

***Electronic supplementary information (ESI)***

A DFT mechanistic study on nickel-catalyzed arylation of amino alcohols with aryl  
electrophiles: insights into the origins of chemoselectivity

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## 1. Free energy changes for activation of alcohols or amines.

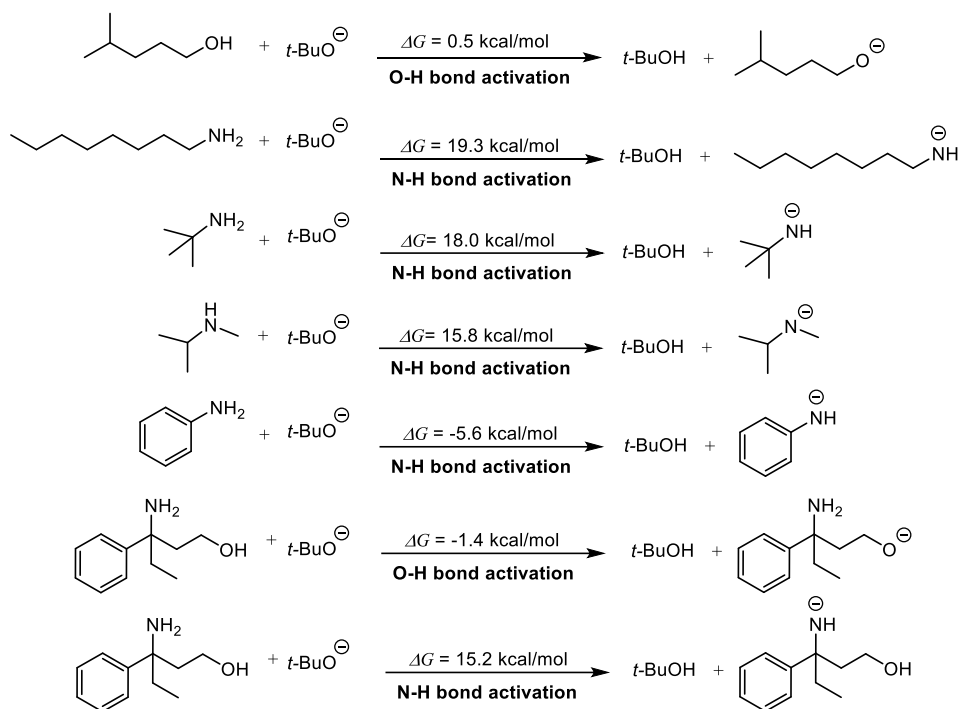


Fig. S1 Free energy changes for activation of alcohols or amines.

