.85895700	-2.70994500	2.82178000
H	-2.18986700	-2.84874300	3.34824000
H	-3.52421100	-1.52343600	5.00574800
H	-2.27840100	-0.49754200	4.27662800
H	-3.96138900	-0.35650200	3.74818000
C	-1.02663900	3.30034000	-0.05503700
C	-1.91685900	2.21027400	-0.10892500
C	-3.27749400	2.36890700	0.16150400
C	-3.70905800	3.65265900	0.48326400
C	-2.81740700	4.74236300	0.53524500
C	-1.45960100	4.58738700	0.26756400
C	0.12020100	1.47118500	-0.60452100
H	-3.96193100	1.52846800	0.12275300
H	-4.75967700	3.81883300	0.70052800
H	-3.19801600	5.72650100	0.79069200
H	-0.77475300	5.42808900	0.30875100
H	0.97605200	0.79578000	-0.86085700
N	-1.15211900	1.10248300	-0.45731300
N	0.23529200	2.78901000	-0.37013300
C	1.48984400	3.53670500	-0.41577200
H	1.65437900	4.03643600	0.54292100
H	2.30825600	2.83838500	-0.60087700
H	1.45334500	4.28304700	-1.21474500

TS₄₁₋₄₂

C	2.18777300	-1.04038200	0.06575000
C	3.73595200	0.34104400	-0.59817700
C	4.30301300	-0.40431200	0.46828200
C	4.50382200	1.32568200	-1.23180200
C	5.60206100	-0.19146600	0.92069100
C	5.81041600	1.54304800	-0.78479900
H	4.09074200	1.89171300	-2.06310000
C	6.35330000	0.79744500	0.27303200
H	6.02321500	-0.76209700	1.74423400
H	6.42100800	2.30138800	-1.26860000
H	7.37262400	0.98866500	0.59742000
C	3.43920800	-2.32400200	1.86217700
H	3.19617800	-1.96709500	2.87209900
H	2.76999900	-3.15033700	1.60963400
H	4.46781000	-2.69839300	1.86340600
N	2.43180500	-0.05516100	-0.81818900
C	0.94534800	-1.72145100	0.21817600
C	-0.00942600	-1.70248100	-0.79710000
H	-1.53389000	-0.27376400	-0.62407600

H	0.73435700	-2.19563700	1.17163800
C	-1.39554600	-1.96034300	-0.72558800
H	0.36884200	-1.32526800	-1.74718400
N	3.30517700	-1.28325200	0.86655100
C	-2.17713200	-2.32026800	-2.01937700
C	-1.56596000	-1.67316200	-3.28074800
C	-2.17679600	-3.85519100	-2.23774000
C	-3.64412700	-1.83630600	-1.92480700
H	-1.47319700	-0.58479800	-3.17845000
H	-0.57483500	-2.07643900	-3.51247900
H	-2.20750800	-1.86841400	-4.14892000
H	-2.64909900	-4.38541800	-1.40323500
H	-2.72323200	-4.12583900	-3.15171900
H	-1.15037900	-4.22819700	-2.33219200
H	-4.22213900	-2.17100400	-2.79572100
H	-4.15018100	-2.21908500	-1.03164100
H	-3.69749500	-0.74015200	-1.89930800
C	-1.92090200	-2.57538500	0.57950100
C	-2.16761000	-1.58537300	1.73561400
H	-1.21932900	-3.34767100	0.93749800
H	-2.86071900	-3.11175700	0.39894400
C	-2.55673400	-2.27342300	3.05059000
H	-1.26786500	-0.97665500	1.89763800
H	-2.96597300	-0.88353300	1.45121900
C	-2.82997300	-1.29069900	4.19452400
H	-3.44705900	-2.89747800	2.88441600
H	-1.75495800	-2.96520200	3.34646500
H	-3.10275300	-1.81367300	5.11880500
H	-1.94656800	-0.67579300	4.40819500
H	-3.65219700	-0.60877500	3.94321600
C	-1.63011900	3.07305700	-0.02219000
C	-2.34772100	1.86914100	-0.18159600
C	-3.73169100	1.82891800	0.01207100
C	-4.35921200	3.01995000	0.36545700
C	-3.63624700	4.21930700	0.52222300
C	-2.25782700	4.26894300	0.33148100
C	-0.22568800	1.44409800	-0.57542300
H	-4.28883700	0.90653200	-0.10933300
H	-5.43329100	3.02619500	0.52457900
H	-4.16628200	5.12584000	0.79846100
H	-1.70270500	5.19362300	0.45390400
H	0.72080100	0.93156500	-0.80772400
N	-1.42979700	0.88580000	-0.53381600
N	-0.29605600	2.75926100	-0.27916400
C	0.84307700	3.66787200	-0.21852500
H	0.73988400	4.45565800	-0.97096400
H	0.90591300	4.12165700	0.77499800
H	1.75366200	3.09753600	-0.40995800

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C	2.40612800	0.00281100	-0.16136300
C	2.93643600	2.08764900	-0.30186500
C	4.14065900	1.39493200	-0.02699900
C	2.95727000	3.48069000	-0.45724100
C	5.36720800	2.04868400	0.10800800
C	4.17665400	4.13905500	-0.32788000
H	2.04205500	4.02101400	-0.68206700
C	5.36435300	3.43395100	-0.04842700
H	6.28603600	1.51285400	0.32862300
H	4.21809400	5.21841000	-0.44578800
H	6.29803100	3.98088400	0.04859700
C	4.69285900	-1.04025900	0.30229400
H	4.82075600	-1.22446000	1.37604900
H	4.32503100	-1.95031000	-0.17468800
H	5.66794800	-0.80261800	-0.13159400
N	1.88154200	1.20049300	-0.37219800
C	1.66726600	-1.25485400	-0.13636200
C	0.39948400	-1.35808200	-0.57347300
H	-1.47443400	-2.20275000	-0.25030200
H	2.18070300	-2.11710000	0.27902500
C	-0.48958400	-2.57853900	-0.56879400
H	-0.06188900	-0.46293200	-0.97800100
N	3.77951900	0.05938800	0.04944800
C	-0.72597500	-3.12500100	-2.03682400
C	-1.04640400	-1.95279200	-2.99067400
C	0.51721700	-3.86935600	-2.55917600
C	-1.93957300	-4.07809200	-2.04236300
H	-1.83288300	-1.30633700	-2.58422900

H	-0.16605500	-1.32794400	-3.17577200
H	-1.38414100	-2.33949200	-3.95997800
H	0.72570300	-4.77805700	-1.98259400
H	0.37037400	-4.16999900	-3.60386600
H	1.40668500	-3.22950500	-2.51904400
H	-2.13416200	-4.43565300	-3.06085000
H	-1.78612200	-4.96091900	-1.41299900
H	-2.84374900	-3.56554500	-1.69141900
C	-0.05343200	-3.66121300	0.44205300
C	-0.27702100	-3.26321400	1.90969300
H	1.00293000	-3.92209000	0.28976400
H	-0.61134000	-4.58547000	0.25165000
C	0.19000900	-4.33323500	2.90552900
H	0.23838800	-2.31769400	2.12363300
H	-1.34752300	-3.06585600	2.06673500
C	-0.05658100	-3.94447300	4.36729200
H	-0.32169100	-5.28192900	2.68810100
H	1.26222700	-4.52705200	2.75483600
H	0.28926900	-4.72537000	5.05454200
H	0.46911200	-3.01645300	4.62439700
H	-1.12439600	-3.78121000	4.55817100
C	-3.49321800	2.60422600	0.39324900
C	-3.61060200	1.33443600	-0.22480000
C	-4.88048900	0.79164800	-0.45713400
C	-5.99281400	1.53145100	-0.06565000
C	-5.85700000	2.79298600	0.54866400
C	-4.60398300	3.35313000	0.78958700
C	-1.51412700	1.73970500	-0.08265000
H	-4.98115600	-0.18020000	-0.93125700
H	-6.98887700	1.13175500	-0.23566400
H	-6.74879200	3.34102900	0.84038400
H	-4.50364900	4.32596200	1.26279900
H	-0.43023300	1.67776300	-0.14560100
N	-2.35105100	0.82226600	-0.50851800
N	-2.12992800	2.83905900	0.47204000
C	-1.47790500	4.00666400	1.03008200
H	-1.75920700	4.91208100	0.47987900
H	-1.74854400	4.13677600	2.08416300
H	-0.39609700	3.87252200	0.96029200

Cartesian coordinates for the stationary points given in Fig. S5.

TS_{1h-43}

C	-1.33377600	-0.66252900	-0.02245500
C	-2.63944900	-2.58570500	0.31211100
C	-3.34982700	-1.76914000	-0.50404700
N	-2.57470900	-0.61149200	-0.70986700
N	-1.42870800	-1.93353800	0.60521700
C	-3.03265600	0.49910200	-1.49839000
C	-3.89186000	1.45458200	-0.90615000
C	-2.65993200	0.58883900	-2.85924200
C	-4.37696100	2.50132100	-1.70565900
C	-3.16830600	1.65495600	-3.61810400
C	-4.02074600	2.60354200	-3.05116300
H	-5.03233000	3.24760200	-1.26567700
H	-2.88630800	1.74426800	-4.66276800
H	-4.40189400	3.42283800	-3.65459200
C	-0.45106900	-2.46751200	1.51938500
C	0.60304300	-3.27207300	1.02406900
C	-0.59895600	-2.21052100	2.90196900
C	1.49529900	-3.83214300	1.95102200
C	0.31993700	-2.79312300	3.78921200
C	1.35609700	-3.60041100	3.32074400
H	2.31817800	-4.44135800	1.59520300
H	0.22840500	-2.59984100	4.85408100
H	2.06310300	-4.03921500	4.01952000
C	-1.72384900	-0.42740300	-3.50970200
H	-1.43315600	-1.14703100	-2.73940500
C	-2.42988700	-1.20485600	-4.64493600
H	-3.32388600	-1.72262700	-4.27631000
H	-2.73990900	-0.53472600	-5.45723000
H	-1.75091000	-1.95458500	-5.06997100
C	-0.42671800	0.24659700	-4.00976300
H	-0.63459400	0.99263700	-4.78812800
H	0.08502200	0.73974100	-3.17688400

H	0.25449800	-0.50271500	-4.43056300
C	0.75697900	-3.55028400	-0.47101700
H	0.28102000	-2.71788200	-1.00115400
C	2.22732300	-3.60656700	-0.93543100
H	2.25598800	-3.73389200	-2.02546600
H	2.77856000	-2.68997200	-0.69427000
H	2.76000700	-4.46338200	-0.50036400
C	0.01645600	-4.85474000	-0.86301700
H	0.45082000	-5.71792400	-0.34094500
H	-1.04916700	-4.80542300	-0.61252400
H	0.10395700	-5.03217100	-1.94263100
C	-1.69908700	-1.29923600	3.44414900
H	-2.30969800	-0.97555900	2.59619400
C	-1.09814100	-0.02446900	4.07955500
H	-0.46232500	-0.26799900	4.94047400
H	-0.49316100	0.51286000	3.34164800
H	-1.89756100	0.64356100	4.42612000
C	-2.62605900	-2.03932400	4.43561700
H	-3.08335200	-2.92054200	3.96937900
H	-2.07609600	-2.37664100	5.32336100
H	-3.43117800	-1.37464300	4.77445700
C	-4.28242700	1.38425800	0.56952200
H	-3.79133900	0.50655500	0.99939700
C	-3.76883300	2.61755000	1.34624000
H	-2.68029600	2.69264800	1.25923000
H	-4.21282500	3.54628700	0.96540200
H	-4.02386100	2.53202800	2.41037000
C	-5.80775600	1.20555100	0.75057400
H	-6.36183600	2.06232700	0.34627900
H	-6.16423400	0.30366300	0.23884500
H	-6.05838600	1.11635800	1.81526800
Ni	0.02517900	0.47857700	0.07567600
C	2.93346500	3.12634100	1.34411200
C	1.59549200	2.83230800	0.98697000
C	0.57885800	3.73860200	1.30615900
C	0.92211700	4.90992500	1.98277500
C	2.25530800	5.18533400	2.34090900
C	3.28312800	4.29409300	2.02519000
C	2.82837000	1.13840700	0.26151300
H	-0.44663600	3.52092100	1.02269200
H	0.14461000	5.62681500	2.23843400
H	2.48963600	6.10734700	2.86892100
H	4.31448300	4.50542000	2.29755000
H	3.48284600	0.10778400	-0.40677000
N	1.56385800	1.60085400	0.33453000
N	3.66874400	2.05382500	0.87671500
C	5.09254900	1.84715600	1.04955000
H	5.67035000	2.64802000	0.56928300
H	5.35425100	1.82155100	2.11603800
H	5.33808900	0.88957800	0.58308600
H	-4.31743800	-1.89677600	-0.95944000
H	-2.87605200	-3.55700700	0.71243200
O	4.28066900	-0.70157700	-0.87601000
C	4.62240900	-0.51186500	-2.21613900
C	5.51822900	-1.69400500	-2.64772800
C	3.36561100	-0.46819600	-3.11897700
C	5.41679900	0.80695500	-2.41496500
H	6.39771700	-1.74599500	-1.99402100
H	4.96838900	-2.63654400	-2.54204600
H	5.86100600	-1.60525600	-3.68944100
H	2.71283200	0.35854800	-2.81799100
H	3.61764000	-0.33980500	-4.18242400
H	2.79463000	-1.39651700	-3.00807300
H	5.71088100	0.96517200	-3.46306100
H	4.81126300	1.66561600	-2.10101400
H	6.32855000	0.79287400	-1.80427200

C	3.85549000	-3.56796200	-1.35908500
H	5.38052900	-2.55565500	-0.23139500
H	2.18130900	-4.32443000	-2.47391300
H	4.37237100	-4.52378700	-1.34322800
C	-0.35801700	2.84247900	-0.60391400
C	-1.58780300	2.97099000	-1.29558400
C	-0.08272100	3.61048400	0.55286500
C	-2.52810900	3.89897500	-0.81888500
C	-1.06085100	4.51330800	0.99979500
C	-2.27145200	4.66336400	0.32049600
H	-3.47414900	4.01385200	-1.34002600
H	-0.86806100	5.10731700	1.88823300
H	-3.01337900	5.37149000	0.67984400
C	0.60136000	-2.11168200	-2.77755400
H	0.12383700	-1.18853700	-2.43613600
C	0.84179300	-1.99430700	-4.30350000
H	1.46999500	-1.12821400	-4.54375500
H	1.33904400	-2.89319500	-4.69222700
H	-0.11358900	-1.88020000	-4.83150600
C	-0.37237600	-3.26446600	-2.45664600
H	0.01857800	-4.23726900	-2.78462600
H	-0.58809300	-3.30111200	-1.38419100
H	-1.32270800	-3.09938400	-2.98006800
C	-1.90745500	2.13154100	-2.53307300
H	-1.10437500	1.39803800	-2.64873300
C	-3.22443700	1.33946100	-2.37509800
H	-3.39616500	0.71304000	-3.25939300
H	-3.18203100	0.68329800	-1.50119800
H	-4.09015000	2.00566300	-2.26693600
C	-1.93976100	3.00360000	-3.81122100
H	-2.72984100	3.76352500	-3.75106300
H	-0.98567400	3.52175300	-3.96381600
H	-2.13556400	2.38203600	-4.69417600
C	1.24745100	3.50402100	1.29710500
H	1.84108900	2.73419800	0.79662100
C	1.05790400	3.04420000	2.76037600
H	0.42610600	3.74382600	3.32421000
H	0.60636700	2.04680900	2.79801700
H	2.03168600	2.99289100	3.26502900
C	2.03279500	4.83565800	1.22295800
H	2.20356400	5.13918200	0.18275700
H	1.49278000	5.64820400	1.72641700
H	3.00886400	4.72828000	1.71322200
C	4.40910900	-0.00632800	-0.05408500
H	3.64402900	0.77386100	0.00500900
C	4.85880200	-0.31591800	1.39003600
H	5.23374500	0.59613600	1.87159800
H	4.02163200	-0.69585000	1.98302900
H	5.66505000	-1.06016100	1.41636000
C	5.59015000	0.54625700	-0.88830700
H	6.38235000	-0.20663100	-0.99437300
H	5.26279800	0.83589800	-1.89319800
H	6.02466800	1.43022100	-0.40359000
Ni	0.08483600	-0.17341900	0.79260700
C	-3.91554900	-1.34595600	0.63185100
C	-3.24466400	-2.54766800	0.26624400
C	-3.97676400	-3.58501700	-0.33055700
C	-5.34385200	-3.40364400	-0.54524000
C	-5.99044500	-2.20851100	-0.17662200
C	-5.28394300	-1.15943500	0.41861500
C	-1.71476900	-1.25010600	1.13093500
H	-3.47814400	-4.50902900	-0.61271900
H	-5.92475600	-4.20021100	-1.00637700
H	-7.05790600	-2.09899100	-0.35719200
H	-5.78466800	-0.23690600	0.70355600
N	-1.91036900	-2.46675100	0.59914900
N	-2.93640500	-0.55171700	1.18046500
C	-3.13054800	0.75979500	1.75845900
H	-2.15614200	1.14082900	2.06920400
H	-3.55926100	1.45573700	1.02725400
H	-3.79605900	0.71027900	2.63177600
H	2.93478000	0.93425500	-3.22819200
H	1.37689800	3.15816500	-2.75607700
H	-0.85168800	-1.00677800	2.14983500
O	-0.05832800	-0.54825100	3.02706000
C	0.65364300	-1.48693400	3.79978400
C	-0.29334500	-2.07611300	4.86963200
C	1.21016400	-2.62920800	2.92254700
C	1.81490900	-0.74976700	4.49517400
H	-0.71586300	-1.26775400	5.47848100

