

镍催化芳烃卤化物还原性交叉偶联的反应机理

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Reaction Mechanism for the Ni-Catalyzed Reductive Cross-Coupling of Aryl Halides

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Table S1 The calculated values of electronic energy ΔE , zero-point energy correction ΔZPE , relative enthalpy ΔH , relative entropy ΔS , Gibbs free energy ΔG , Gibbs free energy in solution

CH₃CN, ΔG_{sol} (298 K) for the Path I and Path II

Sub.	ΔE	ΔZPE	ΔH	ΔS	ΔG	ΔG_{sol}
CA _{0t} +R ₁	0.00	0.00	0.00	0.00	0.00	0.00
CP _{1t}	-65.52	-0.12	-62.89	-150.85	-17.92	-15.37
TS _{1t}	-56.10	-0.92	-55.43	-157.63	-8.42	-15.32
IN _{1t}	-232.92	5.86	-223.32	-123.97	-185.22	-239.15
IN ₂ +R ₂	-206.33	-3.06	-203.69	-101.03	-172.41	-243.76
TS ₂	-135.83	-4.45	-132.68	-277.82	-48.71	-157.72
IN ₃	-294.54	2.68	-284.45	-290.35	-196.78	-342.77
TS ₃	-283.45	0.50	-276.62	-290.27	-188.91	-331.13
P+CA ₁	-511.67	3.94	-507.65	-153.86	-460.63	-573.17
CA _{0s} +R ₁	82.35	0.54	83.28	0.96	82.98	102.95
CP _{1s}	-8.83	3.52	-2.14	-146.16	41.45	32.74
TS _{1s}	30.94	0.25	33.08	-154.03	78.96	81.39
IN _{1s}	-251.59	8.71	-245.61	-204.78	-196.19	-249.66
CA ₁ +R ₁	0.00	0.00	0.00	0.00	0.00	0.00
TS ₇	53.34	-0.59	58.74	-136.45	99.44	37.10
IN ₇	8.12	3.94	18.55	-137.29	59.49	13.73

The unit of relative entropy ΔS is J·mol⁻¹·K⁻¹ and all other energy units are kJ·mol⁻¹. The sum of the energies of R₁ and CA₁ is set as the zero energy, the sum of the energies of R₁ and CA_{0t} is set as the zero energy.

Table S2 The calculated values of electronic energy ΔE , zero-point energy correction ΔZPE , relative enthalpy ΔH , relative entropy ΔS , Gibbs free energy ΔG , Gibbs free energy in solution

CH₃CN, ΔG_{sol} (298 K) for the Path III and Path IV

Sub.	ΔE	ΔZPE	ΔH	ΔS	ΔG	ΔG_{sol}
CA _{0t} +R ₂	0.00	0.00	0.00	0.00	0.00	0.00
CP _{2t}	-72.05	-0.29	-69.38	-152.36	-23.95	-16.41
TS _{4t}	-66.70	-0.67	-65.73	-160.94	-17.75	-26.21
IN _{4t}	-241.62	6.28	-231.61	-126.06	-194.02	-243.63
IN ₅ +R ₁	-222.99	-4.02	-219.47	-95.58	-191.00	-258.49
TS ₅	-173.33	-5.36	-169.65	-281.52	-85.70	-197.49
IN ₆	-297.35	1.13	-287.21	-289.85	-200.80	-343.07
TS ₆	-288.34	-1.05	-281.48	-288.68	-195.40	-337.62
CA ₁ +P	-517.66	2.43	-511.42	-150.10	-466.66	-574.47

CA _{0s} +R ₂	82.35	0.54	83.28	0.96	82.98	102.95
CP _{2s}	-11.39	3.31	-4.56	-138.71	36.76	29.77
TS _{4s}	21.23	0.59	23.70	-155.96	70.21	71.18
IN _{4s}	-261.84	9.50	-250.41	-156.50	-203.77	-260.42
CA ₁ +R ₂	0.00	0.00	0.00	0.00	0.00	0.00
TS ₈	45.72	-0.25	51.29	-146.41	94.96	55.60
IN ₈	4.86	4.02	13.15	-161.48	61.25	12.31

The unit of relative entropy ΔS is $\text{J}\cdot\text{mol}^{-1}\cdot\text{K}^{-1}$ and all other energy units are $\text{kJ}\cdot\text{mol}^{-1}$. The sum of the energies of R₁ and CA_{0t} (triplet Ni⁰) is set as the zero of energy, the sum of the energies of R₂ and CA₁ is set as the zero of energy, the sum of the energies of R₁ and IN₅ is set as the zero of energy.

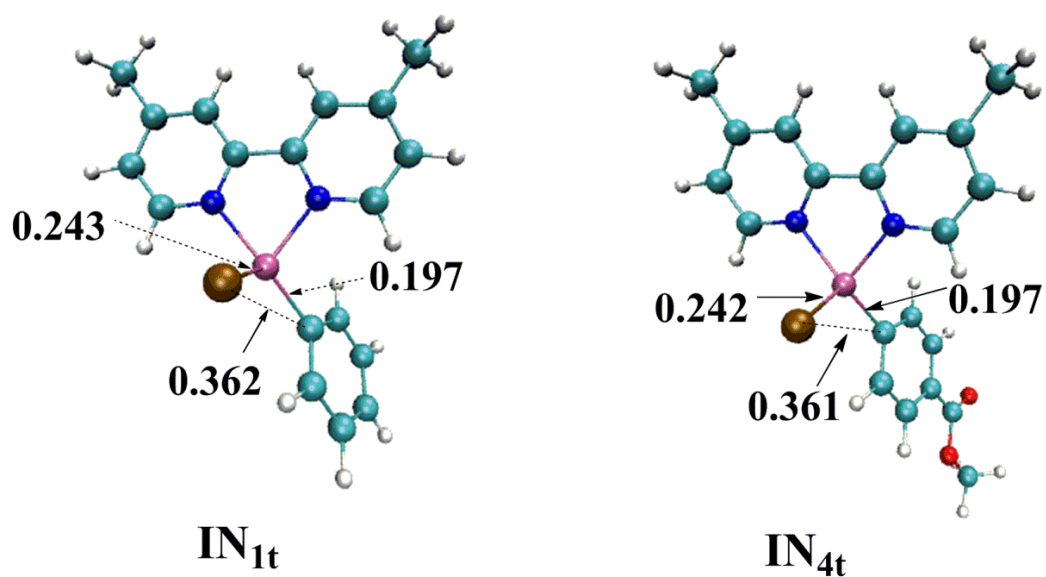


Fig.S1 The optimized structures of IN_{1t} and IN_{4t}

The unit of distance is nm.

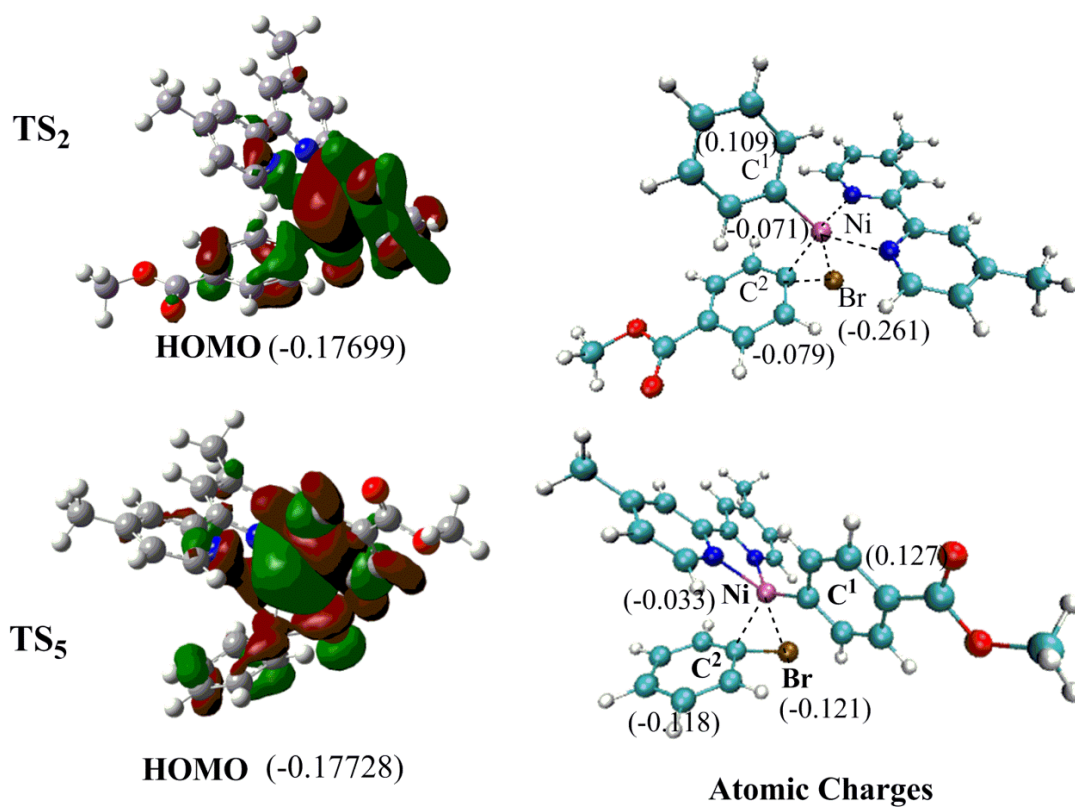


Fig.S2 The HOMO orbitals of TS₂ and TS₅

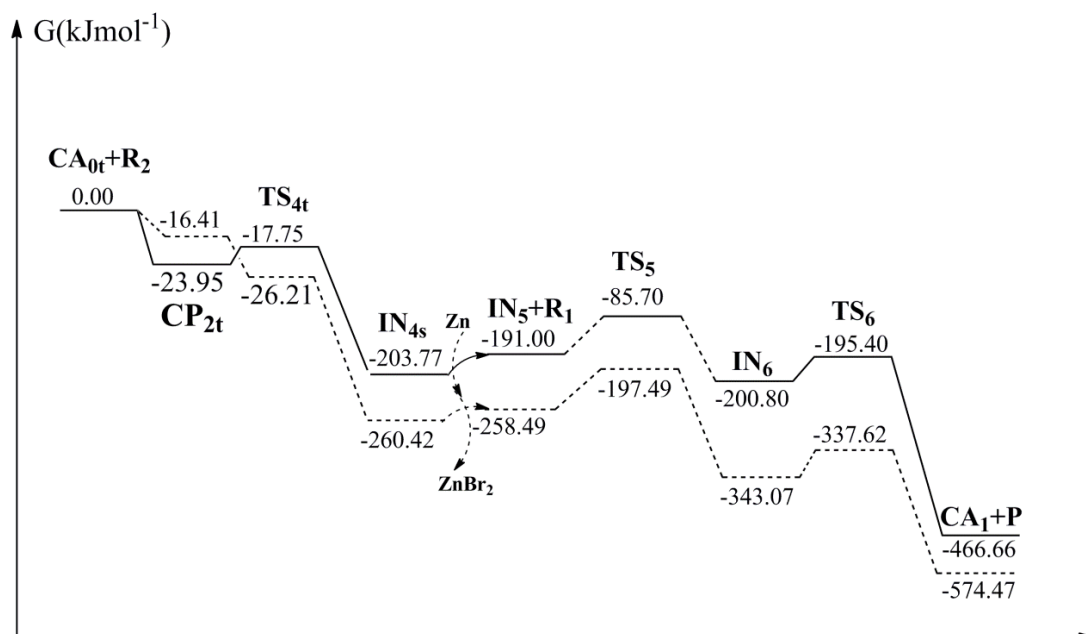


Fig.S3 Gibbs free energies ΔG in gas phase (solid line) and Gibbs free energies in solvent CH₃CN ΔG_{sol} (298K) (dashed line) for the overall catalytic cycles of Path III