## 2. Free energy profiles of Ni-catalyzed competitive arylation of an alkyl alcohol and other amines.

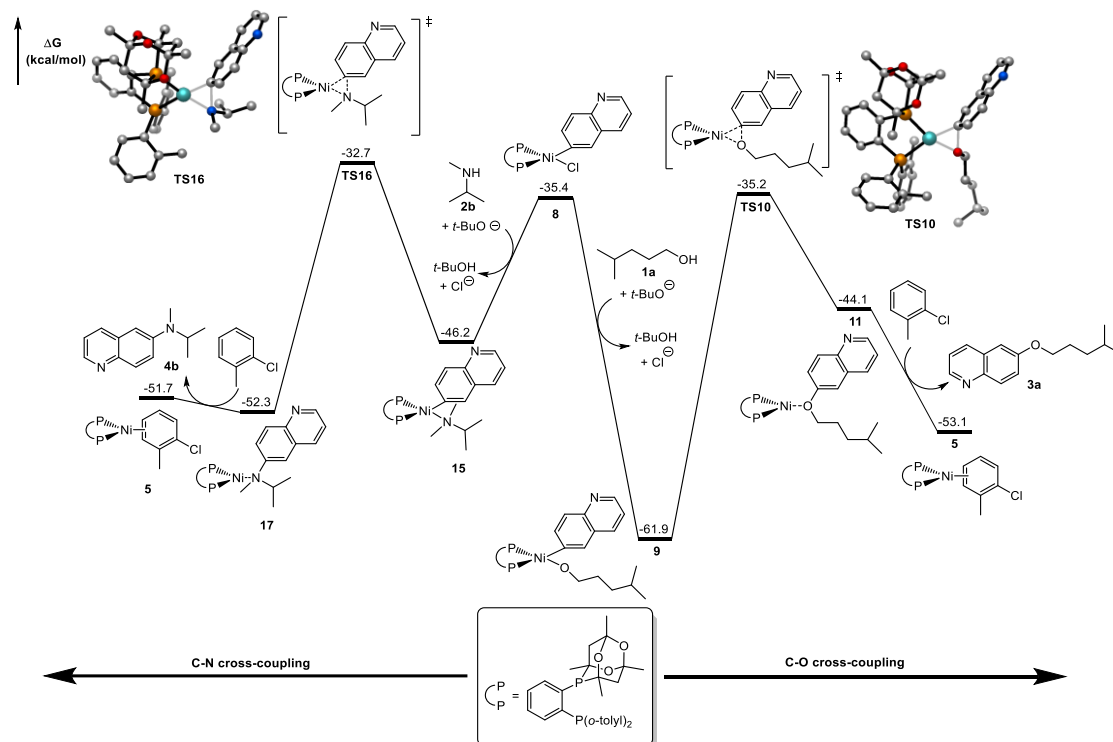
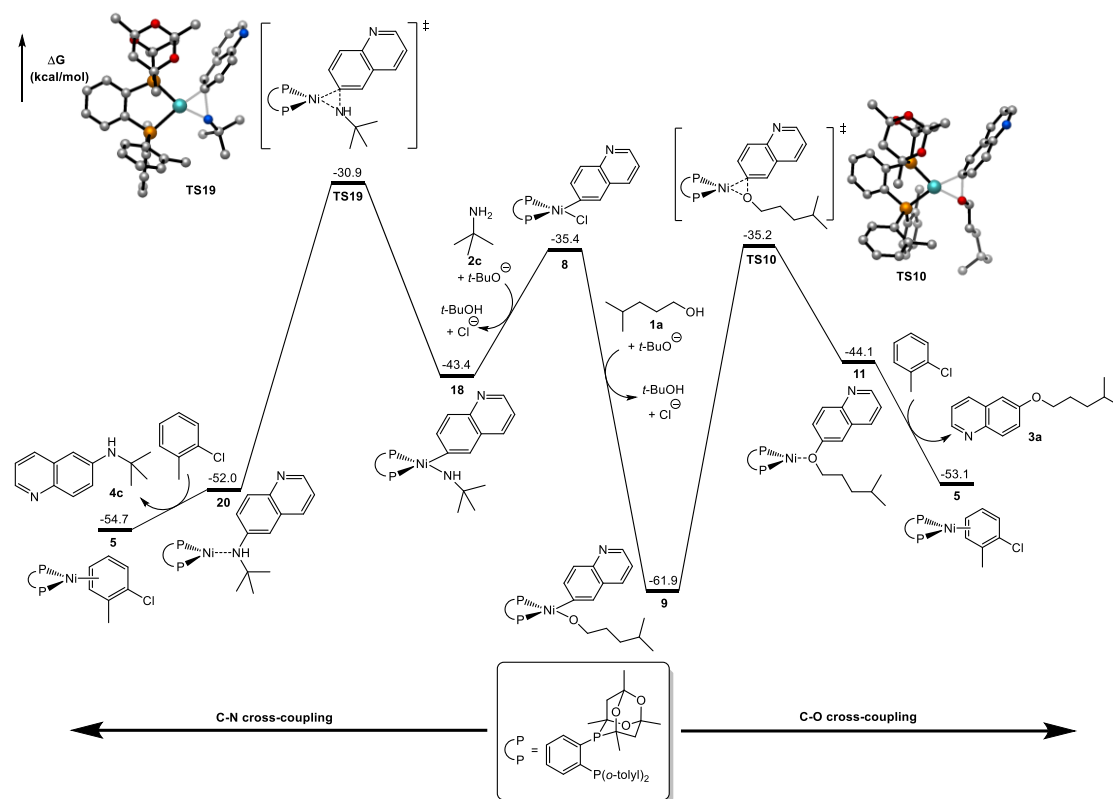
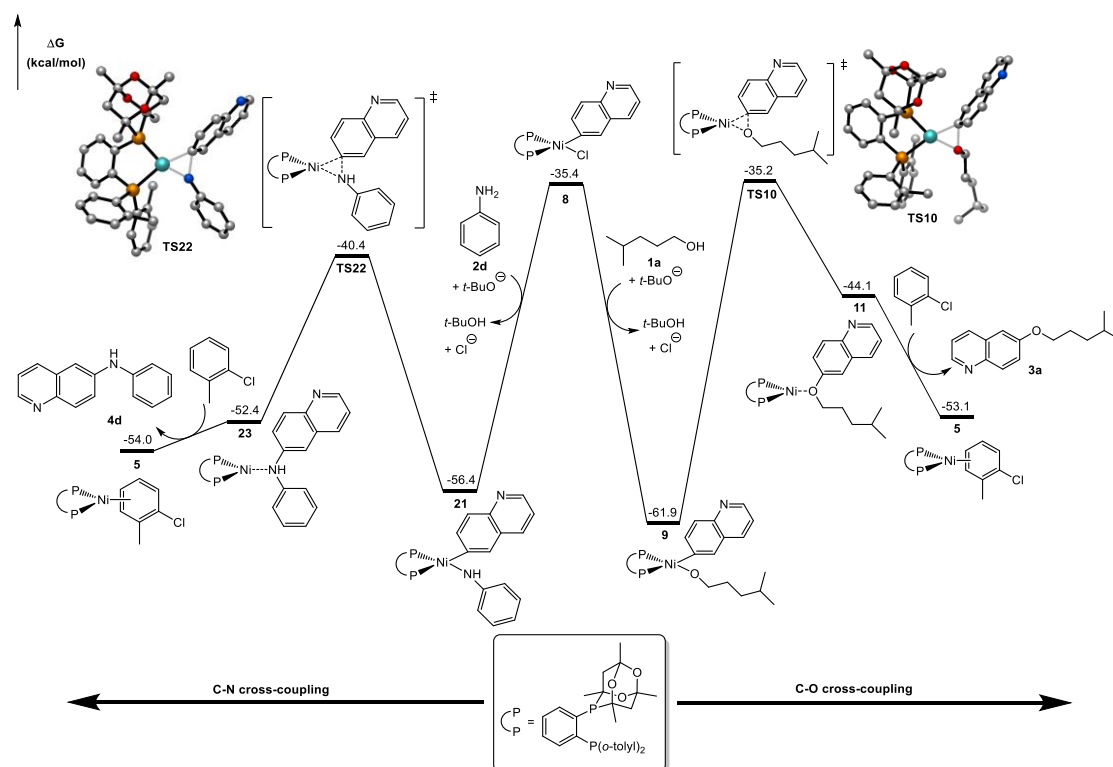