TS_{1h}-

C	0.87232000	0.63057900	-0.57628100
C	1.43009200	2.21618300	-2.23622600
C	2.19737000	1.12425500	-2.46626500
N	1.87871700	0.16791100	-1.48266100
N	0.63287800	1.93933300	-1.10867200
C	2.52421400	-1.11165400	-1.40267700
C	3.76862700	-1.21467400	-0.73662900
C	1.93055000	-2.23079100	-2.03320500
C	4.42289700	-2.45697900	-0.73360200
C	2.61996300	-3.45326700	-1.99853700

H	-1.12269300	-2.60438900	4.38491600
H	0.22119300	-2.78245300	5.53734200
H	1.87576300	-2.21965300	2.15413700
H	1.76947400	-3.36521400	3.51874100
H	0.39421900	-3.14800100	2.40685400
H	2.42460800	-1.42562200	5.11212200
H	2.46233700	-0.28499200	3.74326300
H	1.42230000	0.04733900	5.13835400

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C	1.30187400	-0.69294100	0.13911300
C	2.66121100	-2.61176400	0.11820800
C	3.32779000	-1.67004200	0.82958800
N	2.52190600	-0.51513000	0.84853700
N	1.44537800	-2.03973600	-0.29834900
C	2.93485700	0.71082000	1.47294000
C	3.82141000	1.56985300	0.78070000
C	2.49609600	1.01036800	2.78351800
C	4.27473000	2.72727400	1.43286900
C	2.97278900	2.18172100	3.39265500
C	3.85735500	3.03337600	2.72883600
H	4.95364000	3.39850800	0.91506700
H	2.64151700	2.42978100	4.39645400
H	4.21466600	3.93576300	3.21741800
C	0.52003000	-2.71713100	-1.16870500
C	-0.52801100	-3.48802300	-0.61121900
C	0.71081100	-2.63319900	-2.56739000
C	-1.36690500	-4.19412400	-1.48669800
C	-0.15517500	-3.35687900	-3.40222500
C	-1.18263000	-4.13484700	-2.86933500
H	-2.18350800	-4.78261600	-1.08360600
H	-0.02939700	-3.29787200	-4.47937000
H	-1.84821900	-4.68435700	-3.52944400
C	1.52899100	0.10097800	3.53798500
H	1.23614200	-0.70270500	2.85685100
C	2.20281800	-0.53968600	4.77402000
H	3.09451800	-1.11092500	4.48847700
H	2.50960000	0.22279700	5.50197500
H	1.50572200	-1.22228100	5.27633200
C	0.23603200	0.85142900	3.92631600
H	0.43883200	1.68025100	4.61747100
H	-0.24735900	1.25154700	3.02908500
H	-0.46754500	0.16720200	4.41619100
C	-0.73366600	-3.56826600	0.90097900
H	-0.29591100	-2.65983300	1.32901700
C	-2.22078000	-3.59832000	1.31085900
H	-2.29726500	-3.55638300	2.40509700
H	-2.77793800	-2.74890800	0.90223100
H	-2.71377600	-4.52610900	0.99041500
C	0.01426500	-4.78804500	1.49672800
H	-0.37736100	-5.72496400	1.07820400
H	1.08868100	-4.74353200	1.28704700
H	-0.11807900	-4.82159000	2.58601500
C	1.80024600	-1.75762500	-3.18499800
H	2.36488700	-1.30509000	-2.36484000
C	1.18241700	-0.59833700	-4.00050000
H	0.59441900	-0.97415100	-4.84786800
H	0.52816500	0.00398100	-3.36114300
H	1.97245500	0.05222500	-4.39799900
C	2.79011400	-2.58315200	-4.03851800
H	3.26539800	-3.37176100	-3.44249200
H	2.28632400	-3.06184000	-4.88789800
H	3.57937300	-1.93492500	-4.44049500
C	4.27864500	1.27578000	-0.64790300
H	3.76586600	0.36766900	-0.97720000
C	3.86718900	2.40458600	-1.61972100
H	2.78143900	2.54204800	-1.60585600
H	4.34119000	3.35867800	-1.35578600
H	4.16724700	2.15199900	-2.64480200
C	5.80073200	1.00922200	-0.71474100
H	6.37363100	1.88839500	-0.39275700
H	6.08370000	0.16931900	-0.06911100
H	6.10332600	0.76779000	-1.74170000
Ni	-0.05222600	0.41341000	-0.15772100
C	-2.78699100	3.09744200	-1.71341000
C	-1.48891100	2.77340800	-1.25113800
C	-0.43193800	3.66021400	-1.48209000
C	-0.69347300	4.84209800	-2.17884400

C	-1.98605200	5.14669800	-2.64333600
C	-3.05433000	4.27432800	-2.41519400
C	-2.82028800	1.08545000	-0.61836600
H	0.56204400	3.42133900	-1.11424400
H	0.11751600	5.54350400	-2.36530100
H	-2.15825400	6.07510300	-3.18444600
H	-4.05539700	4.50925800	-2.77039000
H	-3.79931700	-0.15557100	0.28343400
N	-1.54072400	1.54110500	-0.60293400
N	-3.57781800	2.03853300	-1.30595000
C	-4.98652000	1.89039800	-1.59118300
H	-5.57048500	2.72498600	-1.17803900
H	-5.17016500	1.84750700	-2.67423600
H	-5.31991400	0.95794700	-1.13155100
H	4.28340100	-1.70759500	1.32506000
H	2.93238900	-3.62285900	-0.13482100
O	-4.48599000	-0.77176800	0.73427500
C	-4.79170300	-0.30258600	2.03653700
C	-5.72405100	-1.35454400	2.65722400
C	-3.51181600	-0.15952900	2.88375500
C	-5.51934300	1.05817400	1.96953200
H	-6.62110200	-1.47306800	2.03776600
H	-5.21732200	-2.32498000	2.70516200
H	-6.03419300	-1.07106900	3.67170100
H	-2.81821600	0.53988900	2.40620200
H	-3.73479000	0.20387300	3.89687000
H	-3.00346900	-1.12597800	2.96703900
H	-5.80675900	1.41432900	2.96854200
H	-4.87076500	1.81235100	1.51137200
H	-6.42742100	0.97073200	1.36067100

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C	-0.18480300	-1.36841900	0.03499600
C	-0.01756200	-3.64504200	-0.56384600
C	-1.27736000	-3.45573900	-0.10240100
N	-1.39440100	-2.09874000	0.25593000
N	0.64665100	-2.40624800	-0.49097100
C	-2.61700200	-1.51964300	0.73325100
C	-2.81179700	-1.34512300	2.12346500
C	-3.62562700	-1.17644200	-0.19936600
C	-4.04799700	-0.84774000	2.56511500
C	-4.84967000	-0.69360300	0.29100200
C	-5.06349300	-0.53196500	1.66089800
H	-4.21401200	-0.70572100	3.62902000
H	-5.63698300	-0.43168500	0.29100200
H	-6.01517700	-0.15127700	2.02192300
C	1.99844500	-2.21334100	-0.93075200
C	2.24496200	-1.89740500	-2.28741400
C	3.05998800	-2.37953100	-0.01118500
C	3.57748200	-1.77376200	-2.71182500
C	4.37613100	-2.25104400	-0.48210600
C	4.63652200	-1.95355400	-1.82082700
H	3.78501300	-1.52457700	-3.74847800
H	5.20350800	-2.37395600	0.21039100
H	5.66191700	-1.85239300	-2.16619300
C	-3.41155600	-1.32560300	-1.70555600
H	-2.35223200	-1.55039600	-1.86193300
C	-4.23649100	-2.50628200	-2.27343600
H	-3.97821700	-3.44932200	-1.77736100
H	-5.31248600	-2.33570000	-2.13605400
H	-4.04783500	-2.62345800	-3.34839400
C	-3.71839400	-0.02053600	-2.47419100
H	-4.77848500	0.25604200	-2.39201200
H	-3.11272800	0.81442400	-2.10633800
H	-3.49751300	-0.15801800	-3.54111900
C	1.10532900	-1.65879200	-3.27598400
H	0.16725100	-1.85751100	-2.74974900
C	1.06443900	-0.18041400	-3.72764500
H	0.22243400	-0.01414400	-4.41187900
H	0.93417000	0.47371000	-2.85936400
H	1.98847300	0.10314300	-4.24911300
C	1.17874800	-2.61589800	-4.48795900
H	2.09137600	-2.45254000	-5.07550400
H	1.16847800	-3.66487800	-4.16741800
H	0.32105200	-2.45249600	-5.15266600
C	2.80204400	-2.68628100	1.46239200
H	1.72093400	-2.63650400	1.62012100
C	3.44190200	-1.62415400	2.38371600

H	4.53700700	-1.62429600	2.30510200
H	3.07513400	-0.62628800	2.12461600
H	3.18117900	-1.82690400	3.43070200
C	3.27589900	-4.11087700	1.83539400
H	2.77591700	-4.86860000	1.22006800
H	4.35886100	-4.22043000	1.69111900
H	3.05312900	-4.32480000	2.88868700
C	-1.72357800	-1.68994200	3.13869600
H	-0.83999900	-2.00415900	2.57606900
C	-1.30849700	-0.45353300	3.96739200
H	-0.92636000	0.33115500	3.30603200
H	-2.15084300	-0.05268900	4.54683700
H	-0.51208200	-0.72358100	4.67324200
C	-2.15472200	-2.86182400	4.05145300
H	-3.03626400	-2.59924800	4.65096400
H	-2.40209100	-3.75335100	3.46227700
H	-1.34412500	-3.12324300	4.74378200
Ni	0.20606900	0.33722500	0.34420700
C	2.57177800	3.33992100	0.32517700
C	2.16517600	2.57961700	1.45404400
C	2.97877800	2.53780200	2.59069600
C	4.18005300	3.25210600	2.57924300
C	4.56983500	4.00319500	1.45635400
C	3.76904800	4.05850200	0.31070300
C	0.55471000	2.35492500	-0.06708800
H	2.67268100	1.95933600	3.45890100
H	4.82673500	3.22884700	3.45429900
H	5.51164200	4.54816900	1.47642000
H	4.07796800	4.63382200	-0.55931700
H	-1.13324000	2.61243800	-0.99074700
N	0.92425300	2.01580300	1.19082300
N	1.56041900	3.17514700	-0.60227700
C	1.54092500	3.73694300	-1.93333200
H	1.74854700	4.81561100	-1.90537500
H	2.28508500	3.25968800	-2.58664300
H	0.54285000	3.57985500	-2.34823400
H	-2.09327400	-4.14959800	0.01315800
H	0.46830700	-4.53332100	-0.93219200
O	-1.88978300	2.96011200	-1.55687100
C	-2.66268700	3.88339200	-0.79603200
C	-3.86429000	4.24871300	-1.67873700
C	-3.13621100	3.23411200	0.51705700
C	-1.83162300	5.14685400	-0.49244400
H	-3.51915600	4.67323400	-2.62899000
H	-4.45590100	3.35412400	-1.90259800
H	-4.51358300	4.98236400	-1.18393600
H	-2.27475200	2.92592500	1.11887800
H	-3.74756000	3.92802200	1.11091700
H	-3.73127000	2.33903800	0.30680500
H	-2.41978000	5.89514900	0.05641100
H	-0.95538000	4.88757600	0.11071800
H	-1.48145600	5.60093000	-1.42732900

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C	-1.14844100	0.20683400	-0.15767800
C	-3.32143000	0.04507200	-1.04246500
C	-3.01454500	1.36516200	-0.99406300
N	-1.71819500	1.47221200	-0.45937200
N	-2.21067100	-0.65706200	-0.53559000
C	-1.06363300	2.73329300	-0.23139700
C	-1.34377700	3.44205600	0.96014900
C	-0.19307400	3.25739400	-1.21507300
C	-0.76146300	4.70698900	1.13548700
C	0.36299400	4.52743200	-0.99546400
C	0.07941400	5.25102400	0.16379400
H	-0.95653200	5.26326800	2.04787100
H	1.03792700	4.94499700	-1.73566400
H	0.52502300	6.23031600	0.31626800
C	-2.16758100	-2.08896200	-0.42923300
C	-1.67378200	-2.85097800	-1.51339600
C	-2.65595000	-2.70863000	0.74481600
C	-1.68393300	-4.25030800	-1.40076200
C	-2.64302100	-4.11060700	0.81270000
C	-2.16386800	-4.87822100	-0.25030200
H	-1.29978000	-4.85170500	-2.21934000
H	-3.00388200	-4.60425500	1.71024500
H	-2.15872200	-5.96257600	-0.17964600
C	0.14524600	2.48731300	-2.49013700

H	-0.24388300	1.47190400	-2.37072000
C	-0.54428200	3.12584100	-3.72056300
H	-1.63364900	3.16321100	-3.59485000
H	-0.18803600	4.15159800	-3.88449400
H	-0.32409600	2.54424900	-4.62497000
C	1.67026000	2.35700200	-2.70432600
H	2.14260500	3.33741700	-2.85545300
H	2.15251700	1.85980100	-1.85391700
H	1.86473700	1.75641500	-3.60297800
C	-1.11654900	-2.19373500	-2.77448400
H	-1.21699700	-1.11140700	-2.65340200
C	0.39228000	-2.48849800	-2.93764700
H	0.78239100	-1.98514300	-3.83146000
H	0.94363100	-2.11547200	-2.06749500
H	0.58226900	-3.56477800	-3.04423100
C	-1.91275700	-2.60635400	-4.03420300
H	-1.83629100	-3.68503500	-4.22230400
H	-2.97635100	-2.35736600	-3.93287000
H	-1.52202500	-2.08509400	-4.91715200
C	-3.14242100	-1.88993200	1.93960100
H	-3.19451800	-0.84400400	1.62228900
C	-2.12230700	-1.96094500	3.10008000
H	-2.00541100	-2.99131000	3.46140300
H	-1.14632600	-1.59438500	2.76289700
H	-2.45490100	-1.33946300	3.94182600
C	-4.55487100	-2.30857600	2.40499300
H	-5.28153900	-2.23625500	1.58666600
H	-4.56976400	-3.34062400	2.77748600
H	-4.89237400	-1.65760100	3.22140200
C	-2.20243600	2.83846500	2.07060100
H	-2.61534100	1.89722100	1.69529300
C	-1.33034600	2.49338900	3.30083100
H	-1.93663400	2.00872400	4.07767500
H	-0.52404500	1.81087400	3.01128100
H	-0.88094300	3.39681000	3.73322400
C	-3.38940600	3.74811300	2.45932100
H	-3.04601900	4.70561900	2.87085900
H	-4.02466300	3.96416000	1.59170400
H	-4.00799700	3.26060100	3.22370500
Ni	0.55313100	-0.13732300	0.31903400
C	4.49809200	-1.21451200	1.03132200
C	4.61252300	-0.06548500	0.19720300
C	5.88894800	0.38521400	-0.16782000
C	7.00941700	-0.30649300	0.29990000
C	6.87679800	-1.43891700	1.12403400
C	5.61366500	-1.90903600	1.50247500
C	2.44979800	-0.37450300	0.48499200
H	5.99222300	1.26125400	-0.80448200
H	8.00560600	0.03553700	0.02327300
H	7.76806400	-1.95729400	1.47344200
H	5.51281500	-2.78507500	2.14047200
N	3.36096700	0.41968100	-0.11316700
N	3.14338800	-1.38865500	1.19286000
C	2.52572900	-2.44229400	1.95791700
H	1.44334300	-2.34354100	1.83473600
H	2.84000200	-3.43384600	1.59964000
H	2.77569000	-2.36955200	3.02726900
H	-3.58639000	2.23090000	-1.28343400
H	-4.20958400	-0.45892800	-1.38534000