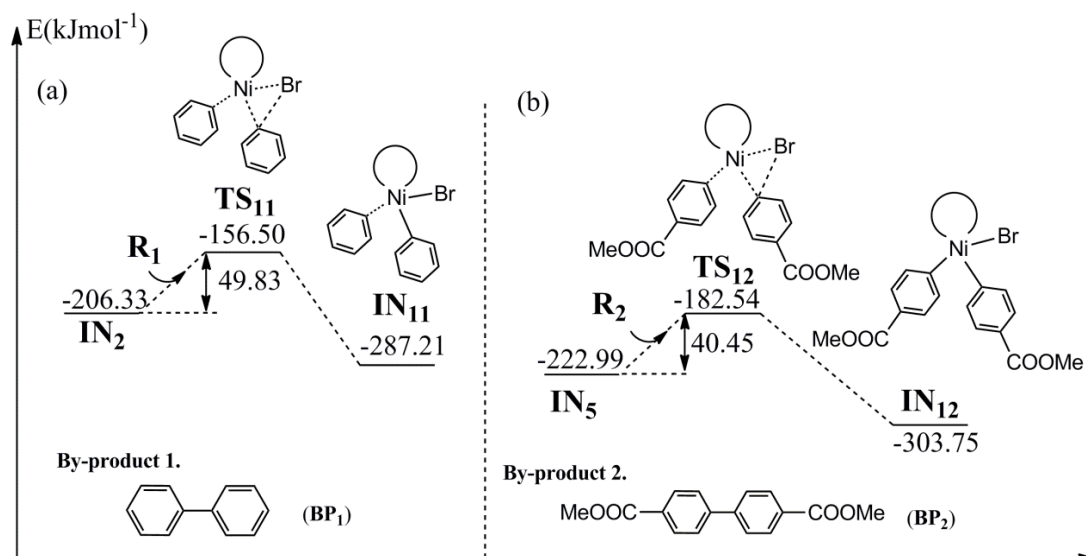


Fig.S4 Energy profiles for the rate-limiting step (the second oxidative addition) to obtain the homocoupling byproducts

The fully optimized structures

R1

C	-2.18478700	-1.20791100	0.00000200
C	-0.78806000	-1.21707200	0.00000000
C	-0.10736600	-0.00000400	0.00000000
C	-0.78805900	1.21707100	0.00000100
C	-2.18478000	1.20791500	0.00000200
C	-2.88500800	0.00000100	0.00000200
H	-2.72271000	-2.15198200	0.00000200
H	-0.23935500	-2.15270300	0.00000000
H	-0.23934300	2.15269600	0.00000000
H	-2.72270700	2.15198400	0.00000300
H	-3.97121500	0.00000700	0.00000300
Br	1.81496200	0.00000000	-0.00000100

CA_{0s}

C	-0.72907200	0.31169500	-0.07047000
C	-2.64280200	-0.97991100	-0.41796600
C	-3.47085400	0.10051800	-0.17482600
C	-2.91549900	1.36468400	0.10915100
C	-1.52504000	1.43888300	0.16294300
C	0.72901800	0.31171100	0.07033300

C	2.64278300	-0.97988200	0.41772900
C	3.47079000	0.10057900	0.17467500
C	2.91540000	1.36478200	-0.10918400
C	1.52495600	1.43895600	-0.16298000
H	-3.05480200	-1.94727000	-0.68723300
H	-4.54812400	-0.02954100	-0.23666200
H	-1.04699800	2.37638200	0.43275100
H	3.05475700	-1.94727200	0.68689400
H	4.54806500	-0.02942300	0.23650600
H	1.04688300	2.37644300	-0.43277500
N	-1.28569900	-0.90686000	-0.40100400
N	1.28565500	-0.90683800	0.40076700
Ni	0.00010300	-2.24964600	0.00012600
C	3.79028800	2.56459600	-0.36847300
H	4.42269700	2.41670600	-1.25360400
H	3.19329800	3.46730400	-0.53254400
H	4.46410300	2.75623700	0.47650400
C	-3.79034300	2.56447800	0.36869200
H	-4.42229900	2.41669800	1.25416800
H	-3.19330200	3.46722600	0.53233200
H	-4.46460100	2.75595300	-0.47596700

CA_{0t}

C	-0.72299000	0.30478600	-0.04871000
C	-2.68221000	-0.99170500	-0.16167300
C	-3.49617400	0.12179900	-0.13113000
C	-2.90136300	1.40562900	-0.00228300
C	-1.52125600	1.47113800	0.04259100
C	0.72298800	0.30479600	-0.04869700
C	2.68220300	-0.99170700	-0.16162700
C	3.49618700	0.12179300	-0.13105800
C	2.90138000	1.40561500	-0.00222400
C	1.52126700	1.47112900	0.04265200
H	-3.10592000	-1.99108200	-0.22428600
H	-4.57392800	0.00817700	-0.19452100
H	-1.04180500	2.43951400	0.14393600
H	3.10592600	-1.99108100	-0.22421400
H	4.57393900	0.00812100	-0.19440000
H	1.04184100	2.43950900	0.14405700
N	-1.33542100	-0.93451600	-0.11826000
N	1.33542500	-0.93451500	-0.11825500
Ni	0.00000300	-2.32317400	0.14991900
C	-3.75969800	2.64133400	0.08279300

H	-3.15296400	3.54932600	0.15586500
H	-4.40559900	2.73591200	-0.79995300
H	-4.42144300	2.60620900	0.95809600
C	3.75966500	2.64136900	0.08268100
H	4.40414200	2.73688000	-0.80101600
H	3.15288700	3.54918400	0.15753800
H	4.42282400	2.60556000	0.95687600

CP₁₅

C	2.70553500	-0.10726500	0.07315400
C	2.48397000	-2.41885800	-0.00280400
C	3.82686700	-2.60208700	0.28366300
C	4.66546300	-1.48651100	0.46130900
C	4.07066200	-0.23065500	0.35521700
C	1.99337200	1.17305000	-0.00910400
C	-0.08531600	2.20219800	0.03382300
C	0.47302700	3.44573100	-0.21602200
C	1.86557500	3.56956500	-0.37290900
C	2.61603200	2.39928600	-0.26897400
H	1.82452100	-3.26311600	-0.17065900
H	4.22446200	-3.61101800	0.35143700
H	4.66565700	0.66247900	0.52151900
H	-1.15670900	2.08791300	0.16676700
H	-0.17155100	4.31849700	-0.27765000
H	3.69106800	2.43465800	-0.41981600
N	1.90876700	-1.20011900	-0.12397100
N	0.64029200	1.06744300	0.14795300
Ni	0.02463600	-0.80280400	-0.17155700
Br	-1.98853300	-1.65513000	-0.58979400
C	-3.52536100	-0.49761400	0.06611400
C	-3.32472500	0.31773500	1.17325700
C	-4.74640000	-0.55606600	-0.59582900
C	-4.38562800	1.10684300	1.62936100
H	-2.35676600	0.33181600	1.67006600
C	-5.79988400	0.23929000	-0.13236400
H	-4.87977700	-1.20464600	-1.45755800
C	-5.62105600	1.06912700	0.97728900
H	-4.24628900	1.74678200	2.49756500
H	-6.76007300	0.20919100	-0.64178100
C	6.13276200	-1.65050600	0.76688400
H	6.63473600	-0.68208000	0.85541500
H	6.28526000	-2.19571400	1.70690600
H	6.63966300	-2.22229000	-0.02055200
C	2.50601000	4.90394300	-0.65995400

H	3.59741700	4.82751100	-0.68789000
H	2.17332000	5.30536600	-1.62572600
H	2.23822000	5.64460500	0.10379800
H	-6.44316000	1.68361300	1.33400700

CP_{1t}

C	2.13662500	-0.67559100	0.08390800
C	0.90121900	-2.64716400	0.43254600
C	2.03103900	-3.43407400	0.41368200
C	3.30105300	-2.81608100	0.22212100
C	3.32622200	-1.44587600	0.05923800
C	2.07185000	0.74891500	-0.07873200
C	0.67289700	2.63467700	-0.14498100
C	1.73115400	3.49029000	-0.36327900
C	3.04760400	2.95468100	-0.44914100
C	3.19035100	1.58938900	-0.30413100
H	-0.08244200	-3.08994100	0.57121000
H	1.94647200	-4.50887100	0.54142300
H	4.27897700	-0.94689100	-0.08967600
H	-0.34254200	3.01357400	-0.07564100
H	1.55457800	4.55649600	-0.46891800
H	4.18130100	1.15000100	-0.36678000
N	0.91633000	-1.30353700	0.27906300
N	0.80090400	1.29758600	-0.00279800
Ni	-0.60481900	-0.07097200	0.29657700
H	-2.47575700	1.49502700	3.04430400
C	-2.59919200	1.42933000	1.96688700
C	-2.45555100	0.16146200	1.34227300
C	-2.92492700	2.55075500	1.22742300
C	-2.65853900	0.07183500	-0.06690900
H	-2.41843600	-0.73702200	1.95244700
C	-3.12052000	2.44747700	-0.17069700
H	-3.04373700	3.51169600	1.71909600
C	-3.00283400	1.22928500	-0.81460200
H	-3.37516200	3.33176500	-0.74832900
H	-3.18089800	1.14119000	-1.88100800
Br	-3.05724000	-1.67448300	-0.85531500
C	4.55826100	-3.64610700	0.20018900
H	4.52357200	-4.39985100	-0.59775700
H	5.44682000	-3.02711200	0.03999400
H	4.69211500	-4.19083600	1.14439300
C	4.22752500	3.85987600	-0.69192100
H	5.16608900	3.29765800	-0.72723500
H	4.12387000	4.40295700	-1.64082800

H	4.31747700	4.61745600	0.09806300
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IN₁₅

C	-1.52136400	1.38429100	-0.00011100
C	0.55749400	2.41088700	-0.00016000
C	-0.02123600	3.67615200	-0.00006800
C	-1.41116800	3.80912100	0.00002500
C	-2.15659300	2.62506900	-0.00001500
C	-2.24292500	0.09559200	-0.00024100
C	-1.99656200	-2.20681300	-0.00085600
C	-3.37645600	-2.39582000	-0.00073100
C	-4.23044500	-1.29039400	-0.00028900
C	-3.63247200	-0.02436100	-0.00004500
H	1.63183700	2.28262900	-0.00023900
H	0.62225200	4.55051900	-0.00006900
H	-3.24007100	2.67776300	0.00000400
H	-1.29597400	-3.03614000	-0.00113800
H	-3.77482300	-3.40582000	-0.00096000
H	-4.25953000	0.86099000	0.00031200
N	-0.16390500	1.27676500	-0.00016900
N	-1.43428600	-0.99117200	-0.00060100
Ni	0.55137300	-0.55397700	-0.00022400
C	2.35644500	0.01057500	0.00038100
C	3.03036800	0.27652100	1.20399200
C	3.03107400	0.27711700	-1.20269800
C	4.32341700	0.81227700	1.20643800
H	2.54966300	0.05624800	2.15538400
C	4.32413400	0.81286800	-1.20411500
H	2.55092800	0.05733200	-2.15448700
C	4.97414500	1.08693500	0.00142000
H	4.82458900	1.00770100	2.15262900
H	4.82586600	1.00875000	-2.14991400
Br	1.29702700	-2.76032600	-0.00028800
C	-2.08864500	5.15548000	0.00012800
H	-2.72903000	5.27395400	-0.88229900
H	-2.72887000	5.27389700	0.88267800
H	-1.35927300	5.97020700	0.00008900
C	-5.73076100	-1.43883200	-0.00006500
H	-6.17339000	-0.96178500	0.88271100
H	-6.17373200	-0.96107800	-0.88228700
H	-6.02846600	-2.49104700	-0.00042500
H	5.98026200	1.49950200	0.00181900