Fig. S2 Free energy profiles of Ni-catalyzed competitive arylation of the alkyl alcohol and secondary dialkylamine from **8**.

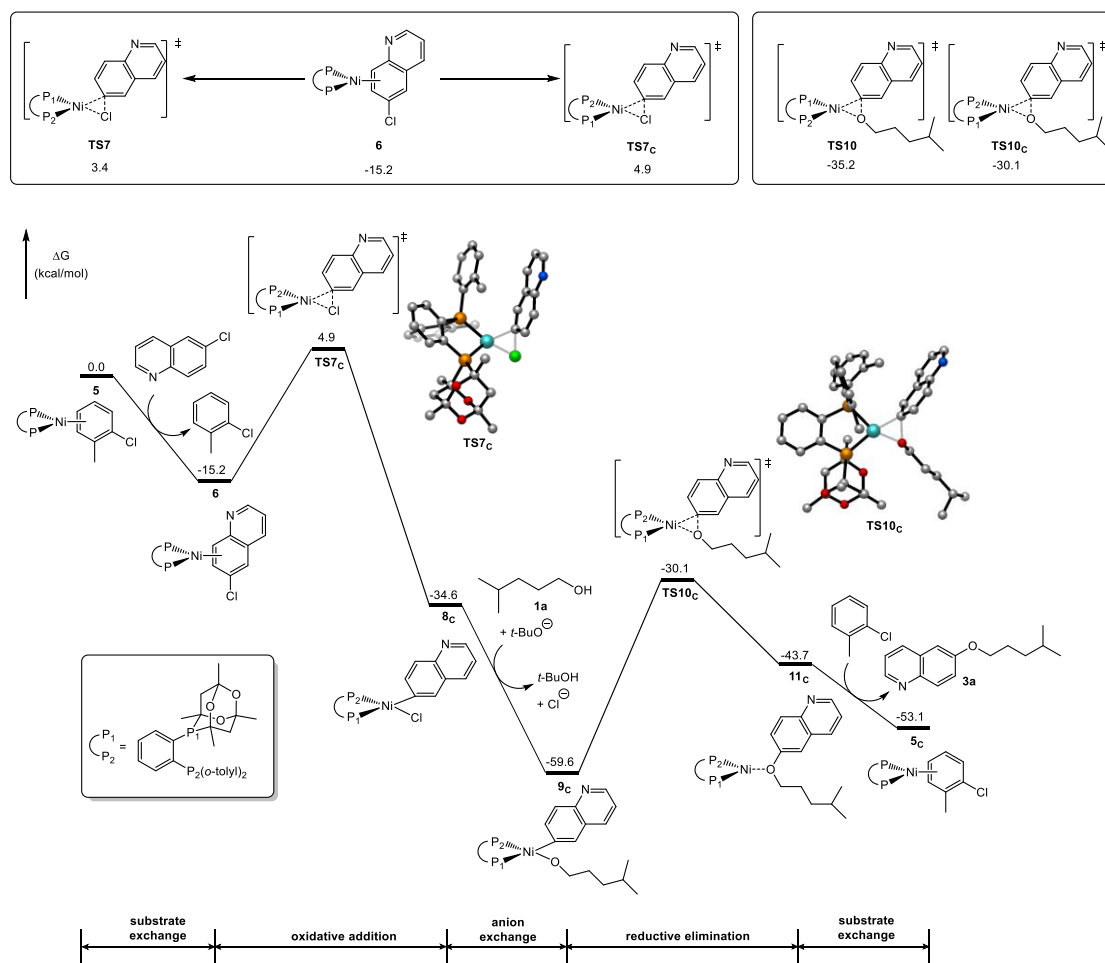


**Fig. S3** Free energy profiles of Ni-catalyzed competitive arylation of the alkyl alcohol and branched primary alkylamine from **8**.