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C	-0.93253000	0.88968600	0.72387900
C	-2.21474700	2.82896700	1.06215000
C	-2.66896400	1.90469800	1.93915700
N	-1.91691600	0.72809500	1.73866600
N	-1.17941400	2.23276900	0.31933100
C	-2.25192500	-0.50521300	2.40320900
C	-3.32130700	-1.28590400	1.89838200
C	-1.55697300	-0.87671400	3.57958100
C	-3.68333100	-2.44819600	2.60011900
C	-1.95512500	-2.04888700	4.24178800
C	-3.00833900	-2.82833500	3.75959200
H	-4.49645400	-3.06201700	2.22761300
H	-1.43537300	-2.35674000	5.14185500
H	-3.30011700	-3.73268200	4.28672100
C	-0.56513000	2.89440700	-0.80503700
C	0.62282300	3.63969800	-0.61293000
C	-1.20813000	2.83902700	-2.06463500

C	1.15384700	4.33272800	-1.71198300
C	-0.63751700	3.55138300	-3.13221500
C	0.53188700	4.29016600	-2.96088000
H	2.06549200	4.90722900	-1.59208900
H	-1.11363600	3.51952400	-4.10660100
H	0.96160200	4.83115400	-3.79968900
C	-0.43291600	-0.00504600	4.14062800
H	0.06293200	0.46668300	3.28451500
C	-0.99879000	1.11719700	5.04744300
H	-0.18255400	1.74449500	5.42779700
H	-1.69314200	1.76216600	4.50043700
H	-1.53017900	0.68951900	5.90834100
C	0.63354000	-0.81026100	4.91039400
H	0.24041000	-1.21620900	5.85194100
H	1.01613900	-1.64136100	4.30883100
H	1.47888600	-0.16033800	5.16008400
C	1.28662300	3.73367000	0.76071800
H	1.03308300	2.81563200	1.30197800
C	2.82482100	3.80936800	0.68067800
H	3.25180800	3.77225300	1.68953200
H	3.22566200	2.96468400	0.11203600
H	3.16786600	4.74289100	0.21588700
C	0.73436400	4.93929900	1.56231200
H	1.19959800	4.98187400	2.55561200
H	0.95130800	5.88265700	1.04352500
H	-0.34947500	4.86677200	1.70003900
C	-2.51640100	2.07668800	-2.27414800
H	-2.64868600	1.41232100	-1.41526600
C	-2.49090300	1.18306600	-3.53205700
H	-2.38447200	1.77350300	-4.45191700
H	-1.67504500	0.45621300	-3.46309900
H	-3.43366800	0.62558300	-3.60677800
C	-3.71796200	3.05402800	-2.31165100
H	-3.78396000	3.64694900	-1.39183500
H	-3.62994400	3.74924600	-3.15702700
H	-4.65709700	2.49807800	-2.42699500
C	-4.10401900	-0.87396600	0.65030300
H	-3.48205100	-0.16462800	0.09564600
C	-4.40584600	-2.05600800	-0.29495200
H	-3.49920000	-2.60461400	-0.56010800
H	-5.11986100	-2.76182000	0.14989000
H	-4.85148000	-1.68173400	-1.22403700
C	-5.42352000	-0.15739400	1.03550300
H	-6.07584500	-0.83042500	1.60747900
H	-5.23889100	0.73506800	1.64203400
H	-5.96381000	0.15239300	0.13212100
Ni	0.41715500	-0.16656400	0.12184800
C	-1.29721400	-2.55765300	-2.64517500
C	-1.17365900	-3.46858100	-1.55383100
C	-1.79453300	-4.71512300	-1.54220200
C	-2.56751100	-5.06563500	-2.66174300
C	-2.70418600	-4.18296000	-3.74352800
C	-2.07791500	-2.93058200	-3.74979400
C	-0.03004500	-1.54241400	-1.17251200
H	-1.69000000	-5.39482100	-0.69925100
H	-3.06592800	-6.03247200	-2.68620000
H	-3.31092100	-4.47909800	-4.59772800
H	-2.18521400	-2.25307200	-4.59340100
N	-0.36894800	-2.82101300	-0.64201600
N	-0.58287200	-1.41430700	-2.40102200
C	0.03751500	-3.35945200	0.63499500
H	0.52020600	-4.33961300	0.50529800
H	0.74793800	-2.66872700	1.09443000
H	-0.81835200	-3.47959100	1.31283000
H	-3.44382500	1.96395300	2.68380800
H	-2.52359900	3.84604400	0.89119800
C	2.32597200	-0.56900600	0.12817500
C	1.71841000	-1.16559500	-1.10708800
C	3.63232500	-0.71105700	0.43698600
C	4.25115800	-0.26156900	1.78292100
C	3.25810500	0.53954700	2.63567400
H	2.35372900	-0.04069700	2.82112400
H	3.71787000	0.81251900	3.59791700
H	2.94548400	1.45189400	2.12412400
C	5.50900700	0.61556400	1.56732900
H	6.29393500	0.08728200	1.01347500
H	5.25844400	1.52509800	1.00868500
H	5.93974800	0.92141900	2.53187300
C	4.66377800	-1.51289400	2.60127400
H	5.12598100	-1.22461100	3.55707100

H	3.78399800	-2.12910800	2.82105300
H	5.38498500	-2.14016700	2.06398200
C	4.61095700	-1.37958200	-0.54066300
H	5.51908900	-1.73108600	-0.02950700
H	4.14765000	-2.28240800	-0.96685100
C	5.04253300	-0.47645800	-1.71514600
H	5.53495800	0.42477000	-1.32350400
H	4.14580900	-0.12716000	-2.24256500
C	5.98101000	-1.16999000	-2.71268500
H	6.88021800	-1.52199000	-2.18436200
H	5.48893100	-2.07129000	-3.10649300
C	6.39843900	-0.26826200	-3.88036100
H	6.92233700	0.62674600	-3.52017800
H	7.06727000	-0.78805800	-4.57855900
H	5.52238000	0.07112800	-4.44705600
H	1.82242300	-0.57713000	-2.02383400
H	2.03084900	-2.20067300	-1.29941900

ZTS₄₄₋₄₅

C	-0.92581100	0.89820000	0.48275300
C	-2.29249600	2.76340700	0.90437900
C	-2.61509800	1.83148300	1.82847900
N	-1.81318100	0.69789600	1.58152000
N	-1.28976400	2.21628600	0.08337800
C	-1.99470200	-0.51700600	2.32980200
C	-3.17764400	-1.27083800	2.12845700
C	-1.03286500	-0.89745800	3.30072200
C	-3.38504900	-2.41030500	2.92493900
C	-1.28093700	-2.05303900	4.05728200
C	-2.44679400	-2.80195000	3.87856500
H	-4.28634600	-2.99894300	2.78481000
H	-0.55590800	-2.36844200	4.79853600
H	-2.61995800	-3.68942800	4.48125200
C	-0.66664600	2.98228900	-0.96500900
C	0.27156600	3.97936000	-0.60777800
C	-1.05260500	2.77611700	-2.31305200
C	0.83466900	4.76251600	-1.62872500
C	-0.44598800	3.57315600	-3.29670500
C	0.48858000	4.55531900	-2.96240700
H	1.55533500	5.53347800	-1.37410400
H	-0.70913300	3.42443200	-4.33697300
H	0.94267100	5.15971800	-3.74308000
C	0.21518200	-0.04782600	3.54506500
H	0.54016300	0.32906200	2.56609100
C	-0.10945200	1.16483400	4.45271700
H	0.78542300	1.78653700	4.58379800
H	-0.89558500	1.79148800	4.01940300
H	-0.44138600	0.83248100	5.44601900
C	1.39834200	-0.84428600	4.12823000
H	1.20713300	-1.18316000	5.15578300
H	1.63235800	-1.71660900	3.50904300
H	2.28992000	-0.20842200	4.15024900
C	0.64965200	4.25162900	0.84875700
H	0.26624600	3.42334500	1.45196200
C	2.17661000	4.29726200	1.06114800
H	2.40481400	4.41526900	2.12779700
H	2.63908100	3.37150300	0.71086800
H	2.63864800	5.13851100	0.52896100
C	-0.00292500	5.56028200	1.35860100
H	0.25162300	5.73076200	2.41257000
H	0.35133800	6.42308900	0.77975000
H	-1.09473000	5.52514000	1.27422300
C	-2.14584800	1.77146600	-2.68336300
H	-2.02498000	0.90096900	-2.03111600
C	-2.04583500	1.25332500	-4.13004200
H	-2.23906500	2.04451100	-4.86813100
H	-1.06646400	0.80480100	-4.31194200
H	-2.79446800	0.46818700	-4.28197600
C	-3.55028000	2.38344500	-2.44051200
H	-3.68785500	2.68842200	-1.39830700
H	-3.70387700	3.26363400	-3.07995400
H	-4.32695700	1.64739600	-2.68377200
C	-4.23532100	-0.87612600	1.09416600
H	-3.81349400	-0.07859800	0.47567600
C	-4.60287100	-2.04036200	0.14824600
H	-3.72269200	-2.43234400	-0.36730200
H	-5.08080500	-2.86756200	0.68860300
H	-5.31077100	-1.69203700	-0.61399000

C	-5.50952500	-0.32457300	1.78057600
H	-5.97500100	-1.09161400	2.41299800
H	-5.28681100	0.54183400	2.41312100
H	-6.24471400	-0.01636000	1.02663800
Ni	0.42310600	-0.14175600	-0.15956700
C	-1.47786800	-2.36807700	-2.91952100
C	-1.53593300	-3.26846400	-1.81372900
C	-2.32655600	-4.41483600	-1.81942900
C	-3.09703600	-4.66717200	-2.96710800
C	-3.05893900	-3.79203100	-4.06203800
C	-2.25634600	-2.64428800	-4.05407900
C	-0.12140600	-1.53601500	-1.41123300
H	-2.35034300	-5.09361300	-0.96958900
H	-3.72702300	-5.55344300	-3.00414800
H	-3.66401500	-4.01219300	-4.94002100
H	-2.22002000	-1.97915900	-4.91308300
N	-0.68476600	-2.73042000	-0.87333500
N	-0.60085500	-1.34680800	-2.66289500
C	-0.34816700	-3.34486000	0.38832300
H	-1.24608100	-3.53170800	0.98979100
H	0.17744000	-4.30120400	0.23873000
H	0.30023500	-2.66625200	0.94571100
H	-3.32865600	1.85690400	2.63371300
H	-2.67309500	3.75805800	0.74824000
C	2.28821800	-0.67707500	-0.15896100
C	1.63344200	-1.44175300	-1.26414100
C	3.56666100	-0.72163200	0.27293000
C	4.71232000	-1.60925000	-0.32516200
C	4.25100800	-3.04738400	-0.66830100
H	3.62064800	-3.08484300	-1.55881600
H	5.12490500	-3.68331400	-0.87028100
H	3.69333000	-3.49353600	0.16337300
C	5.89738900	-1.78802700	0.65698500
H	6.36059600	-0.84240400	0.95194200
H	5.57845500	-2.30340400	1.57172800
H	6.67913300	-2.40189200	0.18809600
C	5.24630300	-0.96256800	-1.62766900
H	6.02283500	-1.58891400	-2.09410000
H	4.43343600	-0.83440400	-2.35048300
H	5.68082700	0.02522700	-1.43936200
C	3.96494700	0.23497300	1.39960100
H	3.03141400	0.62738800	1.81551100
H	4.47944100	-0.29477200	2.21868900
C	4.83909900	1.44097300	0.99207000
H	4.29515500	2.02501300	0.23700300
H	5.76463500	1.10881600	0.50281200
C	5.21668500	2.33922500	2.17851800
H	4.30105400	2.67844200	2.68252900
H	5.76672500	1.74150300	2.92096600
C	6.06041700	3.55612900	1.78086200
H	5.52038800	4.19394400	1.07009100
H	6.32197900	4.17295500	2.65052600
H	6.99686400	3.24708800	1.29810800
H	1.88106000	-1.06787700	-2.26286100
H	1.77475100	-2.52427900	-1.22666900

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C	-1.87102500	0.79566600	0.23439600
C	-3.34889100	2.52539800	0.86213500
C	-4.04896300	1.36841900	0.93781400
N	-3.17995900	0.32811100	0.55968800
N	-2.04586400	2.19743900	0.43898300
C	-3.60397100	-1.04298000	0.49186100
C	-4.29865100	-1.49086900	-0.65722700
C	-3.37691600	-1.90045200	1.59359200
C	-4.77900000	-2.80966800	-0.67478000
C	-3.86799800	-3.21366900	1.52562000
C	-4.56744800	-3.66675700	0.40592800
H	-5.31396100	-3.17052600	-1.54824800
H	-3.69492800	-3.88832500	2.35862000
H	-4.93923000	-4.68708800	0.37245000
C	-1.02778500	3.19295200	0.25584700
C	-0.29862200	3.64904300	1.38051300
C	-0.82758800	3.75553400	-1.02676200
C	0.61404700	4.70083900	1.20157000
C	0.10416300	4.79766700	-1.15884200
C	0.81428600	5.27511800	-0.05557100
H	1.17880800	5.06821600	2.05291200

H	0.27218300	5.23977100	-2.13649300
H	1.52598900	6.08721800	-0.17571600
C	-2.62409200	-1.43525400	2.83816800
H	-2.29835000	-0.40682800	2.65855400
C	-3.53859800	-1.43663500	4.08551800
H	-4.41947600	-0.80095600	3.93311600
H	-3.89075400	-2.44905600	4.32216800
H	-2.99135600	-1.05955300	4.95889300
C	-1.34824700	-2.27475300	3.07317600
H	-1.58659400	-3.32993000	3.26109500
H	-0.69246500	-2.21139900	2.19837800
H	-0.79976100	-1.89307200	3.94401500
C	-0.49352800	3.02715600	2.76283500
H	-1.07838400	2.11261300	2.62463800
C	0.84656700	2.61755900	3.41259300
H	0.66070100	2.09737200	4.36041000
H	1.40546200	1.94207500	2.75795900
H	1.47896200	3.48761600	3.62988100
C	-1.28996800	3.96909600	3.69765700
H	-0.75472400	4.91516100	3.85187100
H	-2.27594400	4.20220800	3.27992600
H	-1.43845000	3.49991600	4.67861500
C	-1.60143400	3.26622000	-2.24931500
H	-2.20792000	2.41359900	-1.93143400
C	-0.65377600	2.75659100	-3.35800300
H	0.00162200	3.55498800	-3.73014600
H	-0.03160900	1.93971700	-2.97925700
H	-1.23528700	2.37633900	-4.20738800
C	-2.55547200	4.35811100	-2.78833800
H	-3.25951000	4.68617400	-2.01437000
H	-1.99916500	5.23914600	-3.13387300
H	-3.13498200	3.97269700	-3.63683000
C	-4.53429800	-0.57703600	-1.85936800
H	-3.96576500	0.34162200	-1.68640300
C	-4.00710300	-1.19890400	-3.17151700
H	-2.94369600	-1.43999400	-3.08472700
H	-4.54806500	-2.11789300	-3.43101700
H	-4.13385900	-0.49210600	-4.00170000
C	-6.02734700	-0.19256200	-1.99080500
H	-6.65081900	-1.08099800	-2.15549900
H	-6.38829900	0.30893800	-1.08519900
H	-6.17623500	0.48711500	-2.83971400
Ni	-0.40133900	-0.15742600	-0.16425600
C	4.98505000	1.18752800	-0.33468500
C	5.63984700	0.13661800	0.35609100
C	7.03849400	0.11777100	0.41719000
C	7.74438700	1.14590100	-0.20810100
C	7.07723600	2.18294800	-0.88788600
C	5.68306400	2.22079400	-0.96198400
C	3.52516800	-0.24980300	0.53240200
H	7.54980100	-0.68461500	0.94248000
H	8.83171400	1.14915200	-0.17179600
H	7.65769300	2.96979400	-1.36447300
H	5.16789300	3.02206100	-1.48542500
N	4.70692600	-0.73491700	0.88432000
N	3.63593500	0.91866600	-0.20850100
C	2.57128800	1.74377500	-0.75416000
H	2.56159300	2.72923900	-0.27397300
H	2.72064900	1.87529200	-1.83252700
H	1.60599000	1.24516700	-0.59808700
H	-5.07073400	1.18266200	1.22372100
H	-3.64609500	3.54108100	1.06280900
C	1.22958000	-1.25787300	-0.23071200
C	2.20969300	-0.86574800	0.92359100
C	1.55072700	-2.36394500	-0.96233800
C	0.60843800	-2.84669100	-2.11219100
C	1.24128000	-3.93174900	-3.01548700
H	1.49027500	-4.84831300	-2.46807900
H	0.53120700	-4.20961600	-3.80659100
H	2.15460200	-3.57346800	-3.50727800
C	0.23179800	-1.66854900	-3.03848200
H	-0.25714500	-0.87331300	-2.46245900
H	1.12743300	-1.24014100	-3.50746000
H	-0.44782400	-2.00209400	-3.83866000
C	-0.69442500	-3.43186300	-1.51582000
H	-1.38589500	-3.75810800	-2.30860300
H	-0.48423900	-4.29968000	-0.87739900
H	-1.19299500	-2.67435200	-0.90285300
C	2.75849100	-3.25452300	-0.65099800
H	3.21219900	-3.65523100	-1.56718700