IN_{1t}

C	-1.54194100	1.23103600	-0.06282700
C	0.41870400	2.33483300	0.51608400
C	-0.26099500	3.52778800	0.73457200
C	-1.64726400	3.57693100	0.54042900
C	-2.28232000	2.40059100	0.12990200
C	-2.13449400	-0.07031700	-0.47072100
C	-1.70321700	-2.29196900	-0.96853400
C	-3.05029700	-2.56140200	-1.17700000
C	-3.98878600	-1.53301600	-1.02029500
C	-3.50525100	-0.27273600	-0.65862000
H	1.49309600	2.24902000	0.64226600
H	0.28870200	4.40876200	1.05190900
H	-3.35427600	2.40578000	-0.03440800
H	-0.95130500	-3.07007900	-1.05799200
H	-3.36276100	-3.56493700	-1.44968500
H	-4.20594300	0.54263500	-0.51570200
N	-0.20631900	1.21647600	0.12788800
N	-1.25109100	-1.07720100	-0.63343000
Ni	0.76813100	-0.59438200	-0.12781800
C	2.62145100	-0.14875900	-0.62403600
C	3.74066200	-0.77755300	-0.04188000
C	2.88604700	0.79534300	-1.63925700
C	5.04526100	-0.48694500	-0.45108500
H	3.58515600	-1.50119900	0.75533400
C	4.18772500	1.09191800	-2.06002400
H	2.06036000	1.32094200	-2.12301900
C	5.27357100	0.44883500	-1.46372000
H	5.88685500	-0.98934500	0.02222900
H	4.35324500	1.82367100	-2.84902500
H	6.28843000	0.67664900	-1.78235000
Br	0.71383000	-1.73021500	2.01893000
C	-2.42464000	4.84602400	0.78053500
H	-3.44645100	4.77255700	0.39693900
H	-2.48405000	5.06438200	1.85414700
H	-1.93860600	5.70367500	0.30269900
C	-5.46158600	-1.78416600	-1.22039400
H	-5.83606900	-2.50539100	-0.48402500
H	-6.04529100	-0.86468000	-1.11962900
H	-5.65671400	-2.20573100	-2.21329800

IN₂

C	-1.99784200	-0.40428200	0.01107900
C	-1.43000300	-2.65365700	0.02495000
C	-2.76043000	-3.04062800	0.08121100

C	-3.76773300	-2.06319000	0.10885800
C	-3.35622300	-0.73007800	0.07195000
C	-1.47868000	0.97942000	-0.03971800
C	0.45006600	2.26560900	-0.13082800
C	-0.28184800	3.44659400	-0.15718000
C	-1.68350000	3.39275800	-0.12304700
C	-2.27578000	2.12912000	-0.06416400
H	-0.63182600	-3.38946600	0.00782400
H	-3.01008400	-4.09747500	0.10502300
H	-4.10246900	0.05747800	0.09204900
H	1.53588700	2.25872500	-0.15521800
H	0.23637500	4.40006800	-0.20497300
H	-3.35781200	2.04898400	-0.04126900
N	-1.03558700	-1.36554600	-0.00984900
N	-0.12952200	1.05796300	-0.07112100
Ni	0.85247200	-0.74062700	-0.03968200
C	2.79809500	-0.59785700	0.01372100
C	3.45570100	0.19322500	0.98715600
C	3.65531200	-1.25449300	-0.90205400
C	4.84675500	0.32799800	1.04468700
H	2.86309400	0.72295200	1.73467500
C	5.04811900	-1.13097200	-0.85941200
H	3.22524600	-1.88204900	-1.68285100
C	5.65229400	-0.33591800	0.11689600
H	5.30340400	0.94910400	1.81429600
H	5.66359200	-1.65519000	-1.58924500
H	6.73511300	-0.23586700	0.15472400
C	-2.51286100	4.65209100	-0.14985700
H	-2.30268700	5.24247300	-1.04976300
H	-3.58393800	4.42964100	-0.13369300
H	-2.28647600	5.28963400	0.71335500
C	-5.22487700	-2.44254900	0.18255300
H	-5.45175200	-2.95043800	1.12831400
H	-5.87349900	-1.56448700	0.10945900
H	-5.49499500	-3.13259700	-0.62561700

IN₃

C	-3.14356800	0.16025000	0.01111600
C	-4.52711400	-0.04798300	0.01207600
C	-5.06619200	-1.21120200	0.56469500
C	-4.16726000	-2.14161500	1.10271900
C	-2.80477400	-1.87823400	1.05856500
C	-2.49472300	1.38605600	-0.51343000
C	-3.20718400	2.51069000	-0.94128900

C	-2.53068100	3.65680100	-1.36555700
C	-1.13154200	3.62149300	-1.33242200
C	-0.48548100	2.47033300	-0.89712300
H	-5.19191600	0.69269300	-0.41839200
H	-4.52126700	-3.06577200	1.54944500
H	-2.08033300	-2.58071000	1.45705700
H	-4.29148800	2.50899600	-0.92862800
H	-0.54402900	4.48349200	-1.63407800
H	0.59616800	2.41616000	-0.84419800
N	-2.30279400	-0.75845000	0.52572300
N	-1.14457500	1.36969200	-0.51256300
Ni	-0.28548800	-0.33686400	0.41291900
C	-0.08672700	-1.68944900	-0.96286700
C	-0.46930100	-1.46223300	-2.28928300
C	0.27315200	-2.98597700	-0.57385000
C	-0.51082200	-2.51696600	-3.20720700
H	-0.74337400	-0.46207300	-2.61757500
C	0.22504800	-4.04268000	-1.49050300
H	0.61387000	-3.18173800	0.44139500
C	-0.16648700	-3.81089600	-2.81008400
H	-0.81316400	-2.32443300	-4.23441200
H	0.51029600	-5.04315400	-1.17298200
C	1.62821100	-0.17627300	0.11948400
C	2.17603900	0.36444900	-1.05401700
C	2.50443300	-0.55867900	1.14798200
C	3.54813200	0.57691400	-1.17623600
H	1.53599200	0.59976700	-1.89967500
C	3.88016000	-0.36691400	1.02228500
H	2.11396900	-0.97043800	2.07265200
C	4.41437300	0.21359900	-0.13714600
H	3.96887800	1.00592100	-2.08063400
H	4.54222300	-0.65335600	1.83258600
Br	-0.35813500	0.54217600	2.70578000
C	-6.55347700	-1.45566500	0.59308800
H	-6.92874300	-1.44410000	1.62375400
H	-7.09825200	-0.69360500	0.02830700
H	-6.79986800	-2.43629900	0.17032600
C	-3.27319100	4.89097500	-1.81024100
H	-4.34106700	4.69381800	-1.94205800
H	-3.16856700	5.69277200	-1.06876300
H	-2.87475800	5.27228200	-2.75701400
H	-0.19421800	-4.62892200	-3.52517800
C	5.86780500	0.45579400	-0.32034500
O	6.37022800	0.96654900	-1.30498200

O	6.60313700	0.04331600	0.74290900
C	8.01466900	0.25540800	0.62645500
H	8.23777600	1.31946200	0.50660700
H	8.44577300	-0.12345600	1.55421000
H	8.41815200	-0.28687800	-0.23350700

CA₁

C	1.38554700	-0.72940700	-0.00004800
C	0.06879100	-2.64046000	-0.00017000
C	1.18751700	-3.46696000	-0.00011300
C	2.46748300	-2.90046900	-0.00001400
C	2.54662000	-1.50290000	0.00001100
C	1.36785600	0.75156400	-0.00003400
C	0.00488200	2.62999900	-0.00019300
C	1.10330200	3.48343200	-0.00008600
C	2.39661000	2.94809800	0.00006900
C	2.50990500	1.55286600	0.00008500
H	-0.93760200	-3.04779800	-0.00023100
H	1.05768200	-4.54487800	-0.00016000
H	3.52101400	-1.02463200	0.00010000
H	-1.01134400	3.01215800	-0.00030900
H	0.94757400	4.55791000	-0.00011700
H	3.49562100	1.09845700	0.00019300
N	0.15385600	-1.30127900	-0.00012800
N	0.12293800	1.29346200	-0.00016500
Ni	-1.37954600	-0.02278100	-0.00011800
Br	-3.67478900	-0.02383600	0.00018400
C	3.62259200	3.82623200	0.00030200
H	4.24420800	3.63597600	0.88356600
H	4.24603200	3.63395100	-0.88122900
H	3.35529300	4.88662200	-0.00116800
C	3.71426700	-3.74873000	-0.00005300
H	4.33144400	-3.54347000	-0.88308500
H	4.33268200	-3.54178400	0.88171000
H	3.47250500	-4.81523000	0.00111500

IN₇

C	-2.28906300	-0.01187100	-0.12449000
C	-3.66303900	-0.25381900	-0.22740700
C	-4.16216400	-1.54940600	-0.07878400
C	-3.23549300	-2.57086100	0.16891100
C	-1.88298400	-2.26463100	0.24057100
C	-1.67533300	1.33342000	-0.21945800
C	-2.42118400	2.51289900	-0.29978400

C	-1.78364800	3.75550800	-0.31836500
C	-0.38657100	3.75591400	-0.23492300
C	0.29656100	2.54811000	-0.16065000
H	-4.35023400	0.56076400	-0.42772400
H	-3.55981700	-3.59928000	0.29538000
H	-1.13420200	-3.03066300	0.40966400
H	-3.50419100	2.47098000	-0.32939100
H	0.17192300	4.68694900	-0.21990900
H	1.37698500	2.51465800	-0.08415000
N	-1.42212700	-1.01713500	0.09688200
N	-0.32439300	1.36131000	-0.17262600
Ni	0.58214500	-0.50990500	0.08751700
Br	0.56290900	-0.45467300	2.51168700
C	-2.56393400	5.04085200	-0.42045100
H	-2.43102100	5.49641700	-1.40981700
H	-3.63460900	4.87594800	-0.26903800
H	-2.22031700	5.77064700	0.32074300
C	-5.63826200	-1.84087500	-0.17173100
H	-6.20287300	-0.96357800	-0.50059900
H	-5.83419200	-2.65757300	-0.87556300
H	-6.03473800	-2.15122400	0.80289100
C	2.50820300	-0.06710000	-0.06223700
C	2.91189400	0.79396400	-1.08447200
C	3.44554600	-0.61744200	0.81114700
C	4.25921000	1.16271500	-1.18815800
H	2.20341700	1.15252000	-1.82432700
C	4.79246200	-0.25514600	0.68689800
H	3.14223100	-1.29734000	1.59793600
C	5.20125900	0.64047000	-0.30185000
H	4.56720200	1.83573800	-1.98507800
H	5.51771100	-0.67433700	1.38028700
H	6.24828500	0.91844700	-0.38979700
Br	0.84632700	-1.73724700	-1.95455500