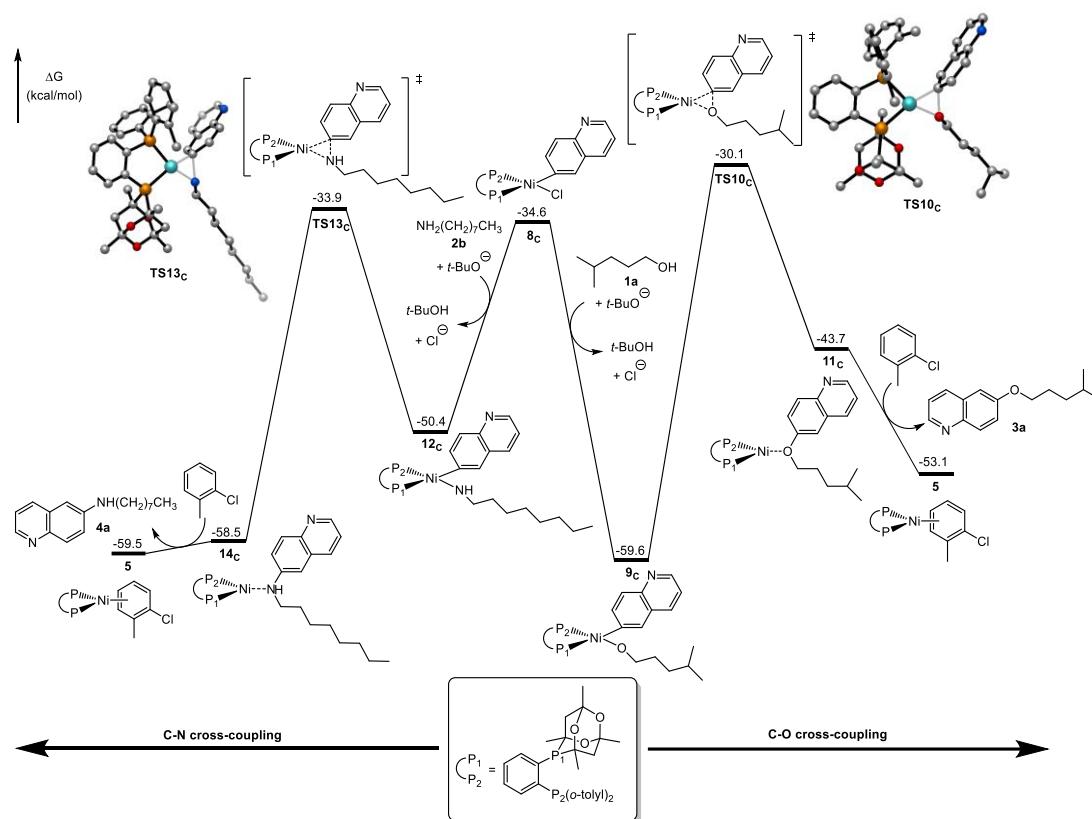


**Fig. S4** Free energy profiles of Ni-catalyzed competitive arylation of the alkyl alcohol and aniline from **8**.

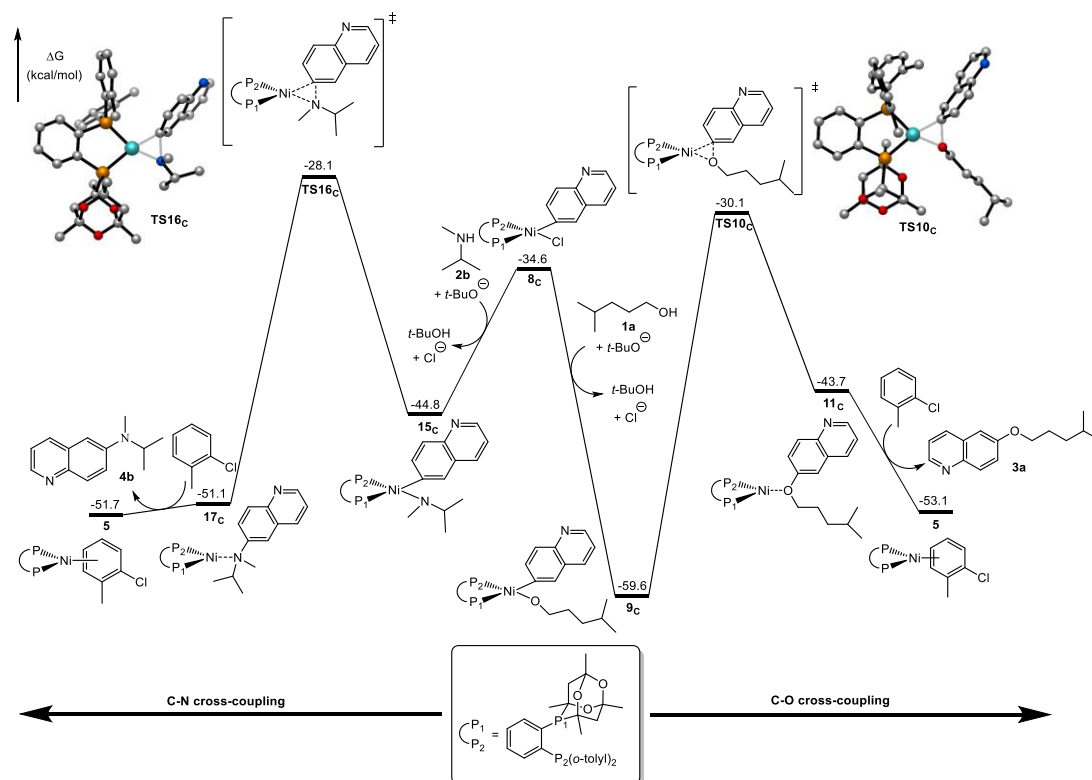
### 3. Free energy profiles for stereoisomers of intermediates and transition states.