H	3.55030200	-2.67128100	-0.17445700
C	2.43567000	-4.44613900	0.28087000
H	1.67509800	-5.09314300	-0.17989200
H	1.98061000	-4.06050300	1.20413300
C	3.66792600	-5.29041900	0.63498800
H	4.12147900	-5.67726700	-0.29000100
H	4.42564700	-4.64165600	1.09612600
C	3.35564000	-6.46078300	1.57515800
H	2.62433600	-7.14615300	1.12653600
H	4.25492500	-7.04343400	1.81463700
H	2.92973800	-6.10233100	2.52114700
H	2.47424300	-1.71514400	1.56704200
H	1.69542700	-0.14501700	1.57395300

TS₄₅₋₄₆

C	-2.15780600	0.58822600	0.52157400
C	-3.51235300	2.07950500	1.73270900
C	-4.34793000	1.25550100	1.05683800
N	-3.54617800	0.35815400	0.32455900
N	-2.19768100	1.68823200	1.42040300
C	-4.10756000	-0.64864400	-0.53504500
C	-4.39762800	-0.32117800	-1.88101900
C	-4.41914200	-1.91983800	0.00290200
C	-5.02154600	-1.29355500	-2.67881500
C	-5.04436500	-2.85751700	-0.83449000
C	-5.34487700	-2.54891200	-2.16236100
H	-5.25249500	-1.06635800	-3.71442600
H	-5.29281200	-3.83951900	-0.44562500
H	-5.82545100	-3.28917400	-2.79593600
C	-1.04472200	2.36896500	1.94804400
C	-0.47129500	1.91546300	3.16005000
C	-0.55658800	3.51508900	1.27861100
C	0.59251100	2.65122100	3.70436600
C	0.50780500	4.21965400	1.86466900
C	1.07587900	3.79662000	3.06708600
H	1.04877200	2.32379100	4.63262500
H	0.89564200	5.10374300	1.36899600
H	1.89772000	4.35553600	3.50632100
C	-4.12491300	-2.25620100	1.46505000
H	-3.36361600	-1.54906200	1.80978400
C	-5.38841900	-2.06715000	2.34091600
H	-5.76390700	-1.03983000	2.28186100
H	-6.19115600	-2.74303600	2.01789700
H	-5.16180200	-2.28571000	3.39230300
C	-3.54700500	-3.67452200	1.65308900
H	-4.27735800	-4.45385500	1.39989500
H	-2.65781100	-3.81974800	1.03301400
H	-3.25898000	-3.82218600	2.70107500
C	-1.01384400	0.68030600	3.87944200
H	-1.55420000	0.08828900	3.13361600
C	0.09990900	-0.22145900	4.45153700
H	-0.33764400	-1.14488200	4.85022600
H	0.82060600	-0.49384300	3.67467800
H	0.64412800	0.26436600	5.27178400
C	-2.01336300	1.08107000	4.99265400
H	-1.52062600	1.69708800	5.75644500
H	-2.85438600	1.65241800	4.58484100
H	-2.41691100	0.18701400	5.48526900
C	-1.17894200	4.00869400	-0.02693700
H	-1.83700300	3.21477100	-0.39320100
C	-0.12537400	4.26580600	-1.12613800
H	0.56275600	5.07510500	-0.84639400
H	0.45862000	3.36267200	-1.33811700
H	-0.62917600	4.57224500	-2.05260100
C	-2.04580900	5.26837500	0.21936700
H	-2.84006100	5.07256700	0.94982700
H	-1.43432600	6.09765400	0.59867100
H	-2.51612000	5.59616300	-0.71636200
C	-4.08640100	1.06439300	-2.44863000
H	-3.34941300	1.52767900	-1.78535700
C	-3.45826200	1.01337900	-3.85770500
H	-2.56472600	0.38292800	-3.86681000
H	-4.16200500	0.63008900	-4.60779800
H	-3.16333700	2.02278700	-4.16864700
C	-5.35365900	1.95507500	-2.45325800
H	-6.13263800	1.52149000	-3.09416900
H	-5.76605600	2.06666300	-1.44443800

H	-5.11596600	2.95565100	-2.83594600
Ni	-0.68507300	-0.23899400	-0.14160100
C	5.61670800	0.40075400	0.23387700
C	5.56640700	-1.01680800	0.29327900
C	6.75100300	-1.75668300	0.18767800
C	7.95249300	-1.06835900	0.02793700
C	7.98562600	0.33856100	-0.02773700
C	6.81765500	1.09576700	0.07487500
C	3.53482700	-0.33778300	0.50571600
H	6.71791700	-2.84201900	0.23015400
H	8.88323700	-1.62496000	-0.05694500
H	8.93907200	0.84660400	-0.15356200
H	6.85112400	2.18150000	0.03282000
N	4.26416600	-1.43933600	0.46791300
N	4.30235300	0.80891500	0.36950700
C	3.81166200	2.18015400	0.36741200
H	2.97664600	2.25511900	-0.33630800
H	3.49981200	2.49043800	1.37174000
H	4.61892400	2.83683800	0.03279300
H	-5.42338700	1.21838600	1.02212900
H	-3.71986800	2.90138600	2.39662500
C	1.22063300	-0.67945600	-0.51809700
C	2.04665800	-0.29277800	0.72911000
C	0.59598000	-1.92746900	-0.56601300
C	0.18548200	-2.55180200	-1.94502400
C	1.43416100	-3.19737500	-2.60144900
H	1.82642200	-4.02957000	-2.00943200
H	1.18936000	-3.58755300	-3.60093900
H	2.23552100	-2.46039200	-2.70291100
C	-0.35371900	-1.49062200	-2.92165300
H	-1.28822100	-1.05999200	-2.54361500
H	0.35248800	-0.67075700	-3.04460500
H	-0.54882600	-1.94319500	-3.90575700
C	-0.90499200	-3.63829200	-1.81317700
H	-1.20396400	-3.99117300	-2.80984800
H	-0.55972800	-4.51457000	-1.25186500
H	-1.79837000	-3.24113400	-1.31781400
C	0.58361400	-2.90971700	0.62406200
H	0.58096600	-2.32518000	1.55054200
H	-0.37123300	-3.45101100	0.64268200
C	1.73176300	-3.93915100	0.73543600
H	2.69134700	-3.42658000	0.59515300
H	1.65060900	-4.69057100	-0.06257600
C	1.73247900	-4.66878800	2.08677900
H	1.83174600	-3.92905000	2.89476500
H	0.75937100	-5.16004200	2.24293600
C	2.85353100	-5.70706700	2.21380400
H	3.83643500	-5.23544500	2.09345500
H	2.83785600	-6.20811200	3.19089500
H	2.76409100	-6.48187200	1.44091500
H	1.86718200	-0.93691500	1.60223600
H	1.77527900	0.72340200	1.03535600
H	1.52314700	0.49021300	-1.56856300
O	1.79470000	1.49799400	-2.00457000
C	2.41576500	1.58032100	-3.26856800
C	3.26201700	0.32885000	-3.57982500
C	1.35184200	1.77899900	-4.37376500
C	3.34317300	2.81515100	-3.26038900
H	3.98323200	0.14738000	-2.77560500
H	2.63035000	-0.55930900	-3.67021100
H	3.81634500	0.44704500	-4.52144200
H	0.76426800	2.68103300	-4.16590900
H	1.80717000	1.88358400	-5.36928800
H	0.66228800	0.92959300	-4.40009200
H	3.78772800	2.99604800	-4.24904600
H	2.77756800	3.70779000	-2.96771000
H	4.15924000	2.67703300	-2.54238000

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C	2.28737600	-0.57588000	0.53332100
C	3.63916400	-2.05932700	1.71126400
C	4.46726600	-1.20032700	1.06711200
N	3.65110100	-0.30462700	0.35010000
N	2.32383800	-1.68504200	1.38878400
C	4.18400100	0.76825700	-0.45249100
C	4.52235200	0.51392900	-1.80249100
C	4.39951200	2.03028200	0.14713900
C	5.09488400	1.55952400	-2.54400300

C	4.97516700	3.04255500	-0.63740100	H	-1.92001100	1.74232600	-4.24873900
C	5.32043400	2.81140100	-1.96924900	H	-2.65617500	1.05407700	-2.78952500
H	5.35989200	1.39355700	-3.58247800	C	-0.16819300	0.03613600	-3.07979200
H	5.14971000	4.02084300	-0.20140300	H	0.81772400	-0.27029900	-2.70580800
H	5.76108200	3.60805500	-2.56167500	H	-0.90584700	-0.71571800	-2.76747000
C	1.15742700	-2.34826900	1.92586500	H	-0.13068700	0.03111000	-4.17956300
C	0.72154700	-1.99977600	3.22456700	C	0.50733700	2.43795700	-3.19504900
C	0.50544000	-3.33960900	1.15331900	H	0.53947600	2.31171800	-4.28512500
C	-0.38803800	-2.67959700	3.75212200	H	0.26272500	3.48863000	-2.99766100
C	-0.60797000	-3.97788000	1.72177300	H	1.51453500	2.24485600	-2.80476700
C	-1.04863000	-3.65712900	3.00757900	C	-0.27056400	2.91202400	-0.38380200
H	-0.74292500	-2.43047400	4.74741600	H	-0.09851000	2.76041900	0.68905700
H	-1.14485600	-4.71832300	1.14206400	H	0.67546100	3.31400700	-0.77140800
H	-1.91365100	-4.16475100	3.42451200	C	-1.36174200	3.99916500	-0.52097500
C	4.05818500	2.29723700	1.61309700	H	-2.32020300	3.59316700	-0.17579400
H	3.44491300	1.46259700	1.96593000	H	-1.48866900	4.27725300	-1.57550900
C	5.34020800	2.34497800	2.47946800	C	-1.02752200	5.26241200	0.28439200
H	5.90697000	1.40986500	2.40328000	H	-0.91004400	4.99294200	1.34414300
H	5.99739500	3.16542000	2.16395600	H	-0.05393200	5.66169900	-0.03976700
H	5.08296800	2.50337300	3.53418000	C	-2.09530600	6.35530600	0.15902900
C	3.22083500	3.58109200	1.79981000	H	-3.06823800	5.98959000	0.50841000
H	3.78157000	4.48041200	1.51602300	H	-1.83800600	7.24505200	0.74848400
H	2.30765800	3.54099100	1.19897200	H	-2.21739800	6.67099000	-0.88528400
H	2.93290800	3.69005800	2.85267000	H	-1.38568700	1.49044200	1.63819300
C	1.42093800	-0.92649300	4.06053900	H	-1.60341500	-0.25942300	1.64294300
H	2.17602000	-0.44973200	3.42781800	H	-1.59289200	-0.31627900	-0.88338300
C	0.44627800	0.18251700	4.51647100	O	-2.50560000	-2.10950200	-1.92995700
H	0.99007000	0.96068700	5.06694800	C	-3.33490600	-2.65162400	-2.87532400
H	-0.04335200	0.64758300	3.65573500	C	-4.48918300	-1.67249600	-3.24709700
H	-0.33339600	-0.21162700	5.17945000	C	-2.55732900	-2.98484500	-4.18470500
C	2.15196500	-1.54897500	5.27445000	C	-3.98281500	-3.97742200	-2.36522700
H	1.44375000	-2.04751000	5.94803200	H	-5.06703600	-1.41812000	-2.34921100
H	2.89058400	-2.29369000	4.95512200	H	-4.06714100	-0.74026700	-3.64194600
H	2.67486300	-0.77302900	5.84775200	H	-5.18677300	-2.07808300	-3.99800700
C	1.01545500	-3.74490100	-0.23067600	H	-1.74072200	-3.68332400	-3.96162900
H	1.48713900	-2.86060200	-0.67396600	H	-3.18986900	-3.43402500	-4.96756800
C	-0.09674400	-4.19887800	-1.19735200	H	-2.10896400	-2.06940400	-4.58963800
H	-0.54805600	-5.14770700	-0.87302900	H	-4.64316000	-4.45811400	-3.10513600
H	-0.89640300	-3.44939000	-1.32810800	H	-3.19441900	-4.69183800	-2.09533200
H	0.34647900	-4.38194600	-2.18520300	H	-4.57596000	-3.78148600	-1.46201900
C	2.09999100	-4.84708200	-0.09664400				
H	2.94429100	-4.52265400	0.52282200				
H	1.67257800	-5.75220600	0.35442700				
H	2.48759600	-5.11435900	-1.08759200				
C	4.31347600	-0.86179900	-2.43680700				
H	3.57717000	-1.39534400	-1.82688000				
C	3.74739600	-0.78568600	-3.87101900				
H	2.82865600	-0.19350200	-3.90391100				
H	4.46859400	-0.34872500	-4.57322700				
H	3.51043100	-1.79442600	-4.22888500				
C	5.62766600	-1.68235600	-2.42032400				
H	6.40629800	-1.18118400	-3.00983700				
H	6.00563800	-1.81459900	-1.40071200				
H	5.46037400	-2.67681300	-2.85190000				
Ni	0.78157600	0.25617000	-0.15141000				
C	-5.46313800	0.43088400	0.90970400				
C	-5.23376300	1.81900100	1.09922300				
C	-6.32072400	2.69944300	1.17871100				
C	-7.60662600	2.17618800	1.06666900				
C	-7.81819600	0.79563800	0.87632000				
C	-6.75165200	-0.09845500	0.79389200				
C	-3.30265600	0.88303100	1.05080800				
H	-6.14920800	3.76308800	1.32172500				
H	-8.46492800	2.84215000	1.12203300				
H	-8.83447500	0.41911000	0.78573100				
H	-6.92233300	-1.15957100	0.63560700				
N	-3.87800600	2.06705400	1.18780900				
N	-4.20686500	-0.14593100	0.89015100				
C	-3.89733500	-1.56606900	0.71336700				
H	-3.40366400	-1.76497400	-0.26524300				
H	-3.25505000	-1.90587800	1.53366200				
H	-4.83658200	-2.12283000	0.76738100				
H	5.54123900	-1.13453500	1.04653200				
H	3.85099000	-2.89122000	2.36030200				
C	-1.19261700	0.52914200	-0.31548400				
C	-1.81423500	0.65701000	1.07707300				
C	-0.54892500	1.55106700	-1.03040800				
C	-0.52222100	1.45977700	-2.58935500				
C	-1.92982200	1.78863200	-3.15034400				
H	-2.27555400	2.78673300	-2.86213000				
H	-1.24336400	0.31365700	-0.00017500				
C	-3.13916000	1.68544200	0.00047500				
C	-3.57445800	0.39983200	0.00044500				
N	-2.43622100	-0.42458100	0.00003400				
N	-1.73288900	1.63574300	0.00010200				
C	-2.49155300	-1.86649000	-0.00003500				
C	-2.52321500	-2.55198900	-1.23574300				
C	-2.52273200	-2.55207600	1.23562200				
C	-2.58216600	-3.95453600	-1.20891600				
C	-2.58172200	-3.95462400	1.20872200				
C	-2.61057600	-4.65161400	-0.00011300				
H	-2.60000200	-4.50429300	-2.14448300				
H	-2.59924200	-4.50443000	2.14426900				
H	-2.65360900	-5.73653400	-0.00014700				
C	-0.86653800	2.78071800	0.00018400				
C	-0.43639200	3.32107800	1.23829700				
C	-0.43659200	3.32143800	-1.23781800				
C	0.48897600	4.38092800	1.21207400				
C	0.48881000	4.38128000	-1.21142400				
C	0.95936300	4.90039200	0.00035900				
H	0.83634100	4.80705200	2.14746800				
H	0.83605700	4.80762600	-2.14676000				
H	1.66833900	5.72269900	0.00043600				
C	-2.46562700	-1.82068100	2.57645900				
H	-2.50058600	-0.74557700	2.37344700				
C	-3.67650700	-2.16451400	3.47374800				
H	-4.62327400	-1.93377100	2.97158100				
H	-3.68985600	-3.22744600	3.74257600				
H	-3.63375100	-1.58735100	4.40525700				
C	-1.12980600	-2.10275500	3.30364800				
H	-1.02009300	-3.16976700	3.53359800				

Cartesian coordinates for the stationary points given in Fig. S6.