R₂

C	-0.57838300	1.35373800	0.00016100
C	0.81154300	1.27161700	0.00011700
C	1.41189700	0.01122600	-0.00003500
C	0.65199300	-1.15930800	-0.00014400
C	-0.73830400	-1.06331700	-0.00009800
C	-1.36145400	0.19193800	0.00005300
H	-1.07605200	2.31785400	0.00027800
H	1.41893400	2.16992900	0.00020100
H	1.13763900	-2.12879200	-0.00026200

H	-1.34224400	-1.96363200	-0.00018100
Br	3.32476700	-0.11620300	-0.00009200
C	-2.84331700	0.35125500	0.00010600
O	-3.41805400	1.42241400	0.00022200
O	-3.48968800	-0.83637900	0.00003800
C	-4.92305000	-0.75369600	0.00001400
H	-5.27492100	-1.78573100	-0.00095100
H	-5.27696400	-0.22659700	0.89005800
H	-5.27686300	-0.22490800	-0.88905400

TS₁₅

C	-2.45703600	-0.11090100	-0.07580800
C	-2.13892500	-2.35550400	-0.58170100
C	-3.40881800	-2.68657800	-0.14408500
C	-4.25589200	-1.68251200	0.37059500
C	-3.74722400	-0.38695200	0.39829500
C	-1.84968100	1.21838200	-0.05115700
C	0.15316100	2.40486700	-0.11939100
C	-0.51246700	3.61681800	-0.16321100
C	-1.92248600	3.64561800	-0.12911100
C	-2.57515600	2.41753400	-0.08243900
H	-1.47704600	-3.11479200	-0.99104600
H	-3.75020900	-3.71613700	-0.21540500
H	-4.34453600	0.41702600	0.81990600
H	1.23776800	2.35927900	-0.11412900
H	0.05974900	4.53989000	-0.20021700
H	-3.66058800	2.38174700	-0.10687900
N	-1.63829300	-1.09760900	-0.56880700
N	-0.47892900	1.21019600	-0.03425000
Ni	0.26802200	-0.54720100	-0.24158700
Br	1.96091100	-2.13046200	-0.14564800
C	3.05844500	-0.53786000	0.12986900
C	3.39647100	-0.16076400	1.43533800
C	3.62757700	0.08706100	-0.98602500
C	4.27222000	0.90813400	1.61510600
H	2.96379800	-0.67617000	2.28568100
C	4.50184300	1.15550400	-0.77908400
H	3.37589200	-0.24055100	-1.98871600
C	4.82491800	1.57463500	0.51476500
H	4.52574400	1.21938600	2.62513100
H	4.93547700	1.65737200	-1.64021600
C	-2.67760900	4.94992100	-0.16633400
H	-3.75943900	4.78766800	-0.12980600
H	-2.40487100	5.59110500	0.68183200

H	-2.45380000	5.51656200	-1.07942300
C	-5.63500800	-2.01047900	0.88346500
H	-6.18177700	-1.10601200	1.16851200
H	-6.22663300	-2.53755200	0.12405400
H	-5.59038300	-2.66510200	1.76376900
H	5.50889200	2.40443600	0.66597300

TS_{1t}

C	2.69339800	0.69737900	-1.07954100
C	2.51911600	0.06383100	0.17720200
C	2.89447600	0.73072300	1.37120300
C	3.32801300	2.04344000	1.30291500
C	3.44715400	2.70510300	0.06056400
C	3.13530200	2.03455300	-1.11607200
Br	2.76649700	-2.07982300	0.13053400
H	2.81024800	0.21712600	2.32375200
H	2.57926000	0.13863500	-2.00416400
H	3.26320800	2.52519200	-2.07815000
H	3.81106400	3.72805200	0.02671000
H	3.57724200	2.57246000	2.21971900
C	-2.17003200	-0.57049400	-0.04510600
C	-1.07494700	-2.62683500	-0.27827300
C	-2.25090600	-3.33418900	-0.12446800
C	-3.45952800	-2.63069000	0.10167300
C	-3.39335000	-1.24679900	0.13940600
C	-2.01884200	0.87344700	-0.04653300
C	-0.51772800	2.65408300	-0.25896000
C	-1.52027100	3.59325700	-0.10676300
C	-2.85243800	3.15663600	0.09467200
C	-3.07826000	1.78954800	0.12146700
H	-0.12725000	-3.13481700	-0.42952400
H	-2.23723500	-4.41897500	-0.16903400
H	-4.30066300	-0.67698200	0.31314900
H	0.51545500	2.95424600	-0.40754000
H	-1.27974300	4.65162300	-0.14050800
H	-4.08826400	1.42142400	0.27107000
N	-1.00797000	-1.27917800	-0.24045400
N	-0.73451700	1.32452000	-0.23003700
Ni	0.61452400	-0.15412500	-0.30152300
C	-3.97099200	4.15131500	0.27021800
H	-4.93559300	3.65296100	0.40761300
H	-3.79556700	4.79439300	1.14227100
H	-4.05315400	4.81273700	-0.60185000
C	-4.75763300	-3.37152200	0.29360500

H	-5.59479500	-2.68419500	0.44999500
H	-4.99025000	-3.99509200	-0.57926900
H	-4.70578500	-4.04360800	1.15987900

TS₂

Ni	0.24755800	0.29458600	0.48827300
C	-1.20523900	-0.63920000	-0.67200600
C	-3.99511300	-0.94213400	-0.38006200
C	-1.73710900	-1.62595300	0.19390600
C	-2.09810700	0.13793600	-1.44910100
C	-3.46579000	-0.00159200	-1.29022900
C	-3.11373400	-1.74354600	0.36023200
H	-1.07250600	-2.31278200	0.70983200
H	-1.70259900	0.85485100	-2.16112000
H	-4.14272500	0.61670400	-1.86991900
H	-3.52857700	-2.47978200	1.04192500
N	1.90221600	1.05539700	-0.52168400
C	4.18754100	1.91709400	-1.89095200
C	1.84506400	2.09700500	-1.35981700
C	3.07934500	0.42414900	-0.33248600
C	4.23440500	0.83948300	-1.00218000
C	2.95340200	2.55668000	-2.06112800
N	1.83830800	-0.99996000	1.15493700
C	4.09473600	-2.49693100	1.89759500
C	1.74425100	-2.00018500	2.04101800
C	3.04835500	-0.71286600	0.62565000
C	4.18577900	-1.44386500	0.98408200
C	2.83133500	-2.76880400	2.43778800
H	0.87311100	2.57045200	-1.45489100
H	5.17623500	0.32553700	-0.84536800
H	2.85235800	3.40451700	-2.73203900
H	0.75300200	-2.18644000	2.44467300
H	5.15154000	-1.19987100	0.55571500
H	2.69196000	-3.56892600	3.15857700
Br	0.43837800	-1.52287000	-1.96145900
C	-0.69176900	1.87471700	1.20899100
C	-2.05379300	1.88930300	1.56825600
C	0.05136400	3.02725200	1.54291100
C	-2.64118700	2.97931600	2.21793800
H	-2.67900700	1.03086200	1.33420100
C	-0.52447100	4.12846600	2.18716100
H	1.11322600	3.07835900	1.29905300
C	-1.87764800	4.10737900	2.52788900
H	-3.69709100	2.94917000	2.48073300

H	0.08380700	5.00022200	2.42331800
H	-2.33260900	4.95961600	3.02777600
C	5.41122600	2.36422300	-2.64950600
H	6.32371500	1.91872400	-2.24242300
H	5.33853200	2.07261000	-3.70486700
H	5.51847600	3.45407400	-2.62147000
C	5.30132500	-3.31667900	2.27721400
H	6.23023400	-2.84602900	1.94213000
H	5.35916500	-3.45770900	3.36206200
H	5.24861600	-4.31419400	1.82302500
C	-5.44790700	-1.13781500	-0.18137400
O	-5.94527300	-1.93644100	0.59348000
O	-6.19641000	-0.31954600	-0.96643800
C	-7.61316300	-0.46218100	-0.81532800
H	-8.05594100	0.25720900	-1.50574200
H	-7.92933400	-1.47882300	-1.06611200
H	-7.91726300	-0.24401200	0.21247600

TS₃

C	-3.09623500	0.62213300	-0.21408800
C	-4.46823100	0.61639700	-0.48923200
C	-5.20865100	-0.55891800	-0.34223000
C	-4.52016500	-1.70191800	0.08437200
C	-3.15441600	-1.62644900	0.33069100
C	-2.24427700	1.83502500	-0.29663000
C	-2.76536600	3.12408300	-0.44658600
C	-1.91896100	4.23544400	-0.44930200
C	-0.54892900	3.99371900	-0.29297700
C	-0.09716800	2.68690200	-0.15172600
H	-4.96561400	1.51983200	-0.82549100
H	-5.03975500	-2.64540500	0.22277100
H	-2.58626700	-2.48853000	0.66389800
H	-3.83597500	3.27196700	-0.53626700
H	0.16407900	4.81257500	-0.27325800
H	0.95765100	2.46768400	-0.02436200
N	-2.45642100	-0.49557200	0.17820000
N	-0.91481600	1.62404900	-0.16598400
Ni	-0.37447400	-0.37434000	0.42845100
C	0.08655900	-1.65483600	-0.95538600
C	-0.15228300	-1.36421000	-2.30648800
C	0.15807700	-2.99651700	-0.55033700
C	-0.34977600	-2.39455700	-3.22808800
H	-0.19602100	-0.33205100	-2.64522400
C	-0.04011000	-4.02498300	-1.47632500

H	0.36895800	-3.23795500	0.48769600
C	-0.29485000	-3.72933100	-2.81701500
H	-0.54536500	-2.15251900	-4.27029800
H	0.01548800	-5.05966900	-1.14633000
H	-0.43913100	-4.53014600	-3.53732200
C	1.54993200	-0.45749700	0.02434000
C	2.13535700	0.39504900	-0.92963600
C	2.39784100	-1.09317000	0.95084400
C	3.50383200	0.65751400	-0.92571900
H	1.52305400	0.84906300	-1.70361600
C	3.76489400	-0.83726200	0.95445300
H	1.97911500	-1.75888000	1.69748300
C	4.33418600	0.04375000	0.02209000
H	3.93344100	1.32462300	-1.66568100
H	4.41291400	-1.31121200	1.68515100
Br	-0.54116500	-0.88756100	2.83737000
C	-2.45846300	5.63681500	-0.58028000
H	-3.50547400	5.63816600	-0.89704800
H	-2.39771800	6.16479600	0.37963500
H	-1.87843800	6.21763500	-1.30583200
C	-6.69104700	-0.59558800	-0.61539200
H	-6.95394000	-1.44426500	-1.25661500
H	-7.25441500	-0.70945200	0.31916900
H	-7.03424600	0.32140100	-1.10353800
C	5.79933700	0.27518100	0.07423400
O	6.56050700	-0.25161100	0.86389200
O	6.22151300	1.15695100	-0.86955800
C	7.63039200	1.41650400	-0.86915500
H	8.19366100	0.49707100	-1.05244900
H	7.79718100	2.13387700	-1.67406600
H	7.94648700	1.83581500	0.09026300

TS₇

Ni	0.71951000	-0.17163700	-0.53339600
C	1.69843300	-0.03250500	1.31635200
C	1.45898200	1.97714500	3.24126200
C	2.50022500	1.12174500	1.21901200
C	0.85930300	-0.23026500	2.43046300
C	0.72501100	0.79122900	3.36786600
C	2.34668700	2.13031000	2.17174100
H	1.35962300	2.76206600	3.98564900
H	3.19606500	1.22865100	0.39496200
H	0.31063700	-1.15946700	2.54004900
H	0.05274400	0.65354400	4.21145500

H	2.94025400	3.03660700	2.08035800
N	-0.80591500	1.22025900	-0.35508600
C	-2.98230500	2.95851600	-0.06352000
C	-0.63814600	2.54498400	-0.45040300
C	-2.04001400	0.72630700	-0.13218100
C	-3.14314200	1.57307500	0.02051200
C	-1.69045300	3.44223200	-0.30771300
N	-0.94151900	-1.40773000	-0.19992200
C	-3.34108400	-2.85263300	0.03841400
C	-0.94565100	-2.74961500	-0.20225800
C	-2.12233900	-0.75632500	-0.08768300
C	-3.32730800	-1.45607500	0.03684200
C	-2.10689400	-3.50340800	-0.08682600
H	0.37437100	2.87228400	-0.66263000
H	-4.13069200	1.16449800	0.20546000
H	-1.50236400	4.50853300	-0.39179400
H	0.02732000	-3.22069300	-0.29477500
H	-4.26466700	-0.91759400	0.12306200
H	-2.04580500	-4.58765400	-0.09657600
Br	1.86780000	0.73501100	-2.46853200
Br	2.50922900	-1.78842200	0.44893600
C	-4.62784300	-3.62940200	0.15422200
H	-5.48060800	-2.97125200	0.34441900
H	-4.83059900	-4.18593900	-0.76901300
H	-4.57376200	-4.36256000	0.96720800
C	-4.15270600	3.89757100	0.08543500
H	-4.36926900	4.40259400	-0.86403300
H	-5.05767600	3.36836500	0.39823800
H	-3.94036800	4.67823100	0.82474500

CP₂₅

C	3.72848500	0.22284600	0.14302900
C	3.88147700	-2.09345300	0.20492100
C	5.21996000	-2.04065900	0.56045100
C	5.85836800	-0.79678200	0.70675000
C	5.07772900	0.33870300	0.49363100
C	2.82917900	1.36789800	-0.05825200
C	0.61792400	2.05106100	-0.19622700
C	0.98935900	3.35776300	-0.47406300
C	2.35153200	3.69584700	-0.55132600
C	3.26825100	2.66584400	-0.34161500
H	3.37464800	-3.04133500	0.06317700
H	5.76838000	-2.96672300	0.70933800
H	5.51446700	1.32375700	0.62803900

H	-0.42859200	1.77205300	-0.12443800
H	0.22108300	4.11226900	-0.61965300
H	4.33187200	2.86868600	-0.42479400
N	3.12711000	-0.99275400	-0.01465300
N	1.50372400	1.05456200	0.01809000
Ni	1.20630500	-0.91136800	-0.17452900
Br	-0.57437800	-2.16107300	-0.59430400
C	-2.35881500	-1.24941000	-0.19494700
C	-2.40923300	-0.28615300	0.80737000
C	-3.48556800	-1.60745300	-0.92817600
C	-3.62368200	0.34212900	1.07785600
H	-1.51007900	-0.03636800	1.36697000
C	-4.69862100	-0.97294900	-0.65589800
H	-3.42394300	-2.36552800	-1.70435000
C	-4.77302000	0.00552200	0.34682300
H	-3.70389900	1.09583600	1.85521900
H	-5.58842600	-1.23121800	-1.21991200
C	-6.03827000	0.71674000	0.67586600
O	-6.14629200	1.57580500	1.53041300
O	-7.07879800	0.30531300	-0.08770200
C	-8.32839000	0.95549400	0.18152200
H	-8.24506700	2.03346400	0.01799200
H	-9.04306500	0.51578100	-0.51517200
H	-8.64017800	0.77855300	1.21458600
C	7.31344500	-0.70288600	1.08981800
H	7.64884900	0.33754900	1.14018700
H	7.49726100	-1.16327800	2.06870000
H	7.94810500	-1.22747200	0.36477600
C	2.79312200	5.10311200	-0.86366200
H	3.88202300	5.20190600	-0.81714500
H	2.47117300	5.40674200	-1.86786100
H	2.35757900	5.82030800	-0.15715100

CP_{2t}

C	2.75722400	0.69495400	0.25220200
C	3.00355500	-1.53011600	0.95450500
C	4.36043900	-1.38243100	1.14412200
C	4.96625900	-0.12587000	0.87385200
C	4.14436700	0.89379600	0.42760700
C	1.82844300	1.70203000	-0.20706600
C	-0.40429700	2.17678700	-0.73364800
C	-0.10896500	3.48332900	-1.06419200
C	1.23121700	3.93820500	-0.96761200
C	2.18148200	3.02856100	-0.53658400

H	2.51441700	-2.48223300	1.14359800
H	4.95222600	-2.22304000	1.49333700
H	4.57595100	1.86539300	0.20820300
H	-1.42041200	1.80232900	-0.80163900
H	-0.90128900	4.14779700	-1.39536300
H	3.21693600	3.34319600	-0.45134600
N	2.19465800	-0.53528500	0.52398500
N	0.51857500	1.28441800	-0.31344300
Ni	0.27032900	-0.62915500	0.16891800
H	-2.76463700	-0.43949500	2.22084700
C	-2.54507600	-0.67044300	1.18422300
C	-1.51318800	-1.58599300	0.88680800
C	-3.30083500	-0.08916200	0.16914500
C	-1.22896300	-1.89788400	-0.48281600
H	-1.07492400	-2.17556700	1.68807800
C	-3.03254500	-0.43489400	-1.18803700
C	-2.03733600	-1.32673000	-1.51298500
H	-3.63893100	0.02339500	-1.96233800
H	-1.85258800	-1.60202200	-2.54598900
Br	-0.31781100	-3.59297000	-0.88104100
C	6.44739200	0.06960100	1.06813300
H	7.02497400	-0.61680300	0.43519700
H	6.75427700	1.09142000	0.82397200
H	6.74165400	-0.13234300	2.10641300
C	1.58977500	5.35764600	-1.32452100
H	1.04558500	6.07440700	-0.69581800
H	2.66082900	5.54590000	-1.20075600
H	1.32516400	5.58354400	-2.36564000
C	-4.38677900	0.87835000	0.43608200
O	-5.04599900	1.43061000	-0.42841700
O	-4.57844100	1.09914800	1.76173400
C	-5.61671800	2.03478600	2.07959900
H	-5.63776500	2.08988400	3.16872900
H	-5.39731700	3.01643400	1.65020600
H	-6.57977700	1.68896900	1.69384100

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C	-2.20173300	1.59453800	-0.01519600
C	0.03439600	2.20687700	0.02775100
C	-0.28963700	3.55689600	0.02058900
C	-1.63151600	3.95396000	-0.00497100
C	-2.58760800	2.93669200	-0.02363000
C	-3.15603700	0.46825000	-0.03545300
C	-3.35772100	-1.83902600	-0.04898300

C	-4.74528800	-1.76017800	-0.07123900
C	-5.37280100	-0.50852600	-0.07542200
C	-4.54521700	0.61698600	-0.05691800
H	1.06402600	1.87580000	0.04855500
H	0.51015400	4.29127600	0.03532700
H	-3.64014200	3.19628600	-0.04550600
H	-2.82830500	-2.78651000	-0.04414100
H	-5.32938900	-2.67566300	-0.08455100
H	-4.99078500	1.60562900	-0.05847100
N	-0.89255800	1.23028500	0.01116700
N	-2.57202200	-0.75139000	-0.03140100
Ni	-0.54334700	-0.70156600	0.01538700
C	1.33419400	-0.50760000	0.07937800
C	2.00205400	-0.35908400	1.30935800
C	2.10007600	-0.41693400	-1.09726600
C	3.37202200	-0.10809600	1.36207300
H	1.44864100	-0.44943600	2.24174700
C	3.47198400	-0.16792500	-1.05369200
H	1.62375000	-0.55511200	-2.06552400
C	4.12094600	-0.00575700	0.18010700
H	3.88430900	0.00717200	2.31274700
H	4.04577000	-0.10333600	-1.97260500
Br	-0.22782500	-3.00782800	0.00107200
C	-2.02129200	5.40947300	-0.00981400
H	-1.57334200	5.93179300	-0.86331400
H	-3.10622200	5.53705200	-0.06419000
H	-1.66528000	5.91150400	0.89780200
C	-6.87484300	-0.38447900	-0.09957700
H	-7.19468300	0.66147700	-0.08456600
H	-7.29094200	-0.85414600	-0.99879000
H	-7.32275500	-0.88973200	0.76419400
C	5.57446200	0.26539100	0.29317300
O	6.17568900	0.43666100	1.33848100
O	6.19424600	0.30962500	-0.91609800
C	7.60338900	0.55566600	-0.86715700
H	7.93857400	0.55256700	-1.90553600
H	7.81359400	1.52220200	-0.39966800
H	8.11421300	-0.22631200	-0.29795700

IN_{4t}

C	-2.46583800	1.29974000	-0.09205200
C	-0.54238900	2.23609700	0.81444000
C	-1.17159800	3.46089100	1.00697000
C	-2.51073900	3.61488700	0.62740900

C	-3.15239700	2.50636200	0.06546400
C	-3.07531000	0.06394100	-0.65127200
C	-2.71716700	-2.15606300	-1.21294700
C	-4.03631900	-2.32073700	-1.61766000
C	-4.92198300	-1.23902600	-1.52999400
C	-4.41582000	-0.03360700	-1.03505000
H	0.49608600	2.07254800	1.08311100
H	-0.61860300	4.28514600	1.44695600
H	-4.18806000	2.59363100	-0.24421500
H	-2.00953400	-2.97881200	-1.24582800
H	-4.36889400	-3.28514100	-1.98944200
H	-5.07681000	0.82124000	-0.94353800
N	-1.17308200	1.18385600	0.27853800
N	-2.24207400	-0.99332500	-0.74982500
Ni	-0.29172700	-0.67566900	0.04622800
C	1.64078100	-0.33872400	-0.16809900
C	2.62722300	-1.08008400	0.51476900
C	2.10464100	0.64612900	-1.06903500
C	3.98978200	-0.86154300	0.31284000
H	2.31775900	-1.83927400	1.22917700
C	3.46281800	0.87680300	-1.28426300
H	1.39098300	1.25676500	-1.62433100
C	4.41948700	0.12187900	-0.59196400
H	4.72580800	-1.44689000	0.85464500
H	3.80464100	1.63617500	-1.98165000
Br	-0.69149100	-1.91796200	2.08920800
C	-3.23680000	4.91945200	0.83498600
H	-4.16438900	4.96184400	0.25660600
H	-3.49620600	5.05054300	1.89317200
H	-2.61125200	5.77096400	0.54696400
C	-6.36838700	-1.37937100	-1.93007600
H	-6.91622700	-1.97644300	-1.19030700
H	-6.86239000	-0.40643700	-2.00668100
H	-6.46378600	-1.89130100	-2.89379500
C	5.85363100	0.40724700	-0.85021500
O	6.27013100	1.25779400	-1.61638800
O	6.68390700	-0.39162900	-0.13161800
C	8.08116200	-0.16114800	-0.33991000
H	8.35052700	0.86353700	-0.06758200
H	8.59591500	-0.87554200	0.30433800
H	8.35007900	-0.32693400	-1.38723100