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H	-0.28268300	-1.79322100	2.68120000
H	-1.08592100	-1.54770600	4.24895500
C	-0.93024100	2.77803700	2.57860100
H	-1.64613200	1.97854400	2.36673400
C	0.22209900	2.15536500	3.40116800
H	-0.16293300	1.75038000	4.34437100
H	0.69215500	1.33426200	2.84706200
H	0.98879600	2.90101500	3.64809200
C	-1.66884900	3.87010700	3.38771100
H	-0.99866200	4.69661500	3.65325000
H	-2.50966300	4.28685200	2.82152100
H	-2.06085000	3.44671200	4.31963500
C	-0.93055000	2.77873700	-2.57822300
H	-1.64678600	1.97951400	-2.36649800
C	0.22167500	2.15567100	-3.40068000
H	0.98869900	2.90106700	-3.64736200
H	0.69127900	1.33431500	-2.84655500
H	-0.16335500	1.75094800	-4.34399600
C	-1.66859700	3.87115800	-3.38734700
H	-2.50924500	4.28830400	-2.82120700
H	-0.99801200	4.69734900	-3.65286800
H	-2.06075200	3.44795300	-4.31929400
C	-2.46628600	-1.82047700	-2.57652700
H	-2.50248400	-0.74541400	-2.37348900
C	-1.12974400	-2.10120500	-3.30294100
H	-0.28330000	-1.79084300	-2.67997000
H	-1.01888300	-3.16813200	-3.53275200
H	-1.08583100	-1.54614800	-4.24824500
C	-3.67628000	-2.16545500	-3.47454100
H	-3.68828700	-3.22830300	-3.74375400
H	-4.62358600	-1.93594100	-2.97282800
H	-3.63366400	-1.58795700	-4.40584800
Ni	0.49607800	-0.25152000	-0.00042300
C	4.28417500	-1.90892200	-0.00000700
C	4.58241900	-0.52453000	-0.00019200
C	5.91834500	-0.10397800	-0.00016400
C	6.92006600	-1.07451200	0.00007000
C	6.60766000	-2.44680200	0.00026000
C	5.28219700	-2.88576900	0.00022500
C	2.36494800	-0.69165000	-0.00039100
H	6.16267400	0.95597600	-0.00030400
H	7.96315800	-0.76777300	0.00010200
H	7.41200800	-3.17799000	0.00044600
H	5.04342700	-3.94605900	0.00037600
N	3.40117800	0.19262500	-0.00046200
N	2.90433300	-1.98017100	-0.00010500
C	2.14167300	-3.21009800	-0.00011500
H	2.36407400	-3.81174900	-0.89088600
H	2.36373000	-3.81157000	0.89086300
H	1.08033500	-2.95043900	-0.00034300
H	-4.57207500	-0.00495600	0.00064900
H	-3.68348100	2.61438200	0.00078200
Na	2.01929400	1.94109900	-0.00059300

TS₄₇₋₄₈

C	-1.02595300	0.78384000	0.95398600
C	-2.22448000	2.75479200	1.32446700
C	-2.54731000	1.90193700	2.32393000
N	-1.84657300	0.70310100	2.09665100
N	-1.31361700	2.08429000	0.48207200
C	-2.09551700	-0.49906700	2.85953100
C	-3.25937900	-1.25369400	2.57038800
C	-1.20849100	-0.86641900	3.89888500
C	-3.50392000	-2.40744000	3.33310500
C	-1.49661500	-2.03248300	4.62639000
C	-2.62817300	-2.79961500	4.34489200
H	-4.38971100	-3.00138700	3.13423100
H	-0.83200500	-2.34184800	5.42437100
H	-2.83149800	-3.69702200	4.92137100
C	-0.84003100	2.62182100	-0.77104500
C	0.24878100	3.53519600	-0.78151500
C	-1.50185300	2.24205900	-1.96929500
C	0.69917000	4.01046500	-2.02908500
C	-1.01312900	2.75158700	-3.18328500
C	0.08139500	3.61601500	-3.21800800
H	1.52177400	4.71558200	-2.06667900
H	-1.49045600	2.46290600	-4.11109900
H	0.44099300	3.99846200	-4.16847500

C	-0.01621600	0.01298900	4.27510300
H	0.29781500	0.54095600	3.36835900
C	-0.43442300	1.06945500	5.32963300
H	0.41544800	1.71783900	5.57551300
H	-1.24938000	1.70368300	4.96422500
H	-0.77009300	0.58343500	6.25443200
C	1.19951100	-0.79049300	4.77802100
H	0.99790000	-1.29056300	5.73306500
H	1.50478300	-1.54328800	4.04429700
H	2.04664500	-0.11500800	4.93987800
C	0.87689200	4.07383400	0.50756900
H	0.75848300	3.30652800	1.28161600
C	2.38208500	4.39629600	0.37058100
H	2.80804800	4.60265100	1.35774600
H	2.95255700	3.56808700	-0.06447700
H	2.54948300	5.28373300	-0.25100700
C	0.14379900	5.35587300	0.98415800
H	0.59642000	5.72738600	1.91115300
H	0.22149300	6.14454100	0.22585400
H	-0.91602400	5.17467000	1.17723600
C	-2.74921500	1.35506300	-1.94908900
H	-2.60671700	0.61539500	-1.15280600
C	-2.98763800	0.58244000	-3.26211400
H	-3.29669400	1.25166700	-4.07534300
H	-2.10057500	0.03254700	-3.58411200
H	-3.79825400	-0.14030300	-3.11607800
C	-4.01161100	2.19544200	-1.61869600
H	-3.93526400	2.69467500	-0.64913600
H	-4.17400400	2.95989200	-2.38893700
H	-4.89612500	1.54728700	-1.59607000
C	-4.27701700	-0.81702900	1.51316400
H	-3.80231300	-0.05820100	0.88362400
C	-4.72110500	-1.96856400	0.58520100
H	-3.86271800	-2.44522000	0.10470500
H	-5.27955500	-2.73905100	1.12946600
H	-5.38047200	-1.58046100	-0.20032900
C	-5.51701700	-0.17138500	2.18164800
H	-6.02861400	-0.89458400	2.82847900
H	-5.24052800	0.69153000	2.79633900
H	-6.22944100	0.16711000	1.41968200
Ni	0.30031200	-0.38445500	0.44854200
C	0.13161400	-1.35646700	-3.40879800
C	-0.70130400	-2.43157100	-2.99792800
C	-1.38298300	-3.23553400	-3.90754400
C	-1.22206700	-2.94870700	-5.26962700
C	-0.40478400	-1.88996200	-5.69328100
C	0.27673800	-1.08428900	-4.77543100
C	0.20279700	-1.39313100	-1.20084000
H	-2.01124600	-4.06050700	-3.58216000
H	-1.73456400	-3.56067500	-6.00692600
H	-0.29625200	-1.69458400	-6.75721300
H	0.91121100	-0.26628400	-5.10836200
N	-0.65515200	-2.42167300	-1.61160700
N	0.68005500	-0.74238600	-2.30484900
C	-1.28881700	-3.38601000	-0.74383500
H	-1.40087800	-2.94795900	0.25114000
H	-2.28286900	-3.63642500	-1.12929600
H	-0.70631200	-4.31514700	-0.66393700
H	-3.20905200	2.02248800	3.16369600
H	-2.56164000	3.75571300	1.12308000
C	2.21412000	-0.83110200	0.64777700
C	1.52292300	-1.93515200	-0.09695000
C	3.56066400	-0.77343200	0.79124200
C	4.27873900	0.29920800	1.64606500
C	3.30590300	1.35345300	2.19213900
H	2.53640200	0.89301000	2.81349200
H	3.85059800	2.09813100	2.78822700
H	2.78211200	1.87481100	1.38787400
C	5.38051000	1.02501800	0.83693400
H	6.13679100	0.33327600	0.45079000
H	4.95356300	1.56213400	-0.02225600
H	5.89924800	1.76307500	1.46271700
C	4.94485900	-0.37986600	2.87249500
H	5.43112700	0.37148700	3.50864300
H	4.19508000	-0.90279000	3.47602900
H	5.71102400	-1.10723400	2.58443900
C	4.47327400	-1.85083600	0.18193600
H	5.43644300	-1.89930700	0.70493700
H	4.01469100	-2.83953000	0.31931400
C	4.76763800	-1.66045800	-1.32350800

H	5.25974200	-0.68943300	-1.47938600
H	3.82140100	-1.61558500	-1.88070000
C	5.64854400	-2.76778800	-1.91838300
H	6.59887100	-2.81087000	-1.36685800
H	5.16086500	-3.74037900	-1.76031000
C	5.93195300	-2.57683800	-3.41244500
H	6.44982600	-1.62731500	-3.59925900
H	6.56181800	-3.38189200	-3.80896300
H	5.00081200	-2.56614000	-3.99269200
H	2.05890700	-2.40426500	-0.92505800
H	1.12591600	-2.72092400	0.55978000
Na	1.85378700	0.94590200	-1.29036500

C	-0.00349000	-1.24971800	-3.67791300
C	-0.89030000	-2.28862300	-3.28949000
C	-1.62095400	-3.03059600	-4.21405000
C	-1.45004600	-2.71877200	-5.56887900
C	-0.57582000	-1.69698800	-5.97123600
C	0.15295100	-0.95321700	-5.03822100
C	0.07180200	-1.34236900	-1.47327700
H	-2.29338800	-3.82639300	-3.90481700
H	-1.99943100	-3.28183800	-6.31847000
H	-0.46079800	-1.48248100	-7.03074400
H	0.83164800	-0.16466100	-5.35456000
N	-0.83279800	-2.31906800	-1.90478900
N	0.58275100	-0.69578300	-2.56161800
C	-1.54211000	-3.24817800	-1.05825900
H	-1.53966600	-2.86094700	-0.03694600
H	-2.58108800	-3.34425600	-1.39304000
H	-1.08153600	-4.24619700	-1.06782100
H	-3.26269400	1.91828000	3.08957700
H	-2.84865500	3.64712700	0.98031100
C	2.10472100	-0.85161100	0.33515500
C	1.35580500	-1.94391500	-0.35178700
C	3.40218600	-0.82932800	0.71759200
C	4.38574000	-2.04319500	0.61025200
C	3.71991700	-3.35401000	1.09367600
H	2.90853200	-3.68341000	0.44196700
H	4.46114900	-4.16366600	1.12219600
H	3.31165100	-3.23422600	2.10397000
C	5.65181400	-1.87151500	1.48418500
H	6.24472400	-0.99185100	1.21469900
H	5.39978900	-1.79620800	2.54854000
H	6.30104700	-2.74775500	1.36282400
C	4.84656400	-2.22884900	-0.85766200
H	5.50287500	-3.10503600	-0.95326400
H	3.99604000	-2.37423300	-1.53133000
H	5.40578600	-1.35570600	-1.21369100
C	3.96522600	0.47005900	1.29353400
H	3.11482500	1.09619600	1.58625600
H	4.53870100	0.28020400	2.21113400
C	4.86596200	1.28184400	0.33529700
H	4.25421400	1.65517700	-0.50652400
H	5.62309400	0.63480000	-0.12479900
C	5.57244900	2.46814500	1.00589300
H	4.82933500	3.10323100	1.50720100
H	6.22646700	2.08417500	1.80147300
C	6.39814900	3.31469800	0.03116300
H	5.76396200	3.74834300	-0.75325100
H	6.90302300	4.14196500	0.54355900
H	7.16814900	2.71062600	-0.46463700
H	1.87147800	-2.44817600	-1.17273700
H	0.90111700	-2.69633200	0.30355800
Na	1.74873400	0.99558800	-1.52276700

ZTS₄₇₋₄₈

C	-1.14720400	0.77011200	0.76715500
C	-2.45032800	2.66685600	1.17430500
C	-2.65428400	1.81765000	2.20816200
N	-1.88822900	0.66318200	1.96155900
N	-1.55314300	2.03424400	0.29135700
C	-1.89672500	-0.48280500	2.84015600
C	-2.97499700	-1.39856200	2.76146000
C	-0.85752900	-0.63238200	3.78991600
C	-2.97946300	-2.48726700	3.64888200
C	-0.90801000	-1.74207200	4.64871600
C	-1.95412600	-2.66296000	4.57825800
H	-3.79318100	-3.20346100	3.61352800
H	-0.12336900	-1.88433800	5.38287800
H	-1.97409200	-3.51333000	5.25317500
C	-1.04011700	2.64465000	-0.90697700
C	0.04529900	3.55172900	-0.79923400
C	-1.63476400	2.33485500	-2.15601800
C	0.57080200	4.09748500	-1.98592000
C	-1.07547500	2.91110200	-3.30875100
C	0.02279400	3.77061100	-3.22953900
H	1.39144200	4.80547200	-1.93224600
H	-1.49851600	2.68019800	-4.27829600
H	0.43612200	4.20497900	-4.13490100
C	0.24662900	0.41510200	3.94091300
H	0.34519400	0.92871500	2.97912600
C	-0.14946900	1.46112000	5.01395400
H	0.62547500	2.23303300	5.09832000
H	-1.09529600	1.95493100	4.76458300
H	-0.26385800	0.98669700	5.99679100
C	1.62683000	-0.19302700	4.26129000
H	1.64783900	-0.68113300	5.24336600
H	1.91972700	-0.91779000	3.49583200
H	2.38253900	0.60085900	4.27650200
C	0.57209600	4.01615800	0.56068900
H	0.24434800	3.28858600	1.30979400
C	2.11041200	4.08843300	0.63402400
H	2.42069600	4.37646500	1.64489100
H	2.56674300	3.11758500	0.41690000
H	2.52415000	4.83109800	-0.05854700
C	-0.03732300	5.39341900	0.92839400
H	0.29782600	5.70467000	1.92488900
H	0.27449400	6.16035700	0.20876700
H	-1.13160800	5.36292000	0.93262300
C	-2.87714200	1.44519300	-2.24264900
H	-2.75363100	0.64988200	-1.49763000
C	-3.07156600	0.77746200	-3.61823900
H	-3.35919600	1.50905400	-4.38437000
H	-2.17246300	0.25718400	-3.95562200
H	-3.88151200	0.04228700	-3.55544800
C	-4.15389900	2.25166400	-1.88451300
H	-4.11225100	2.66535900	-0.87344800
H	-4.29359500	3.07929900	-2.59123800
H	-5.03538400	1.60229200	-1.94714200
C	-4.14296200	-1.19891400	1.79192000
H	-3.79905600	-0.53732900	0.98897900
C	-4.62387400	-2.51381700	1.13934000
H	-3.79517200	-3.06935400	0.69255700
H	-5.11953500	-3.16913500	1.86522600
H	-5.35286500	-2.29240400	0.35094100
C	-5.33920600	-0.51223200	2.49936400
H	-5.70700500	-1.13682700	3.32270300
H	-5.06272700	0.46219800	2.91251600
H	-6.16417000	-0.35885500	1.79301400
Ni	0.20049900	-0.33035200	0.18076800

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C	-1.80023000	0.68641500	-0.48252200
C	-3.02797900	2.30016100	-1.64739300
C	-3.78760300	1.91221400	-0.59333200
N	-3.05161200	0.94077000	0.11221500
N	-1.83095600	1.56831100	-1.58182000
C	-3.56488000	0.28393800	1.28845000
C	-4.41391000	-0.83547000	1.13335100
C	-3.25675100	0.81320400	2.56513800
C	-4.96364800	-1.41265300	2.29013700
C	-3.82895100	0.19944600	3.68994600
C	-4.67735100	-0.90237000	3.55588200
H	-5.62183300	-2.26994200	2.19649400
H	-3.61571300	0.58786400	4.67999400
H	-5.11456400	-1.36030100	4.43799300
C	-0.75011100	1.73459300	-2.51995900
C	0.15841900	2.80266000	-2.33269600
C	-0.64727800	0.85578000	-3.62278400
C	1.18375200	2.97219400	-3.27734700
C	0.39931500	1.06266600	-4.53585100
C	1.30717700	2.10981000	-4.36890000
H	1.88585900	3.79207200	-3.15963100
H	0.49949200	0.39885900	-5.38873000
H	2.10329100	2.25890900	-5.09253400
C	-2.35707200	2.04021900	2.71914900
H	-1.71366000	2.08088400	1.83270600
C	-3.18986500	3.34543900	2.76785600