IN₅

C	2.73401900	0.95087500	-0.06959300
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C	0.83447300	2.27896200	-0.15280500
C	1.59263700	3.44224500	-0.21528800
C	2.99249300	3.35674800	-0.20440100
C	3.55656100	2.08049500	-0.13066500
C	3.22485500	-0.44387700	0.00073000
C	2.61131700	-2.67966900	0.06843200
C	3.93462100	-3.09349700	0.11533200
C	4.96120200	-2.13712300	0.10844200
C	4.57670500	-0.79622300	0.04924900
H	-0.25132400	2.29868400	-0.15818100
H	1.09503300	4.40605900	-0.27248500
H	4.63663600	1.97595500	-0.12473300
H	1.79818000	-3.39901200	0.07631600
H	4.16260800	-4.15455900	0.15811600
H	5.33938300	-0.02451800	0.04288600
N	1.38701200	1.05971500	-0.07919300
N	2.24429600	-1.38510900	0.01215900
Ni	0.36902000	-0.71846300	-0.00529300
C	-1.56978300	-0.51917700	0.06072900
C	-2.19677800	0.30162200	1.03283100
C	-2.45475200	-1.15352800	-0.84655000
C	-3.57613600	0.48555500	1.09499200
H	-1.58390500	0.81521800	1.77413000
C	-3.83858300	-0.98567900	-0.80246400
H	-2.05038800	-1.80062500	-1.62426300
C	-4.41554300	-0.15809400	0.17317900
H	-4.02815700	1.12252700	1.85035200
H	-4.47792500	-1.48968700	-1.52084400
C	6.41121600	-2.54457100	0.17011500
H	6.65455500	-3.25928400	-0.62485800
H	7.07649200	-1.68229600	0.06651500
H	6.64104100	-3.03425900	1.12461800
C	3.85003700	4.59538300	-0.27160600
H	4.91583300	4.34955400	-0.24965500
H	3.65151300	5.16121600	-1.18976900
H	3.63889000	5.26475500	0.57090500
C	-5.87550300	0.06991700	0.27476800
O	-6.42067200	0.78966900	1.09342100
O	-6.58244000	-0.62051400	-0.66216400
C	-7.99935400	-0.43611200	-0.60829500
H	-8.26216800	0.61504300	-0.76087900
H	-8.40740000	-1.05126700	-1.41219600
H	-8.39793500	-0.75755700	0.35861300

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C	1.46307500	-2.06409700	-0.11032100
C	1.60709200	-3.44258900	-0.30146800
C	1.08377000	-4.05652400	-1.44099400
C	0.41777400	-3.23717400	-2.36193200
C	0.30028800	-1.87766700	-2.10543000
C	2.03029300	-1.32808900	1.04548100
C	2.87871900	-1.91400300	1.99010500
C	3.43366100	-1.14403100	3.01500900
C	3.10553700	0.21672300	3.04149700
C	2.25338200	0.73511600	2.07345000
H	2.12564700	-4.04575600	0.43558000
H	-0.01019500	-3.65093300	-3.27000000
H	-0.21583300	-1.21654000	-2.79369700
H	3.12965500	-2.96676200	1.92190800
H	3.51483900	0.87447600	3.80246800
H	1.99111300	1.78719700	2.05431400
N	0.80634700	-1.30338800	-1.00802100
N	1.71212600	-0.01711000	1.10667300
Ni	0.63438900	0.71017400	-0.56567600
C	-1.24484900	0.45100800	-0.17988000
C	-1.69126500	-0.08876900	1.03393100
C	-2.17221600	0.62881700	-1.21810800
C	-3.02427200	-0.46139400	1.20493800
H	-0.99655700	-0.22781100	1.85897700
C	-3.50422000	0.25035900	-1.05611400
H	-1.86476000	1.08326500	-2.15799200
C	-3.94251500	-0.29879500	0.15699100
H	-3.35744800	-0.88181900	2.14815300
H	-4.22471100	0.38480800	-1.85719000
C	0.16431600	2.54740800	-0.12427100
C	-0.16157300	2.95778900	1.17481500
C	0.20779700	3.51264200	-1.14076100
C	-0.38119000	4.30849100	1.46830100
H	-0.27627600	2.22617500	1.97037500
C	-0.03144700	4.85935200	-0.85008100
H	0.46669600	3.22808300	-2.15544600
C	-0.31781600	5.26484600	0.45498500
H	-0.62376300	4.60442800	2.48671200
H	0.02127500	5.59407200	-1.65033400
H	-0.49796700	6.31352000	0.67730600
Br	2.59866600	1.16615600	-1.96536900
C	1.23394600	-5.53740900	-1.67953900
H	1.86183000	-5.72723800	-2.55861600

H	1.69300600	-6.03948800	-0.82299600
H	0.26144500	-6.00576500	-1.86967800
C	4.37389900	-1.74299400	4.02972400
H	4.36545900	-2.83625000	3.99222800
H	5.40276500	-1.40915900	3.84581200
H	4.10961200	-1.43154500	5.04626400
C	-5.37266200	-0.68026900	0.27708500
O	-6.19824000	-0.57475700	-0.61088100
O	-5.67943500	-1.17333200	1.50441200
C	-7.04932000	-1.55419700	1.68131500
H	-7.32739000	-2.34015500	0.97332900
H	-7.12232900	-1.91941700	2.70670600
H	-7.71142800	-0.69680400	1.53147300

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C	-3.11558600	0.26084400	-0.21783900
C	-4.50237000	0.21628400	-0.39581600
C	-5.17913700	-1.00412200	-0.34889300
C	-4.41326500	-2.15561500	-0.12259400
C	-3.03786200	-2.04343300	0.02940900
C	-2.32170500	1.51160900	-0.20587800
C	-2.89527300	2.78521300	-0.26229700
C	-2.09653300	3.92760200	-0.17855800
C	-0.71917600	3.73158600	-0.02344500
C	-0.21108000	2.43932000	0.02171600
H	-5.06195200	1.12770300	-0.57409200
H	-4.87979600	-3.13468400	-0.07249600
H	-2.41041400	-2.91391300	0.18635500
H	-3.96998800	2.89461900	-0.35414800
H	-0.04143300	4.57488400	0.06874600
H	0.84900000	2.25602800	0.15135100
N	-2.40559300	-0.86489300	-0.01705100
N	-0.98461900	1.35064500	-0.08610000
Ni	-0.36316300	-0.64008400	0.11643800
Br	-0.52028400	-0.66861700	2.53003200
C	-2.68902500	5.31205100	-0.23707700
H	-2.29263000	5.86962700	-1.09403600
H	-3.77854900	5.28141500	-0.32707300
H	-2.43728000	5.88306500	0.66422000
C	-6.67331000	-1.08513100	-0.53076900
H	-7.10867700	-0.10344100	-0.73832000
H	-6.93094900	-1.75461200	-1.35965400
H	-7.15402800	-1.48575400	0.36977800
C	1.60385800	-0.47428000	0.10474100

C	2.19244100	0.37578900	-0.83678200
C	2.40098900	-1.19973900	0.99307600
C	3.57747600	0.55350700	-0.84747400
H	1.59041500	0.87281200	-1.59032300
C	3.78584400	-1.03012000	0.96708900
H	1.95702300	-1.87045800	1.71845900
C	4.38389500	-0.14721200	0.05865400
H	4.03285800	1.21439200	-1.57727600
H	4.41883800	-1.57426400	1.66107300
C	5.86384100	-0.00616600	0.08823700
O	6.60356900	-0.60471500	0.84575800
O	6.31983600	0.87805000	-0.83434300
C	7.74257900	1.04934900	-0.86097400
H	7.93526700	1.78006800	-1.64767800
H	8.10569400	1.41747100	0.10271000
H	8.24134300	0.10257200	-1.08628900
Br	-0.12918900	-1.79441500	-1.96711700

TS_g

Ni	1.02508300	-0.88061200	0.44468100
C	-0.52691700	-1.48800400	-0.81165100
C	-3.17747900	-0.57861700	-0.85720900
C	-1.48666700	-2.08038100	0.04156100
C	-0.92763700	-0.53054500	-1.77170100
C	-2.23354900	-0.06382400	-1.76709900
C	-2.78774500	-1.59469500	0.03311900
H	-1.19128600	-2.87489200	0.71704400
H	-0.20827700	-0.14672900	-2.48695400
H	-2.53641400	0.69848800	-2.47693600
H	-3.53034900	-2.00499000	0.71034200
N	0.23529100	0.85702800	1.24438500
C	-0.74983000	3.30637600	2.17458300
C	-0.68501700	0.89621200	2.21561500
C	0.69740900	2.01132800	0.72439700
C	0.22114800	3.24821600	1.17095700
C	-1.20319400	2.09073600	2.70268400
N	2.03530200	0.57847400	-0.66351100
C	3.39536800	2.71677600	-1.87577500
C	2.98920000	0.36011300	-1.58104400
C	1.74143800	1.85433500	-0.32147500
C	2.40350600	2.93319400	-0.91599800
C	3.68597800	1.38695400	-2.20601800
H	-0.99206900	-0.06759800	2.60782900
H	0.59713300	4.17122600	0.74321900

H	-1.95124900	2.06985700	3.48953600
H	3.18296200	-0.68084500	-1.81768400
H	2.15703000	3.94951300	-0.62922300
H	4.44733000	1.14805700	-2.94253600
Br	1.44388500	-2.13450000	2.46058100
Br	1.06887900	-2.74574900	-1.38806600
C	-4.58228800	-0.11377100	-0.81359500
O	-5.42629800	-0.51960300	-0.03480000
O	-4.84710900	0.83675100	-1.74845000
C	-6.19774100	1.31482600	-1.76094800
H	-6.23992400	2.05480300	-2.56145200
H	-6.89583600	0.49651700	-1.95825300
H	-6.45621600	1.77209400	-0.80148600
C	4.13574800	3.86260200	-2.51688800
H	4.16016800	3.75585400	-3.60710200
H	3.67513200	4.82528100	-2.27696400
H	5.17672700	3.89268100	-2.17172300
C	-1.28709400	4.62299200	2.67566900
H	-1.09594500	4.73983400	3.74896500
H	-0.83007200	5.47003100	2.15579100
H	-2.37262000	4.68200200	2.53326100

TS₄₅

C	-3.26872200	0.55013700	0.04466700
C	-3.80156100	-1.68532900	-0.27884600
C	-5.03881300	-1.52900600	0.32371400
C	-5.41763000	-0.26896900	0.82586200
C	-4.49997300	0.76916200	0.67438900
C	-2.24594500	1.58673000	-0.12869500
C	0.00825500	1.99388000	-0.53335300
C	-0.20312400	3.36102100	-0.59661100
C	-1.49781900	3.88034800	-0.40361800
C	-2.51809900	2.95952900	-0.17526600
H	-3.49770100	-2.64656600	-0.68424200
H	-5.71388000	-2.37813000	0.39112300
H	-4.72954000	1.75273500	1.07459200
H	1.00184800	1.57314300	-0.65250500
H	0.63915600	4.02374600	-0.77527500
H	-3.54161300	3.30555200	-0.06407200
N	-2.90862200	-0.68183700	-0.43379100
N	-0.97709100	1.10193200	-0.28376400
Ni	-0.90708700	-0.81927600	-0.44009000
Br	0.24385500	-2.80817300	-0.44224900
C	1.77807200	-1.68250400	-0.07046500