H	-3.78908100	3.46753000	1.86005000
H	-3.87073300	3.33986900	3.62814800
H	-2.53171900	4.21842800	2.85912800
C	-1.43390000	1.96259200	3.95484100
H	-1.99206600	2.05876000	4.89354900
H	-0.89450000	1.00606900	3.99715500
H	-0.69793500	2.77466400	3.92584500
C	0.04492800	3.76747000	-1.15245000
H	-0.76202200	3.40846900	-0.50643600
C	1.33258000	3.78909500	-0.29857300
H	1.20482600	4.45854600	0.56096400
H	1.56283000	2.78734200	0.07868900
H	2.19493900	4.15003300	-0.87253400
C	-0.32936700	5.19240200	-1.62513700
H	0.44652200	5.61131700	-2.27762700
H	-1.27227700	5.19128800	-2.18401900
H	-0.44329600	5.86277600	-0.76459300
C	-1.63184700	-0.29076700	-3.84660400
H	-2.35248200	-0.27488000	-3.02350900
C	-0.92164600	-1.66305100	-3.80163000
H	-0.17555800	-1.75560200	-4.60096300
H	-0.41871300	-1.80190000	-2.83801100
H	-1.65167500	-2.47189400	-3.92856800
C	-2.41965600	-0.11029000	-5.16543400
H	-2.95812200	0.84451400	-5.18026000
H	-1.75361000	-0.13402400	-6.03656800
H	-3.15233900	-0.91780100	-5.28295700
C	-4.76240200	-1.39991300	-0.24392000
H	-4.06509100	-0.96172800	-0.96507000
C	-4.58811900	-2.93263000	-0.31630600
H	-3.57540900	-3.22725700	-0.02608700
H	-5.29917900	-3.45566400	0.33468500
H	-4.76498600	-3.27970000	-1.34145600
C	-6.19705600	-0.99494200	-0.66297700
H	-6.93891800	-1.40323000	0.03466200
H	-6.31599500	0.09409500	-0.68234500
H	-6.42549900	-1.37998700	-1.66410400
Ni	-0.44196300	-0.46787000	-0.08768700
C	4.67312400	1.67183300	1.00647500
C	3.86838700	1.32168200	2.11358500
C	4.10226100	1.90905500	3.36217000
C	5.13418400	2.83864900	3.46792400
C	5.92468200	3.18125700	2.35435600
C	5.70783000	2.60433200	1.10374600
C	3.13331900	0.15816000	0.43450600
H	3.49656500	1.63848800	4.22338800
H	5.33615600	3.30827200	4.42653500
H	6.72049900	3.91165200	2.47043900
H	6.31973200	2.87852500	0.24920700
N	2.92056700	0.38491500	1.72474700
N	4.18827800	0.90970000	-0.04745300
C	4.64754600	0.96220300	-1.42472500
H	4.65948700	-0.04251800	-1.85357000
H	3.99811000	1.59842000	-2.03693100
H	5.66448300	1.35967800	-1.44598400
H	-4.77046100	2.22206800	-0.28248800
H	-3.21968900	3.01499200	-2.42921000
C	1.17728400	-1.52772700	0.16992100
C	2.36014600	-0.76439800	-0.47050500
C	1.43173000	-2.78882800	0.63912100
C	0.27879800	-3.69319100	1.18715900
C	-0.63372100	-4.11665700	0.00897800
H	-0.06859800	-4.67058300	-0.75029100
H	-1.45296800	-4.76272700	0.35647700
H	-1.05888600	-3.22807200	-0.46901100
C	-0.59762800	-2.94831500	2.21910400
H	-0.00501400	-2.67013300	3.10789900
H	-1.04343300	-2.04738500	1.77665200
H	-1.41585700	-3.58851900	2.57452700
C	0.77757800	-4.97882400	1.88605300
H	-0.08367500	-5.56121700	2.23638500
H	1.35538100	-5.62736700	1.21893500
H	1.39880300	-4.75682700	2.76296300
C	2.81745500	-3.43854100	0.55079100
H	3.59509500	-2.66796300	0.61307600
H	2.99999300	-4.08500900	1.41660100
C	3.06837400	-4.26914900	-0.72802200
H	2.89058400	-3.63696800	-1.60972900
H	2.33248900	-5.08225300	-0.79425700
C	4.48212400	-4.86258100	-0.79786200

H	5.21975900	-4.04948900	-0.72716600
H	4.65137600	-5.49975900	0.08213800
C	4.73883800	-5.67397000	-2.07255000
H	4.60955900	-5.05443900	-2.96903100
H	5.75661900	-6.08154900	-2.09301400
H	4.04107100	-6.51686500	-2.15283200
H	1.96258600	-0.13942500	-1.28384600
H	3.09546500	-1.42495800	-0.95906900
Na	0.75107700	-0.29101600	2.26832700

TS₄₈₋₄₉

C	1.94594600	0.32534300	0.66819500
C	3.65098900	0.17468700	2.25628400
C	3.82888000	1.34643000	1.59948000
N	2.80628800	1.44328800	0.63975200
N	2.51772300	-0.44435100	1.70287400
C	2.69107900	2.57897900	-0.24538000
C	3.42975100	2.59063500	-1.45292900
C	1.90182500	3.68205900	0.15399800
C	3.33645000	3.73105500	-2.26704100
C	1.83877200	4.79639800	-0.69711300
C	2.54543600	4.82043300	-1.89956700
H	3.88781000	3.76575300	-3.19968800
H	1.23911400	5.65486500	-0.41200200
H	2.48560600	5.68974000	-2.54688100
C	2.06437600	-1.75238600	2.12212500
C	1.26317500	-1.86142900	3.28395400
C	2.48383000	-2.88969600	1.39211200
C	0.86196700	-3.14327600	3.69185800
C	2.05190800	-4.14748000	1.84109500
C	1.24634800	-4.27562400	2.97294300
H	0.24901900	-3.25696400	4.57995400
H	2.34437300	-5.03401900	1.29173900
H	0.92139400	-5.25910700	3.29763900
C	1.17052700	3.71542300	1.49578600
H	1.25787200	2.71530100	1.93938000
C	1.84463800	4.70484900	2.47677100
H	2.89504900	4.44267000	2.64312800
H	1.81064500	5.72794200	2.08432100
H	1.33228200	4.69738100	3.44693400
C	-0.33215600	4.04665500	1.33787000
H	-0.48003300	5.07644300	0.99349200
H	-0.81581200	3.39232800	0.60244300
H	-0.85207600	3.95484600	2.30146400
C	0.88819900	-0.64468300	4.13341500
H	1.10385700	0.25529700	3.53967200
C	-0.60624600	-0.62051300	4.53400400
H	-0.85021300	0.32423000	5.03695800
H	-1.27812200	-0.74184400	3.67585100
H	-0.84025400	-1.42748600	5.23696600
C	1.77149700	-0.56140900	5.40353600
H	1.61447700	-1.44287400	6.03612700
H	2.83494200	-0.51606500	5.14799100
H	1.52226300	0.33012000	5.99214700
C	3.43380900	-2.77817500	0.19917200
H	3.31489100	-1.77406800	-0.22148700
C	3.11786100	-3.78131700	-0.92897900
H	3.34657800	-4.81276400	-0.62886800
H	2.06479900	-3.72319100	-1.22827200
H	3.74436200	-3.55620900	-1.80109500
C	4.90419300	-2.92702800	0.66933600
H	5.17279500	-2.17505200	1.42015000
H	5.07046300	-3.91923100	1.10730700
H	5.58563900	-2.81549500	-0.18273400
C	4.35190500	1.43556800	-1.84729200
H	4.01566700	0.54517500	-1.30474600
C	4.30274200	1.10494800	-3.35455100
H	3.27793600	0.93635100	-3.69489800
H	4.74199500	1.90594000	-3.96147000
H	4.87999100	0.19420500	-3.55099000
C	5.81336700	1.72932300	-1.42123200
H	6.19157600	2.62371600	-1.93157500
H	5.89830200	1.89363300	-0.34212200
H	6.46223000	0.88630200	-1.68690200
Ni	0.53172900	-0.09143200	-0.44368300
C	-5.15674300	0.43239900	0.91565400
C	-4.19876400	0.94999000	1.81542100
C	-4.57286100	1.92319900	2.74943900

C	-5.89988400	2.34840300	2.75726700
C	-6.84381400	1.81963300	1.85678600
C	-6.48869900	0.84955300	0.91969100
C	-3.16704100	-0.51821700	0.58268600
H	-3.84852500	2.32550600	3.45313400
H	-6.21564200	3.10067700	3.47465700
H	-7.87075600	2.17155100	1.89364700
H	-7.22162300	0.43993800	0.23110600
N	-2.97472200	0.33907700	1.58518900
N	-4.46972500	-0.49138400	0.13817600
C	-5.07441000	-1.30975700	-0.90144600
H	-4.29995200	-1.71361700	-1.55254500
H	-5.64954900	-2.13583500	-0.46732500
H	-5.74267000	-0.68928700	-1.50545200
H	4.57386600	2.11398900	1.71620900
H	4.21804200	-0.28073000	3.04920700
C	-1.11353600	-1.06874400	-1.10848400
C	-2.11170100	-1.43081200	0.02229700
C	-1.05371800	0.09001800	-1.87795200
C	-0.31194300	0.02928400	-3.26710200
C	-1.25421300	-0.59625600	-4.32702700
H	-2.17276500	-0.01984100	-4.47106200
H	-0.74568800	-0.65339600	-5.29945100
H	-1.53124800	-1.61149500	-4.03042100
C	0.95054700	-0.86050400	-3.22382700
H	1.67581400	-0.48747400	-2.48513400
H	0.71660500	-1.89644100	-2.96965900
H	1.44253500	-0.84210100	-4.20672800
C	0.12819800	1.42915800	-3.75397200
H	0.68873000	1.33303800	-4.69262000
H	-0.71446800	2.09975300	-3.95411500
H	0.78233100	1.91766000	-3.02260200
C	-1.90004700	1.36044800	-1.65255800
H	-2.24207200	1.37956100	-0.61370700
H	-1.25262300	2.24170500	-1.75935900
C	-3.14783300	1.58762100	-2.53650700
H	-3.77785200	0.68736000	-2.52909600
H	-2.85459900	1.74151600	-3.58129500
C	-3.97742700	2.79701400	-2.08080500
H	-4.30161600	2.64902700	-1.04132000
H	-3.33564400	3.69038100	-2.07701800
C	-5.20350900	3.05809000	-2.96302200
H	-5.88297300	2.19601900	-2.96283700
H	-5.77247400	3.92777800	-2.61387300
H	-4.91164100	3.24523600	-4.00390900
H	-1.51601900	-1.77313300	0.87959700
H	-2.62530900	-2.34308200	-0.31138500
H	-0.59708800	-2.40254400	-1.45425100
O	-0.12935100	-3.46564500	-1.66139800
C	-0.93621900	-4.59050800	-1.88586000
C	-2.15837300	-4.25698400	-2.77184700
C	-0.07528100	-5.64208400	-2.61769000
C	-1.42333400	-5.19204000	-0.54579600
H	-2.78956800	-3.49601900	-2.29554600
H	-1.82896100	-3.86100300	-3.73873700
H	-2.78253100	-5.14120200	-2.95773200
H	0.78953000	-5.91521900	-2.00232800
H	-0.63995400	-6.55700400	-2.84358500
H	0.30083200	-5.22311000	-3.55781800
H	-1.99680300	-6.11862400	-0.68817400
H	-0.56125100	-5.41029900	0.09395700
H	-2.06112100	-4.47996100	-0.00789300
Na	-0.72259900	0.84771100	1.62631100

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C	-2.30349200	-0.64161600	0.30716000
C	-3.90120400	-1.96948300	1.36225700
C	-4.55948600	-1.16711300	0.49055000
N	-3.59752200	-0.36265500	-0.14044600
N	-2.53592200	-1.65632700	1.24596400
C	-3.95880100	0.64745600	-1.11285500
C	-4.47091500	1.88223300	-0.64953700
C	-3.85429000	0.34121000	-2.49011700
C	-4.86897300	2.82457200	-1.61154400
C	-4.26348600	1.32129000	-3.40767000
C	-4.76300100	2.55112300	-2.97499100
H	-5.26370500	3.78110500	-1.28713600
H	-4.19374200	1.11973300	-4.47040100

H	-5.07281900	3.29497600	-3.70220700
C	-1.50590500	-2.35504300	1.96951800
C	-1.09052100	-3.62838100	1.49892500
C	-0.94987100	-1.76256200	3.13320900
C	-0.05808900	-4.28222400	2.19902300
C	0.07843300	-2.46008100	3.79078600
C	0.52654800	-3.70064900	3.32721800
H	0.28165300	-5.25630600	1.86307200
H	0.53417700	-2.02810300	4.67351300
H	1.32568900	-4.21616600	3.84942100
C	-3.38436900	-1.03043300	-2.97959600
H	-2.78539400	-1.48097000	-2.18081200
C	-4.59877300	-1.95684700	-3.24238100
H	-5.20994600	-2.08285300	-2.34172400
H	-5.23978800	-1.54264500	-4.03003400
H	-4.26081000	-2.94870100	-3.56676600
C	-2.48300600	-0.95554600	-4.22989600
H	-3.03078800	-0.60211200	-5.11143500
H	-1.63186900	-0.28731600	-4.06612900
H	-2.09443600	-1.95286300	-4.46731800
C	-1.73138800	-4.30947400	0.28493400
H	-2.47822400	-3.62763200	-0.13211000
C	-0.70628900	-4.60550400	-0.83587300
H	-1.19882100	-5.11357500	-1.67248200
H	-0.26647800	-3.68252300	-1.23690400
H	0.10531400	-5.25364300	-0.48527900
C	-2.46778300	-5.60402000	0.70656600
H	-1.76983700	-6.34817100	1.10755700
H	-3.21964500	-5.40012600	1.47686900
C	-2.97502100	-6.04912600	-0.15688600
C	-1.48662600	-0.44541400	3.69490100
H	-1.92726200	0.11182600	2.86189500
C	-0.40074400	0.45488200	4.31861100
H	0.03203400	0.01569800	5.22538600
H	0.40958400	0.66314000	3.61371200
H	-0.84292900	1.41522400	4.60453900
C	-2.61002900	-0.73252600	4.72540500
H	-3.42975700	-1.30825600	4.84159300
H	-2.21851400	-1.29877400	5.57932400
C	-3.02203000	0.21002700	5.10357400
C	-4.65204900	2.18956100	0.83942300
H	-4.09347700	1.43810900	1.40814100
C	-4.09606700	3.57298300	1.24499500
H	-3.03806400	3.67100400	0.98821900
H	-4.64219100	4.38940400	0.75831900
H	-4.19939900	3.71008000	2.32780300
C	-6.14409600	2.07724100	1.24288200
H	-6.74782100	2.81949700	0.70691900
H	-6.55346300	1.08658100	1.01594700
H	-6.26271900	2.25712400	2.31790000
Ni	-0.72247000	0.24503600	-0.16639500
C	5.15578900	-1.03378100	-0.50226800
C	4.28603400	-2.13806200	-0.35773400
C	4.69836500	-3.41281500	-0.76496600
C	5.97418300	-3.54490000	-1.30789300
C	6.83140200	-2.43505500	-1.44434500
C	6.43722500	-1.15974400	-1.04370900
C	3.23376600	-0.38842000	0.39187300
H	4.04005100	-4.27102700	-0.65538600
H	6.31868500	-4.52307300	-1.63234200
H	7.82050200	-2.57637200	-1.87093000
H	7.09798800	-0.30475500	-1.14780500
N	3.09654800	-1.70509100	0.20480700
N	4.46278300	0.06445400	-0.01408700
C	5.00757200	1.42378500	0.05338100
H	4.31050900	2.11339200	0.57302000
H	5.95776100	1.39119700	0.59810700
H	5.19915300	1.78526300	-0.96346400
H	-5.60716500	-1.08427500	0.26120000
H	-4.26029300	-2.72271800	2.04168900
C	1.06613200	1.13875400	0.24092200
C	2.19613100	0.47061500	1.03791900
C	0.81633900	1.30804700	-1.12433400
C	0.30720600	2.70701600	-1.60240200
C	1.51561300	3.68227800	-1.63892800
H	2.24699000	3.40464300	-2.40420600
H	1.16339700	4.69534400	-1.87831900
H	2.02231800	3.70625000	-0.66437400
C	-0.72961600	3.32062300	-0.63413600
H	-1.56996900	2.63626000	-0.46486200

H	-0.28984100	3.58183700	0.33292300
H	-1.13037200	4.24494500	-1.06860400
C	-0.36032500	2.63322600	-2.99167100
H	-0.68960500	3.63368800	-3.29736300
H	0.31846100	2.26768700	-3.76849200
H	-1.24436800	1.98475300	-2.97654400
C	1.37990100	0.35804500	-2.18627100
H	1.63778000	-0.59301800	-1.70736800
H	0.57851800	0.11579600	-2.89941300
C	2.61895200	0.79326900	-3.00250300
H	3.41382000	1.11688400	-2.32133700
H	2.38045300	1.66007100	-3.62895100
C	3.14101600	-0.33636100	-3.90283700
H	3.40197800	-1.20545800	-3.28313600
H	2.33329600	-0.66624900	-4.57336300
C	4.36014800	0.07352500	-4.73602800
H	5.19884600	0.35977600	-4.09001400
H	4.70110600	-0.74817200	-5.37667300
H	4.13102000	0.92950900	-5.38305200
H	1.77904300	-0.09133800	1.88880700
H	2.67084000	1.38775400	1.49425100
H	0.73057000	1.96570000	0.86523200
O	2.96237500	3.10831100	1.50856000
C	3.19922400	4.01008200	2.52120800
C	3.97090300	5.24294300	1.97779900
C	1.85740400	4.50459000	3.13040600
C	4.04140200	3.36777100	3.65828100
H	4.93232600	4.92196900	1.55682300
H	3.39416500	5.70981400	1.16997600
H	4.17056800	6.00528400	2.74562600
H	1.29530100	3.64739200	3.52534500
H	1.98720600	5.23384100	3.94420200
H	1.24908800	4.97053000	2.34474800
H	4.24940100	4.05853700	4.48887500
H	3.51191800	2.49567800	4.06511900
H	5.00220900	3.01857000	3.25849700
Na	0.84298700	-1.90146900	0.48367000

Cartesian coordinates for the stationary points given in Fig. S7.