C	2.17355000	-1.47803600	1.26188500
C	2.55633800	-1.21943100	-1.14365800
C	3.32387900	-0.74478200	1.51018400
H	1.57668500	-1.86967700	2.07818300
C	3.70566200	-0.48705900	-0.87247600
H	2.25472500	-1.41799600	-2.16643100
C	4.10243300	-0.23372200	0.45408600
H	3.64758400	-0.55803100	2.52904100
H	4.30996600	-0.11425600	-1.69219400
C	5.31891200	0.53399600	0.79437900
O	5.70143200	0.76724000	1.92812500
O	5.98851500	0.96525000	-0.30762400
C	7.18405300	1.70734500	-0.04005400
H	7.89977500	1.09956000	0.52088000
H	7.59054400	1.97154200	-1.01738800
H	6.96013500	2.60826100	0.53839200
C	-1.76221700	5.36333600	-0.46580300
H	-2.80991400	5.59333900	-0.24879000
H	-1.14036200	5.90715700	0.25623600
H	-1.52799600	5.76826500	-1.45866900
C	-6.74482400	-0.06625700	1.51154900
H	-6.91639000	0.98821400	1.74941600
H	-7.57400700	-0.41038000	0.88090300
H	-6.79967000	-0.63364100	2.44969000

TS_{4t}

C	1.66759300	-1.35354500	-1.17380200
C	1.14122500	-1.72767800	0.10173900
C	1.89810600	-1.43680600	1.27754800
C	3.04298100	-0.67661700	1.18505900
C	3.51744700	-0.21356300	-0.07397200
C	2.82258200	-0.57137600	-1.23858800
Br	0.09179000	-3.56318000	0.10117300
H	1.54194000	-1.78733500	2.24109600
H	1.21220600	-1.72413300	-2.08768700
H	3.21461300	-0.24636800	-2.19770200
H	3.59041500	-0.41218800	2.08342800
C	-2.89193800	0.76643400	-0.00358300
C	-3.33649600	-1.51899300	-0.20007700
C	-4.68847700	-1.32904900	0.01804500
C	-5.17648500	-0.02555900	0.25921300
C	-4.25320200	1.01260500	0.24653600
C	-1.86154100	1.80082900	-0.06404600
C	0.40856200	2.23229500	-0.38946900

C	0.22397100	3.59729700	-0.25370400
C	-1.07087900	4.09916300	-0.00051900
C	-2.10610000	3.17699000	0.09140600
H	-2.92401000	-2.50988500	-0.36447200
H	-5.35965900	-2.18252700	0.00991400
H	-4.59257400	2.02651600	0.43201300
H	1.39216000	1.81344200	-0.57903000
H	1.07419400	4.26669200	-0.34242700
H	-3.11512400	3.52859000	0.28049100
N	-2.44162400	-0.50982300	-0.21249600
N	-0.59511800	1.33993200	-0.29486300
Ni	-0.47408100	-0.66276200	-0.32372900
C	-1.30970900	5.57862900	0.15988900
H	-2.36675400	5.79961700	0.33620700
H	-0.73441600	5.98144800	1.00296300
H	-0.99282800	6.12870500	-0.73497300
C	-6.64083100	0.21640000	0.52022400
H	-6.85218300	1.27856400	0.67651700
H	-7.25424800	-0.13089800	-0.32075100
H	-6.97918500	-0.33019900	1.40952000
C	4.73116000	0.61238300	-0.21525300
O	5.15357600	1.06275600	-1.26837400
O	5.35055800	0.83779700	0.97566700
C	6.53683000	1.63567400	0.90105400
H	6.90034100	1.71841800	1.92643100
H	7.28748400	1.15605900	0.26636200
H	6.31458700	2.62586200	0.49241200

TS₅

Ni	-0.27246700	-0.51415600	-0.11848000
C	-0.60020000	-1.61560000	1.65886400
C	-1.27506400	-0.57427500	4.16766200
C	0.41695200	-1.31750500	2.58903800
C	-1.95515400	-1.50544600	2.03294400
C	-2.27962200	-0.95293900	3.27208500
C	0.06876700	-0.76986800	3.82140200
H	1.45546600	-1.47316300	2.32321200
H	-2.73369800	-1.83035500	1.35133200
H	-3.32620300	-0.83738000	3.54424200
H	0.85644100	-0.50114500	4.52120200
N	-1.18387200	1.30353300	0.40971900
C	-2.59431500	3.63049000	1.08858100
C	-0.70843600	2.14817500	1.33413300
C	-2.35588300	1.58770300	-0.19591100

C	-3.07971300	2.74093300	0.12676000
C	-1.37473700	3.31181900	1.70079100
N	-2.07536400	-0.55627500	-1.23278600
C	-4.23923200	-0.18141500	-2.99472700
C	-2.41986400	-1.50166600	-2.12295700
C	-2.79949700	0.58790100	-1.19798700
C	-3.87720700	0.79609700	-2.06587200
C	-3.48098200	-1.36062400	-3.00746300
H	0.24022700	1.86770500	1.77978500
H	-4.02890300	2.94762000	-0.35650500
H	-0.94544900	3.96173400	2.45767900
H	-1.81347100	-2.40165100	-2.10686300
H	-4.43050900	1.72848700	-2.03237800
H	-3.70985600	-2.16292700	-3.70285700
Br	-0.20519900	-3.20035600	0.29570700
C	1.66533000	-0.06172200	-0.30228600
C	2.73823800	-0.97697100	-0.18955700
C	2.04186700	1.25701900	-0.65548500
C	4.07030600	-0.61837600	-0.39312500
H	2.52854300	-2.01499500	0.06448500
C	3.36534400	1.64005300	-0.86726800
H	1.27384900	2.02184500	-0.77446100
C	4.39956800	0.70306100	-0.73361700
H	4.86037200	-1.35621200	-0.29157800
H	3.62178800	2.66099900	-1.13698300
C	-5.38289700	0.02429900	-3.95489500
H	-5.94326200	0.93554200	-3.72593000
H	-5.01628900	0.10502500	-4.98577100
H	-6.07930800	-0.82162500	-3.92613800
C	-3.34561100	4.88685200	1.45061900
H	-2.80530100	5.77687900	1.10467600
H	-4.34262200	4.90415300	1.00055400
H	-3.45877200	4.98031100	2.53661300
H	-1.53455800	-0.16125700	5.13837400
C	5.79194100	1.15549200	-0.95864100
O	6.12460200	2.29123300	-1.25027200
O	6.70139700	0.15453300	-0.80386100
C	8.06387400	0.53673100	-1.01016300
H	8.65132500	-0.36902000	-0.85030900
H	8.21326100	0.91457900	-2.02603200
H	8.36197600	1.31543600	-0.30169400

TS₆

C	-1.45546200	2.12787300	-0.03691800
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C	-1.50151700	3.52338400	-0.12515500
C	-0.74018700	4.19287900	-1.08635200
C	0.05611000	3.41087200	-1.93252600
C	0.06145300	2.02919700	-1.78198400
C	-2.26750500	1.33536900	0.92005500
C	-3.29598400	1.88863100	1.69003900
C	-4.07430200	1.07926400	2.52043200
C	-3.78398100	-0.29058000	2.52977600
C	-2.74677900	-0.77498500	1.74215300
H	-2.12224300	4.09690000	0.55480300
H	0.67060300	3.87023000	-2.70100100
H	0.66809900	1.39194400	-2.41713800
H	-3.51345200	2.94918200	1.62788900
H	-4.36426900	-0.98028600	3.13551400
H	-2.50400100	-1.83188700	1.71763000
N	-0.67021200	1.40149900	-0.85541000
N	-1.98905500	0.01309600	0.96578100
Ni	-0.64865500	-0.67163700	-0.53715200
C	1.20537800	-0.75739600	0.01326600
C	1.62954700	-0.22122700	1.24189100
C	2.14040800	-0.85798600	-1.03361300
C	2.93436000	0.23126900	1.41095800
H	0.93190600	-0.14117500	2.07139000
C	3.44478500	-0.40077900	-0.86768000
H	1.84706300	-1.30239700	-1.98127700
C	3.85698900	0.14868800	0.35504100
H	3.24473000	0.65528700	2.36016600
H	4.16573800	-0.46994200	-1.67646700
C	-0.04917300	-2.45246100	0.09060300
C	-0.16298600	-2.85366800	1.43094100
C	0.12319100	-3.44595400	-0.88885000
C	-0.16503700	-4.20724900	1.78051100
H	-0.22680400	-2.11068900	2.22101600
C	0.12802100	-4.79600300	-0.53789200
H	0.21122800	-3.16861600	-1.93405100
C	-0.02090200	-5.18524700	0.79631100
H	-0.26114400	-4.49178800	2.82594700
H	0.24051500	-5.54764300	-1.31543800
H	-0.01321200	-6.23817900	1.06525900
Br	-1.91394100	-1.12609700	-2.59525900
C	-5.18639200	1.65018300	3.36272300
H	-4.94666400	1.56988900	4.43029000
H	-5.36315900	2.70552000	3.13590800
H	-6.12231800	1.10393500	3.20000500

C	-0.78681000	5.69372500	-1.22214100
H	0.21676600	6.11074900	-1.35866600
H	-1.38041700	5.98369300	-2.09843300
H	-1.23808200	6.16442100	-0.34357700
C	5.25998000	0.61530300	0.47568800
O	6.08525800	0.57758300	-0.41845100
O	5.54272000	1.10404700	1.71074100
C	6.88746200	1.56592800	1.88800500
H	7.11161400	2.38136600	1.19437200
H	6.94430100	1.91483800	2.92005800
H	7.60055200	0.75451100	1.71753100

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C	-1.17399400	1.32411700	-0.33093600
C	0.21373000	1.25530000	-0.31577400
C	0.87659300	0.05121700	-0.01576600
C	0.09340100	-1.08193400	0.26770900
C	-1.29604600	-1.01872300	0.25299800
C	-1.94314400	0.18784600	-0.04671600
H	-1.68453200	2.25118800	-0.57043300
H	0.79569300	2.13782500	-0.56482500
H	0.58157400	-2.01630900	0.52896200
H	-1.88449900	-1.90002200	0.48253800
C	2.35905200	-0.02051800	0.00206800
C	3.03291700	-1.16027100	-0.46916200
C	3.12693300	1.05037400	0.49076800
C	4.42511300	-1.22656100	-0.45318600
H	2.46062900	-1.98899200	-0.87663000
C	4.51904900	0.98356500	0.50855600
H	2.62645900	1.93053900	0.88460300
C	5.17444600	-0.15505800	0.03619900
H	4.92544400	-2.11404700	-0.83159300
H	5.09240200	1.81989600	0.89965100
H	6.25972400	-0.20683900	0.04919400
C	-3.42506200	0.31992400	-0.07749300
O	-4.02148300	1.34788500	-0.33510500
O	-4.05498600	-0.84268300	0.21660100
C	-5.48849200	-0.78004100	0.20553700
H	-5.82695700	-1.78496000	0.46026100
H	-5.84762200	-0.05508400	0.94100600
H	-5.85353800	-0.49024900	-0.78350300

Zn

Zn	0.00000000	0.00000000	0.00000000
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ZnBr₂

Zn	0.00000000	0.00000000	0.00000000
Br	0.00000000	0.00000000	2.23771700
Br	0.00000000	0.00000000	-2.23771700