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C	-1.51304900	-0.61530900	-0.29902600
C	-3.48300600	-1.38906500	0.07012400
C	-3.66234800	-0.10996900	-0.51929900
C	-4.60324300	-2.15031300	0.42425000
C	-4.92807900	0.42364600	-0.76928400
C	-5.87088500	-1.62227000	0.17901700
H	-4.47360000	-3.12942400	0.87792800
C	-6.03108300	-0.35320700	-0.40932500
H	-5.05513200	1.40147800	-1.22625900
H	-6.75377400	-2.19918400	0.44596000
H	-7.03309400	0.03017200	-0.58885300
C	-2.02850900	1.66045600	-1.32012900
H	-1.95665000	1.58150400	-2.41402100
H	-2.81857900	2.37850300	-1.07737700
H	-1.07466200	2.03011400	-0.89150200
N	-2.13502600	-1.67435600	0.18927500
C	-0.03667700	-0.42046700	-0.41778200
C	0.78367000	-1.51626100	0.19998500
H	0.22537800	0.58305100	0.01578900
H	0.20864800	-0.29480100	-1.48394700
C	2.05097600	-1.82073800	-0.13327300
H	0.28035100	-2.06188700	0.99100600
N	-2.38483000	0.37117600	-0.73450000
C	2.83940500	-2.94290400	0.56687000
C	2.08060900	-3.54901600	1.76310300
C	3.11987200	-4.08639200	-0.44055500
C	4.18782700	-2.39562100	1.09432600
H	1.85372700	-2.78914400	2.51893600
H	1.13628300	-4.01021400	1.45446400
H	2.69310900	-4.32644800	2.23832600
H	3.68164300	-3.73470800	-1.31281300
H	3.70744700	-4.88598300	0.03172100
H	2.17948200	-4.52024500	-0.80008400
H	4.76561000	-3.19543200	1.57783100

H	4.80501500	-1.98110300	0.29023000
H	4.02187100	-1.60081000	1.83035900
C	2.75188900	-1.05727500	-1.25365500
C	3.14776000	0.39320000	-0.89939100
H	2.08006000	-1.01792100	-2.12437500
H	3.64136400	-1.60114400	-1.59974300
C	3.57860100	1.21634700	-2.12248400
H	2.30762000	0.91771800	-0.42702700
H	3.96071200	0.38213900	-0.15790200
C	3.69401600	2.70857600	-1.78908500
H	4.52332300	0.83228200	-2.54132900
H	2.82310600	1.09139600	-2.91304600
H	3.93330000	3.30812800	-2.67813400
H	2.74344200	3.05241500	-1.36253900
H	4.48150200	2.88885200	-1.04446800
O	0.61841000	2.43581600	0.06900700
C	0.59376600	3.23362500	1.18253200
C	0.50949900	4.73386200	0.77085200
C	-0.63290000	2.91750300	2.08996800
C	1.87894500	3.03929600	2.03944500
H	1.37423800	4.99120300	0.14591600
H	-0.39379100	4.89623400	0.16816200
H	0.48219600	5.42797000	1.62658000
H	-0.60047400	1.86573200	2.40149000
H	-0.68081100	3.54145600	2.99689100
H	-1.56339100	3.06865400	1.52722700
H	1.90203000	3.66364900	2.94740100
H	1.95818600	1.98759500	2.34278000
H	2.76367400	3.27771700	1.43583900

TS₅₀₋₅₁

C	1.48024900	-0.51716500	0.41124500
C	3.44728000	-1.24481500	-0.10121400
C	3.65626100	-0.10443100	0.72316900
C	4.55550700	-1.94835100	-0.58803800
C	4.93009000	0.34089600	1.07094200
C	5.83611400	-1.50563800	-0.24535900
H	4.40809500	-2.82077600	-1.21957800
C	6.02311800	-0.37737300	0.57070200
H	5.07776500	1.21008500	1.70774500
H	6.70609200	-2.04398500	-0.61657500
H	7.03173800	-0.05615800	0.82200900
C	2.04766100	1.56663700	1.74720900
H	1.79732300	1.35746800	2.79706800
H	2.91092600	2.23939900	1.72632700
H	1.20108900	2.05685300	1.24867700
N	2.09865300	-1.47581600	-0.27368100
C	0.04045600	-0.27836900	0.51380500
C	-0.82383600	-1.31050300	-0.09197900
H	-0.19253300	0.91881900	-0.00928500
H	-0.23963600	-0.01478300	1.54225200
C	-2.11431400	-1.58118200	0.21010900
H	-0.33610400	-1.87279800	-0.88300300
N	2.38635600	0.35167900	1.02542200
C	-2.91626900	-2.68435600	-0.50475600
C	-2.16421500	-3.28419500	-1.70873400
C	-3.21076600	-3.84070500	0.48560700
C	-4.26336500	-2.12883500	-1.02935800
H	-1.92052300	-2.51476300	-2.44968800
H	-1.22880700	-3.76621900	-1.40540600
H	-2.78803100	-4.04317200	-2.19974500
H	-3.76689800	-3.49294100	1.36359800
H	-3.80902900	-4.62889200	0.00591400
H	-2.27456800	-4.28824900	0.83890200
H	-4.84805400	-2.92293300	-1.51530100
H	-4.87747500	-1.71478200	-0.22218800
H	-4.09486100	-1.33191300	-1.76282700
C	-2.81613100	-0.80730500	1.32056700
C	-3.23743100	0.62690400	0.93402300
H	-2.14317700	-0.73621300	2.18913900
H	-3.70016400	-1.35285000	1.68147900
C	-3.79302900	1.43856300	2.11187500
H	-2.37674000	1.16244300	0.51527000
H	-3.99359400	0.58358300	0.13591700
C	-4.08243100	2.89449900	1.72780200
H	-4.70524600	0.96564500	2.51018000
H	-3.06064600	1.42426700	2.93286900
H	-4.44473500	3.48119400	2.58268200

H	-3.17256600	3.36956700	1.34277800
H	-4.84367200	2.95085300	0.93830200
O	-0.43770600	2.21713900	-0.19146900
C	-0.32882700	2.68960300	-1.49705900
C	-0.50110900	4.22625900	-1.46410800
C	1.05745400	2.35375100	-2.10315600
C	-1.43252400	2.07993500	-2.39795900
H	-1.47664700	4.47913700	-1.03080300
H	0.27265300	4.67121800	-0.82628500
H	-0.43404400	4.68394100	-2.46266400
H	1.20781600	1.26855900	-2.13924000
H	1.17780800	2.74782700	-3.12340300
H	1.85142800	2.77986300	-1.47747800
H	-1.38115900	2.44324500	-3.43548900
H	-1.34574000	0.98712800	-2.41073800
H	-2.42115600	2.32926100	-1.99385900

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C	-1.37625900	-0.67703200	-0.60989700
C	-3.34497900	-1.24726700	0.11261200
C	-3.57869400	-0.28489700	-0.91633400
C	-4.45003700	-1.80748200	0.77044800
C	-4.85507900	0.11871100	-1.28731000
C	-5.73961400	-1.40366500	0.40019800
H	-4.29324600	-2.54182600	1.55688200
C	-5.94649200	-0.45577400	-0.61012800
H	-5.01733000	0.85346600	-2.07405700
H	-6.59975600	-1.83574400	0.90969900
H	-6.95822200	-0.15803200	-0.87797500
C	-1.98692400	1.12520400	-2.28539500
H	-1.41206700	0.75203800	-3.14410500
H	-2.91167900	1.57134200	-2.66131000
H	-1.39780200	1.90226600	-1.78129600
N	-2.00421900	-1.47016600	0.28585000
C	0.01413100	-0.52460000	-0.79781500
C	0.95511200	-1.34062200	-0.08392100
H	0.07465400	1.34229700	0.10372600
H	0.34273000	0.04738400	-1.66168500
C	2.30914300	-1.43488700	-0.24864600
H	0.48093800	-1.95443800	0.67824400
N	-2.31321600	0.05942800	-1.36804800
C	3.17712500	-2.41193800	0.56088100
C	2.39897800	-3.09971000	1.69978800
C	3.72440100	-3.53172900	-0.36528000
C	4.38376500	-1.68167300	1.20350400
H	1.97867300	-2.36610700	2.39681200
H	1.57226100	-3.70748800	1.31704400
H	3.06795800	-3.76232500	2.26564700
H	4.31814700	-3.12125700	-1.19049200
H	4.36916400	-4.23055500	0.18849400
H	2.89648400	-4.10170300	-0.80242200
H	5.02096800	-2.38599600	1.75842600
H	5.01268500	-1.19302700	0.45079600
H	4.03997500	-0.91019800	1.90279800
C	2.99640500	-0.59359700	-1.31381700
C	3.24430600	0.88125200	-0.92316500
H	2.38694900	-0.59879600	-2.23227800
H	3.96118100	-1.03568500	-1.60535700
C	3.81771100	1.73041600	-2.06562200
H	2.30585200	1.33051500	-0.57886900
H	3.93129700	0.92076800	-0.06548600
C	4.02818000	3.19766900	-1.67361300
H	4.77167200	1.29978000	-2.40862000
H	3.13682900	1.68056800	-2.92833900
H	4.41936000	3.79309300	-2.50932100
H	3.08409200	3.65036000	-1.34733600
H	4.73870400	3.28537700	-0.84105900
O	0.09790900	2.30967400	0.32326700
C	-0.13173800	2.46271900	1.72673100
C	-0.16667400	3.97739400	1.96480000
C	-1.47405300	1.82163800	2.11915700
C	1.02422700	1.82058200	2.51538200
H	0.77623100	4.43277000	1.64029400
H	-0.97975300	4.43166300	1.38712000
H	-0.32040900	4.20952100	3.02583900
H	-1.47070000	0.74450300	1.91799400
H	-1.68986600	1.97139600	3.18555800
H	-2.28903100	2.26660900	1.53723000
H	0.87915700	1.92462600	3.59898900

H	1.09926400	0.75373000	2.27778000
H	1.97577000	2.29260300	2.24453800

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C	-1.62031300	0.71346600	-0.49368400
C	-3.53325300	-0.31127400	-0.66862400
C	-3.83123700	0.95426000	-0.07624200
C	-4.59115700	-1.20189300	-0.90779800
C	-5.11886900	1.33281500	0.27893900
C	-5.89404000	-0.82229900	-0.55743700
H	-4.38857900	-2.17017600	-1.35891600
C	-6.16269600	0.42198900	0.02590100
H	-5.32481600	2.29622800	0.74236500
H	-6.71615700	-1.51266200	-0.74124500
H	-7.18301100	0.69010000	0.29231900
C	-2.36986900	2.92977900	0.49597400
H	-1.67239000	3.45200600	-0.17038600
H	-3.31410300	3.48322200	0.51002200
H	-1.94378900	2.94344900	1.51103700
N	-2.19307000	-0.44132100	-0.91005200
C	-0.25992800	1.05632300	-0.52729900
C	0.70610500	0.23741100	-1.18489900
H	1.56823200	-1.26432100	0.41617000
H	0.04273200	1.99347900	-0.07103800
C	2.06189000	0.42961800	-1.30219300
H	0.26826400	-0.63962500	-1.65713500
N	-2.60413900	1.59466400	0.01470500
C	2.96615000	-0.48043000	-2.15272500
C	2.25603000	-1.77293500	-2.60300700
C	3.42101900	0.27433500	-3.43063900
C	4.22757700	-0.90797700	-1.35821500
H	1.91938900	-2.35698300	-1.74025100
H	1.38711000	-1.56289000	-3.23618500
H	2.94849700	-2.39579500	-3.18556400
H	3.95752400	1.19943600	-3.18701900
H	4.09421200	-0.34563500	-4.04154700
H	2.55335700	0.54462000	-4.04407400
H	4.89046700	-1.52396700	-1.98351900
H	4.81030500	-0.04235500	-1.02116300
H	3.94526200	-1.49274300	-0.47631900
C	2.69382000	1.66372200	-0.67659300
C	2.90193400	1.58832500	0.85250000
H	2.06603000	2.54633600	-0.88622800
H	3.66658600	1.88272400	-1.14027500
C	3.52880700	2.85767400	1.44438100
H	1.93287900	1.40133400	1.33238200
H	3.52946100	0.72005100	1.09411000
C	3.72307300	2.78984700	2.96370500
H	4.50014200	3.04522400	0.96121700
H	2.89763400	3.72426200	1.19635600
H	4.17233400	3.71007900	3.35995500
H	2.76487300	2.63797500	3.47625200
H	4.37681000	1.95282300	3.24028100
O	1.87530700	-2.00295900	0.98074300
C	0.79529400	-2.44371400	1.81475400
C	1.41597000	-3.51920100	2.71485300
C	0.27351100	-1.26674300	2.65546900
C	-0.33532500	-3.04035200	0.95911900
H	1.81752300	-4.33661700	2.10476300
H	2.24050800	-3.09565500	3.30005000
H	0.67160300	-3.93315500	3.40556200
H	-0.11521900	-0.47880600	1.99987100
H	-0.53573400	-1.58197200	3.32680200
H	1.08523300	-0.84605600	3.26144500
H	-1.12792400	-3.46031700	1.59294500
H	-0.79590800	-2.28406900	0.31180000
H	0.06169900	-3.84574900	0.32922200

TS₅₂₋₅₃

C	2.05891900	0.14565700	0.38917400
C	3.96702800	-0.81368700	0.06117100
C	4.21337500	0.58204500	-0.06446200
C	5.03260600	-1.70990300	-0.10190000
C	5.47776000	1.09835300	-0.33746300
C	6.30239900	-1.19917600	-0.38048200
H	4.85841000	-2.77862500	-0.01152900

C	6.52571900	0.18301100	-0.49770400
H	5.65624400	2.16818300	-0.42034400
H	7.13758500	-1.88461200	-0.50918900
H	7.52637400	0.55097000	-0.71255000
C	2.69674700	2.59187500	0.05830100
H	2.65466500	3.06412100	1.04957000
H	3.48028000	3.08168700	-0.52712800
H	1.74028900	2.75623100	-0.44605600
N	2.64342900	-1.05192600	0.34191500
C	0.68147200	0.42982100	0.67719000
C	-0.26409100	-0.55423700	0.83368200
H	-2.23991100	-0.56854700	-0.12019000
H	0.40791000	1.47336900	0.79063000
C	-1.68586100	-0.41187200	1.06299900
H	0.11859700	-1.56380200	0.69641000
N	2.97915100	1.17639000	0.13743700
C	-2.35087100	-1.58571700	1.87590600
C	-1.91233300	-2.96245600	1.33104900
C	-1.97031700	-1.50872400	3.37201300
C	-3.89117100	-1.52995900	1.73338900
H	-2.10449500	-3.02500800	0.25560500
H	-0.85118000	-3.16947300	1.50855900
H	-2.48217900	-3.76056300	1.82661400
H	-2.29539500	-0.56224300	3.82136700
H	-2.43939800	-2.32346900	3.94359700
H	-0.88365000	-1.58454000	3.50413500
H	-4.34886800	-2.39601100	2.23293900
H	-4.31987900	-0.63212500	2.19428700
H	-4.16298000	-1.53251900	0.67306500
C	-2.11818600	0.99906300	1.53243800
C	-2.40751700	2.00864400	0.40549500
H	-1.35779400	1.42503800	2.21025300
H	-3.03096300	0.92366100	2.13591300
C	-2.91924500	3.35796000	0.92548800
H	-1.49949400	2.17455700	-0.19135100
H	-3.13061800	1.55390500	-0.28148400
C	-3.19682400	4.37098500	-0.19167500
H	-3.84046600	3.19804500	1.50635700
H	-2.19047600	3.78636800	1.63165600
H	-3.57208300	5.32471100	0.20300700
H	-2.28600100	4.58300300	-0.76649500
H	-3.94231100	3.98206300	-0.89633800
O	-3.11907500	-0.67541300	-1.15760900
C	-2.64013500	-0.86508500	-2.44613100
C	-3.84573600	-0.75350800	-3.41206800
C	-1.58974000	0.20674500	-2.83866600
C	-2.00108300	-2.26905700	-2.61422000
H	-4.60137400	-1.50174800	-3.14281600
H	-4.30686600	0.23653300	-3.31026900
H	-3.56526300	-0.90259500	-4.46608200
H	-0.72903200	0.16288600	-2.16112300
H	-1.22136800	0.07685900	-3.86750100
H	-2.03170200	1.20731800	-2.75644400
H	-1.67393400	-2.46864600	-3.64596000
H	-1.12756800	-2.36813100	-1.95908100
H	-2.72805100	-3.03944900	-2.32777400

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C	-2.43908800	0.02240400	-0.21632800
C	-4.23795100	-0.94561400	0.46800200
C	-4.57117700	0.42655700	0.31963300
C	-5.21697900	-1.84728700	0.90678700
C	-5.84743600	0.92087400	0.58965500
C	-6.49382300	-1.35979000	1.18229800
H	-4.97099400	-2.89859800	1.02549000
C	-6.80641400	0.00366600	1.02678600
H	-6.09637500	1.97175000	0.46440700
H	-7.26631400	-2.04475900	1.52396200
H	-7.81272400	0.35120500	1.24763500
C	-3.23401900	2.44711700	-0.36633100
H	-3.42043000	2.70026300	-1.41841700
H	-3.93430800	3.01015500	0.25764900
H	-2.22064700	2.75785000	-0.10371300
N	-2.92181000	-1.16311300	0.12727300
C	-1.09162400	0.30844300	-0.67218000
C	-0.08735900	-0.59528300	-0.62325900
H	1.96998100	-0.50625700	-0.11524000
H	-0.91041100	1.30257000	-1.06681400
C	1.33715500	-0.41128500	-1.03658500

H	-0.34803200	-1.56272800	-0.19897100
N	-3.40239900	1.03141300	-0.10879600
C	1.85713700	-1.60321800	-1.94051900
C	1.68315500	-2.93779100	-1.18289400
C	1.10182900	-1.66692700	-3.28181400
C	3.37500200	-1.42959800	-2.18648500
H	2.18533900	-2.87892400	-0.21063000
H	0.63218100	-3.20485900	-1.02229100
H	2.13960200	-3.75773900	-1.75341500
H	1.21657800	-0.73327800	-3.84703000
H	1.48878100	-2.48212800	-3.90928600
H	0.02749000	-1.83740300	-3.13374900
H	3.79632500	-2.36164100	-2.58961600
H	3.58661000	-0.64384900	-2.92241200
H	3.86970700	-1.17466200	-1.23756400
C	1.64039600	0.99731100	-1.60045400
C	1.88140300	2.03473400	-0.48993100
H	0.84716100	1.33266800	-2.28924200
H	2.55356000	0.95438500	-2.20135500
C	2.28843400	3.41288700	-1.02472100
H	0.98063400	2.14206100	0.13351200
H	2.66544500	1.61531500	0.15847700
C	2.53935900	4.43681600	0.08880700
H	3.20034800	3.30899600	-1.63135800
H	1.51455500	3.80035400	-1.70792900
H	2.84525400	5.41265300	-0.31182900
H	1.63552400	4.59260900	0.69263300
H	3.32720600	4.08719100	0.76652100
O	3.65304400	-0.33889200	0.75595700
C	4.20328200	-0.60210900	1.97128100
C	5.56753400	0.14183100	2.11678400
C	3.27394800	-0.13510000	3.13321500
C	4.47102500	-2.12796200	2.15911400
H	6.23615300	-0.17390300	1.30535500
H	5.40294300	1.22171100	2.00610300
H	6.07807100	-0.03526700	3.07818100
H	2.30778900	-0.65030100	3.05497800
H	3.68547000	-0.32389900	4.13864000
H	3.08310100	0.94170000	3.03659800
H	4.94100000	-2.38571300	3.12281300
H	3.52212500	-2.67558900	2.08476800
H	5.12367500	-2.48294800	1.35099000

Cartesian coordinates for the stationary points given in Fig. S8.

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C	-1.81002100	-0.86882200	-0.81709800
C	-2.41507600	-2.91284700	-0.54336300
C	-3.60757600	-2.14298200	-0.55504500
C	-2.48915900	-4.30159000	-0.38425800
C	-4.86955300	-2.72407700	-0.41785300
C	-3.74690800	-4.88822200	-0.24493400
H	-1.57980900	-4.89662400	-0.37295800
C	-4.92040700	-4.11053100	-0.26111900
H	-5.77768300	-2.12723300	-0.43294900
H	-3.82576600	-5.96614100	-0.12143500
H	-5.88643700	-4.59814100	-0.15093000
C	-4.03688100	0.35533000	-0.75422900
H	-4.30909100	0.60858100	-1.78838200
H	-4.95476000	0.14046700	-0.19827000
H	-3.51760100	1.20326300	-0.26382900
N	-1.31546000	-2.09003500	-0.71047700
C	-1.04330800	0.39760300	-1.01302900
C	0.44631000	0.22086100	-1.06476500
H	-1.34915700	1.10978800	-0.19719600
H	-1.41623100	0.89417300	-1.92355600
C	1.31948900	1.14196300	-1.50278600
H	0.82140700	-0.72526600	-0.69435900
N	-3.19147400	-0.83498600	-0.71919200
C	2.83491600	0.87727400	-1.47509700
C	3.35024000	0.64104800	-2.91056700
C	3.59210100	2.06264100	-0.84190000
H	3.12108300	1.48675000	-3.56762700

H	4.43653500	0.48991400	-2.90196000
H	2.87626800	-0.25649500	-3.31878500
H	4.66776600	1.85292600	-0.82147800
H	3.43668500	2.98508300	-1.40977500
H	3.24907200	2.24752700	0.18189200
C	0.84080300	2.45947100	-2.10078100
C	0.32137500	3.49580400	-1.08129000
H	0.01959500	2.24102100	-2.79995500
H	1.62900800	2.91685700	-2.71541400
C	-0.35004300	4.70416200	-1.75112700
H	-0.41527400	3.03564300	-0.40972400
H	1.15239700	3.84068900	-0.44738300
C	-1.11695000	5.56174800	-0.73792200
H	0.39001800	5.31001000	-2.29934100
H	-1.06090500	4.33630000	-2.50637100
H	-1.64969000	6.39024000	-1.22445300
H	-1.83766300	4.92642200	-0.20909600
H	-0.43890800	5.99528100	0.00984800
O	-2.30138000	2.45816800	0.72031300
C	-2.44817800	2.56622000	2.07898300
C	-3.69061300	3.44227800	2.41996200
C	-2.64557400	1.17473100	2.75118000
C	-1.19949100	3.23049700	2.73033600
H	-3.57163600	4.43725400	1.97228100
H	-4.58960800	2.98827600	1.98269900
H	-3.85978200	3.56715900	3.50178000
H	-1.78188000	0.53379700	2.53308500
H	-2.76242400	1.22961900	3.84529100
H	-3.53697700	0.68245300	2.34133800
H	-1.27977300	3.33623100	3.82415200
H	-0.30892100	2.62797400	2.50896800
H	-1.04234100	4.22706600	2.29910300
O	3.15918700	-0.34038000	-0.79012000
Si	3.36095500	-0.74749200	0.86022400
C	3.52228300	-2.68109800	0.78835400
C	1.93388000	-0.20897200	2.00091100
H	2.20145000	-0.39888500	3.04804000
H	1.71549900	0.85924000	1.89921100
H	1.00571300	-0.74511300	1.78143500
C	4.98391100	0.00027100	1.55513200
H	5.24680600	-0.47731700	2.50775300
H	5.82221200	-0.14533200	0.86512300
H	4.88457700	1.07467200	1.74226400
C	3.52586800	-3.26040900	2.21719000
H	2.58882600	-3.04709100	2.74535700
H	3.64045200	-4.35436800	2.18309900
H	4.35184900	-2.86611000	2.82448100
C	2.33895500	-3.27594000	-0.00139300
H	2.32945100	-2.91172700	-1.03318000
H	2.41828500	-4.37407800	-0.02801500
H	1.36537000	-3.02478100	0.43419100
C	4.83639600	-3.06502000	0.07921200
H	4.87692700	-2.64787700	-0.93350500
H	5.71970500	-2.71179300	0.62690900
H	4.91859600	-4.15956500	-0.00548500

TS₅₄₋₅₅

C	-2.01591800	-0.42883100	-0.82097000
C	-2.95398900	-2.36570800	-0.62890000
C	-4.01557500	-1.43011500	-0.77069400
C	-3.25512800	-3.72616600	-0.49387800
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C	-4.59566900	-4.12114000	-0.50528500
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C	-5.63133100	-3.18257800	-0.64794600
H	-6.15732900	-1.09328400	-0.90258500
H	-4.84385800	-5.17570700	-0.40243000
H	-6.66570800	-3.51955300	-0.65500500
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H	-4.11956600	1.45241500	-1.98812000
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C	-1.07317600	0.68833600	-0.87484900
C	0.34839800	0.31096100	-0.98241600
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H	-1.38407700	1.42460200	-1.62850700
C	1.36482800	1.07009800	-1.44385000

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C	3.84105200	1.50900300	-1.01291400
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H -1.66261000 1.85150500 1.60225700
H -2.16563300 1.96704000 3.30269900
H -0.90929000 3.05986800 2.67065200
H -1.59189700 -0.55102700 3.62659500
H -1.13466500 -0.64479300 1.91598000
H 0.02732400 -1.12654900 3.17386600
O 2.37520900 -0.52950300 -0.90189000
Si 3.39149900 -1.59373300 -0.05427900
C 5.11308000 -1.75160900 -0.88836800
H 5.72739000 -2.49559400 -0.36587800
H 5.02666800 -2.06076500 -1.93587900
H 5.65845900 -0.80118100 -0.86577500
C 3.64289600 -1.07369200 1.76636800
H 4.48214700 -0.37653700 1.87118200
H 2.74424100 -0.56972600 2.13905100
H 3.84988000 -1.94397200 2.40180900
C 2.46273500 -3.29370200 -0.16763100
C 3.34788700 -4.40992400 0.42415200
H 3.59265400 -4.22769800 1.47891700
H 2.82083000 -5.37468400 0.37634500
H 4.29177400 -4.52586900 -0.12415600

C	2.15589300	-3.61790200	-1.64347600
H	1.60457300	-4.56759400	-1.71730600
H	1.54134700	-2.83477600	-2.09803000
H	3.07150400	-3.72316000	-2.24158400
C	1.13511500	-3.23735400	0.61700000
H	0.64206000	-4.22121000	0.58505800
H	1.29622000	-2.98822800	1.67360500
H	0.42968900	-2.50893200	0.20374100

H	5.02776400	-2.66536500	1.08414000
C	1.94184300	-3.63602800	0.22651100
C	2.78550500	-4.91024700	0.43398600
H	3.59457400	-4.75684000	1.15993000
H	2.15318300	-5.72441000	0.81946500
H	3.23691300	-5.26468800	-0.50176700
C	0.82098400	-3.92822500	-0.79110800
H	0.19423200	-4.76077000	-0.43644300
H	0.16844400	-3.06056700	-0.92968600
H	1.22184800	-4.21673600	-1.77203500
C	1.30019000	-3.23082700	1.56840400
H	0.66003600	-4.04400300	1.94354600
H	2.05386600	-3.02259500	2.33812400
H	0.67445700	-2.33946600	1.46002300

TS_{57-TP2}

C	-2.73402700	0.10838200	-0.34771500
C	-4.00585800	-1.57531200	0.11748800
C	-4.88132900	-0.46412500	-0.03442500
C	-4.54687900	-2.83113700	0.42581800
C	-6.26287600	-0.57423500	0.10406500
C	-5.93105900	-2.94777500	0.57060100
H	-3.88911700	-3.68739500	0.54707900
C	-6.77944300	-1.83880500	0.41303100
H	-6.92356000	0.28012500	-0.02557100
H	-6.36358500	-3.91721000	0.80927600
H	-7.85385800	-1.96161900	0.52884500
C	-4.45988400	1.97546500	-0.51488700
H	-4.52491200	2.24246100	-1.57876900
H	-5.44304400	2.12285300	-0.05856000
H	-3.75219700	2.65323200	-0.02905900
N	-2.69994100	-1.19813100	-0.08295000
C	-1.61970600	0.95938400	-0.65997800
C	-0.32304800	0.51519800	-0.60934900
H	1.38291500	1.63611100	0.29774100
H	-1.84367300	1.97422300	-0.97250800
C	0.89957500	1.24192100	-0.86945300
H	-0.19453200	-0.51506800	-0.28888300
N	-4.04708900	0.60406800	-0.31902300
C	2.04459800	0.32196700	-1.41889400
C	1.80423600	-0.03749700	-2.89948800
C	3.42080500	0.98358700	-1.22957900
H	1.72971000	0.86526800	-3.51605500
H	2.62015900	-0.64943200	-3.30384000
H	0.86725000	-0.59588400	-2.99740500
H	4.22398600	0.30684500	-1.55151600
H	3.50940800	1.89232800	-1.83514200
H	3.54618200	1.26425400	-0.17980800
C	0.72989300	2.55451700	-1.67175200
C	0.38706500	3.80362400	-0.83815900
H	-0.03690000	2.42371300	-2.45575900
H	1.66031300	2.78019400	-2.20958200
C	0.30322400	5.07985400	-1.68486900
H	-0.56843500	3.65692300	-0.31505200
H	1.14288800	3.90119300	-0.05050100
C	-0.03795300	6.32867300	-0.86298700
H	1.26287000	5.23809100	-2.20042800
H	-0.44712800	4.95199400	-2.48102600
H	-0.08446100	7.23080600	-1.48752600
H	-1.00917200	6.21840100	-0.36332200
H	0.71236600	6.49883700	-0.08107300
O	2.10264700	2.25628600	1.26328900
C	1.69447200	2.10183200	2.58134600
C	2.54386100	3.06158200	3.45014100
C	0.19629600	2.45721900	2.76838500
C	1.92916200	0.65021000	3.07157100
H	3.60801500	2.82908300	3.31992000
H	2.38581800	4.09539000	3.11923400
H	2.30035300	2.99641400	4.52163600
H	-0.43179900	1.80735100	2.14842300
H	-0.13115900	2.35418200	3.81375300
H	0.01882200	3.49335900	2.45433400
H	1.64426500	0.50179200	4.12419600
H	1.35254200	-0.04995700	2.45741000
H	2.99133400	0.39760800	2.96239200
O	1.98709200	-0.90732600	-0.65818000
Si	3.06861700	-2.19551300	-0.43134300
C	3.94787900	-2.76288000	-2.04004000
H	4.59325700	-3.62504300	-1.82950400
H	3.23458700	-3.05728600	-2.81709900
H	4.58244200	-1.97033900	-2.45187300
C	4.43057300	-1.77712100	0.84160800
H	5.10924400	-1.01067100	0.45280200
H	3.99553700	-1.38896800	1.76763100