TS₉

Br	1.49071700	-1.19271200	-0.00001300
C	-0.65375600	0.15566400	-0.00002300
C	-1.30772400	0.01505500	-1.22357700
C	-1.30767900	0.01500900	1.22355700
C	-2.69365000	-0.17044000	-1.20834400
H	-0.76773300	0.05939800	-2.16227700
C	-2.69360100	-0.17049900	1.20836600
H	-0.76766100	0.05937000	2.16224000
C	-3.38866700	-0.26048000	0.00002100
H	-3.22188400	-0.25518100	-2.15444500
H	-3.22180200	-0.25527600	2.15448200
H	-4.46325800	-0.41649000	0.00003900
Zn	1.08459000	1.50157500	0.00001400

IN₉

Br	-2.83192000	0.00000000	0.00000100
C	1.35533300	0.00000000	-0.00000100
C	2.07680400	1.20810400	0.00000000
C	2.07680400	-1.20810400	0.00000000
C	3.47382400	1.20826900	0.00000100
H	1.55451800	2.16222900	-0.00000100
C	3.47382400	-1.20826900	0.00000100
H	1.55451800	-2.16222900	0.00000000
C	4.17333800	0.00000000	0.00000100
H	4.01472500	2.15136000	0.00000100
H	4.01472500	-2.15136000	0.00000100
H	5.26031100	0.00000000	0.00000200
Zn	-0.56870500	0.00000000	-0.00000200

TS₁₀

Br	2.66542200	-1.28446300	-0.00365700
C	0.66786500	0.24199600	0.02978400
C	-0.06935800	0.08844100	-1.14761300
C	0.07032800	0.22510600	1.29367700
C	-1.45849900	0.02146800	-1.05358000
H	0.41706200	0.03501900	-2.11465000
C	-1.31884800	0.15732200	1.36180100

H	0.66302900	0.27729900	2.19954500
C	-2.09371900	0.06069000	0.19664300
H	-2.05077000	-0.07087700	-1.95739900
H	-1.82054900	0.16978100	2.32425900
Zn	2.49470300	1.42012400	-0.14046300
C	-3.57189600	-0.01545400	0.34811700
O	-4.15418800	0.01229800	1.41534300
O	-4.20703300	-0.11949400	-0.84124400
C	-5.63863000	-0.20172400	-0.76597600
H	-6.04992200	0.69274900	-0.29049500
H	-5.98091200	-0.28040700	-1.79822700
H	-5.94246700	-1.08057600	-0.19108100

IN₁₀

Br	4.29533400	-0.10063100	0.00000200
C	0.11247000	0.07827700	-0.00000200
C	-0.65872500	-1.09906500	-0.00000500
C	-0.56052600	1.31502400	-0.00000100
C	-2.05247000	-1.04727400	-0.00000600
H	-0.17688100	-2.07392500	-0.00000600
C	-1.95261100	1.37246500	-0.00000300
H	-0.00172000	2.24782200	0.00000100
C	-2.70615000	0.19185600	-0.00000500
H	-2.63504900	-1.96197400	-0.00000800
H	-2.47521600	2.32365400	-0.00000200
Zn	2.03765900	-0.00208600	0.00000000
C	-4.19339800	0.31443100	-0.00000700
O	-4.79438600	1.37093600	0.00000400
O	-4.81053000	-0.88826900	0.00000100
C	-6.24554000	-0.84053300	0.00000900
H	-6.57229000	-1.88078500	0.00001000
H	-6.61213600	-0.32128600	0.88953300
H	-6.61214500	-0.32128400	-0.88951000

IN₁₁

C	-2.29834300	-0.18685300	-0.02857900
C	-3.62563800	-0.62990300	-0.03978900
C	-3.96393100	-1.86059600	0.52573300
C	-2.92576000	-2.61424700	1.08899500
C	-1.62839000	-2.12056200	1.05554900
C	-1.86279000	1.12469900	-0.56632200
C	-2.75294100	2.10781000	-1.01059300
C	-2.27746600	3.34651400	-1.44656300
C	-0.89242200	3.54834300	-1.40882100

C	-0.06360600	2.52825300	-0.95708200
H	-4.40196800	-0.02141700	-0.49045200
H	-3.12167700	-3.57895300	1.54731000
H	-0.79961700	-2.68110600	1.47495400
H	-3.82144800	1.92333800	-0.99995600
H	-0.45769000	4.49420400	-1.71821900
H	1.01170700	2.65604500	-0.89893800
N	-1.31908600	-0.93919800	0.50966700

TS₁₁

Ni	0.58040400	-0.31359000	-0.31358800
C	1.21850100	-0.46548700	1.70613100
C	0.92588100	1.51946100	3.66113900
C	2.26319600	0.45621200	1.93165800
C	0.08454200	-0.46392400	2.54558500
C	-0.06687200	0.55000200	3.49154200
C	2.09090700	1.45734600	2.88368700
H	0.81055100	2.29612200	4.41203400
H	3.16426000	0.40802800	1.33236600
H	-0.66959800	-1.23585100	2.43791800
H	-0.95949700	0.56755500	4.11270800
H	2.87949700	2.19275300	3.02467500
N	-0.76857100	1.28099700	-0.14881300
C	-2.70793500	3.28957000	0.11298200
C	-0.41281300	2.54962800	0.09323100
C	-2.07869300	0.97902600	-0.26803000
C	-3.06550800	1.96324500	-0.14041100
C	-1.34072800	3.57521600	0.23132500
N	-1.29811100	-1.28049200	-0.44270400
C	-3.84532600	-2.29602500	-1.08239500
C	-1.48874900	-2.59172700	-0.66707100
C	-2.36708400	-0.45223700	-0.52642300
C	-3.64114400	-0.93551700	-0.84659700
C	-2.72658700	-3.13573000	-0.98166400
H	0.65461000	2.72808700	0.17134600
H	-4.11535700	1.70293700	-0.22437000
H	-0.99899800	4.58687300	0.42998500
H	-0.60353700	-3.21351500	-0.57946200
H	-4.47914600	-0.25119000	-0.92670800
H	-2.81532400	-4.20501100	-1.15048800
Br	1.78650000	-2.39343700	1.03426800
C	2.06952500	0.37936500	-1.44557400
C	3.38908500	-0.12568500	-1.46072300
C	1.80960600	1.39932900	-2.38945500

C	4.37384900	0.34980100	-2.33267400
H	3.66308600	-0.92275100	-0.77020200
C	2.78085300	1.88719300	-3.27187000
H	0.81138800	1.83599400	-2.44930800
C	4.07423700	1.36382800	-3.24553700
H	5.37676700	-0.07375200	-2.30164500
H	2.52673200	2.67500100	-3.98007900
H	4.83629600	1.73815100	-3.92586600
C	-5.20437800	-2.84267900	-1.43854500
H	-5.50838600	-3.62875900	-0.73714200
H	-5.96958600	-2.06098100	-1.42501400
H	-5.19639700	-3.29031900	-2.43984000
C	-3.74702900	4.37396100	0.24970200
H	-3.67384500	5.09157600	-0.57692800
H	-4.76102100	3.96312700	0.24850400
H	-3.60852100	4.93818000	1.17914600

TS₁₂

Ni	-0.19952300	-0.76688300	-0.47698200
C	0.62202700	0.71832700	-1.72186400
C	2.07151400	2.97463800	-0.88311700
C	-0.04684500	1.94763400	-1.50383500
C	2.03597800	0.67231000	-1.65359600
C	2.74123200	1.78009300	-1.20406800
C	0.67390200	3.04210200	-1.05406000
H	-1.11995300	2.00895400	-1.63797000
H	2.55958900	-0.23602600	-1.93012100
H	3.82128300	1.73146600	-1.11454200
H	0.16912400	3.97683100	-0.83039800
N	0.85620600	-0.36316900	1.28910500
C	2.43216100	0.08495000	3.56299000
C	0.66658900	0.72229600	2.04988800
C	1.81820100	-1.24508200	1.63092800
C	2.61878700	-1.04394500	2.76004900
C	1.42632700	0.98375100	3.18452200
N	1.22671800	-2.33837700	-0.42177700
C	2.84797600	-4.57799300	0.09671100
C	1.30147400	-3.35785700	-1.29244800

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C	-3.03474000	-1.07637800	-0.02758100
C	-4.42630800	-1.00274000	-0.14849400
C	-5.00813200	-0.38331600	-1.25665000
C	-4.14258600	0.15386400	-2.21827500

C	-2.77005700	0.05667100	-2.03144300
C	-2.33896700	-1.75549000	1.09204800
C	-3.00248200	-2.50210200	2.07084600
C	-2.27913000	-3.17178900	3.06040800
C	-0.88371200	-3.06541600	3.01384300
C	-0.28763400	-2.30515900	2.01479200
H	-5.06486500	-1.42402100	0.62002400
H	-4.52982900	0.64823200	-3.10395800
H	-2.07244800	0.46877600	-2.75291400
H	-4.08370600	-2.58320200	2.05766000
H	-0.26032600	-3.57540300	3.74218000
H	0.79036900	-2.21631600	1.94025000
N	-2.22710300	-0.53976800	-0.96397000
N	-0.99297200	-1.64797000	1.08476400
Ni	-0.19752900	-0.67978600	-0.62445600
C	-0.14306800	1.21460200	-0.22560700
C	-0.54555700	1.73261900	1.01215700
C	0.12694100	2.10576900	-1.27516400
C	-0.69786200	3.10705100	1.19553000
H	-0.75008400	1.06430500	1.84522400
C	-0.03163900	3.47982900	-1.09973000
H	0.48069500	1.73485700	-2.23526400
C	-0.44634800	3.99246500	0.13712500
H	-1.01401500	3.49807200	2.15699700
H	0.17398300	4.17402800	-1.90880200
C	1.70629200	-0.49850000	-0.27697200
C	2.22448400	-0.26776300	1.00630700
C	2.60709000	-0.66506900	-1.34072900
C	3.59922300	-0.26616200	1.23613200
H	1.55818800	-0.05953000	1.83865000
C	3.98390400	-0.64414300	-1.11849900
H	2.23908400	-0.85482100	-2.34348000
C	4.49279400	-0.45560900	0.17455700
H	3.99940900	-0.09943600	2.23157600
H	4.66735200	-0.79057200	-1.94816800
Br	-0.09798000	-2.67235500	-2.04686300
C	-6.50446900	-0.30863500	-1.42245900
H	-6.84091200	-0.99920900	-2.20597100
H	-7.02614300	-0.57235100	-0.49782700
H	-6.81971800	0.69731300	-1.72021300
C	-2.96613900	-3.99740100	4.11798100
H	-4.05299800	-3.88078900	4.07860100
H	-2.73604900	-5.06194800	3.98810600
H	-2.62704100	-3.71366200	5.12075300

C	-0.59527500	5.46486400	0.26937600
O	-0.40576100	6.26551300	-0.62718100
O	-0.97479300	5.84003700	1.51689900
C	-1.12715900	7.25239100	1.70731600
H	-1.89081200	7.65344300	1.03488000
H	-1.42933200	7.37707900	2.74802700
H	-0.18377000	7.77174000	1.51708800
C	5.94747900	-0.44036500	0.47507900
O	6.42613600	-0.29342400	1.58493500
O	6.71054400	-0.61143700	-0.63285200
C	8.12488300	-0.61116300	-0.40473500
H	8.40728800	-1.42168600	0.27320800
H	8.58005700	-0.75652100	-1.38534300
H	8.44631000	0.33919300	0.03077400