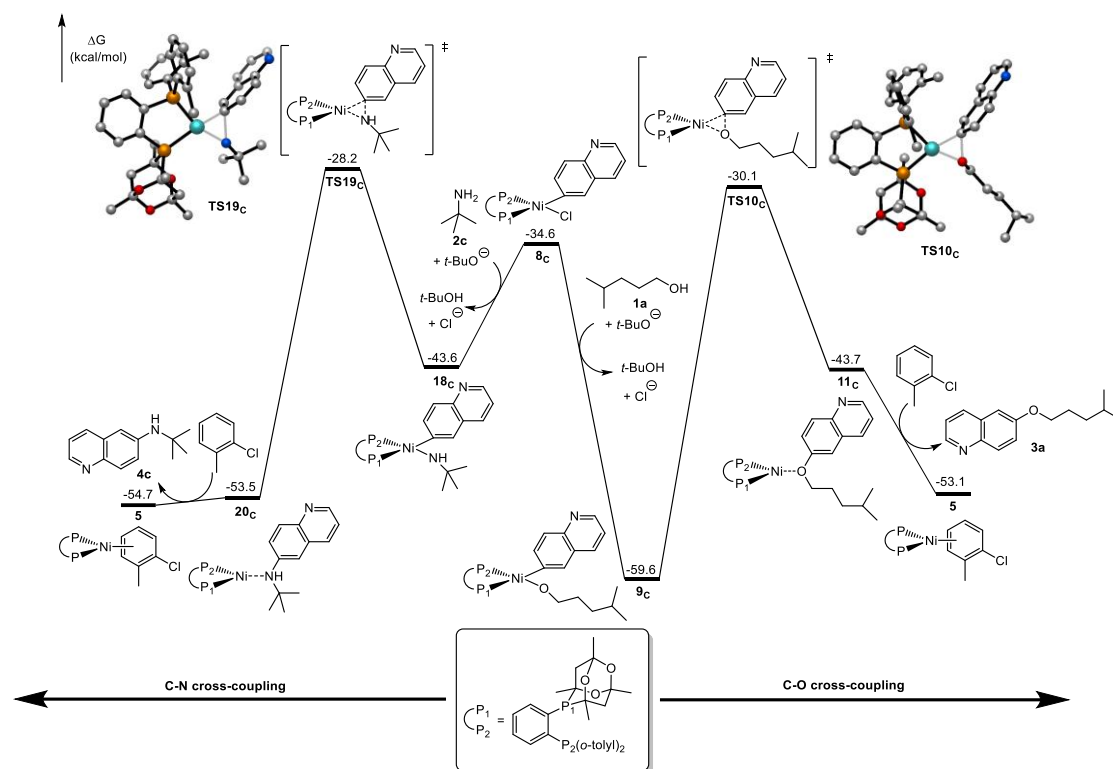
**Fig. S5** Free energy profile of Ni-catalyzed C-O cross-coupling of an alcohol and heteroaryl chloride.



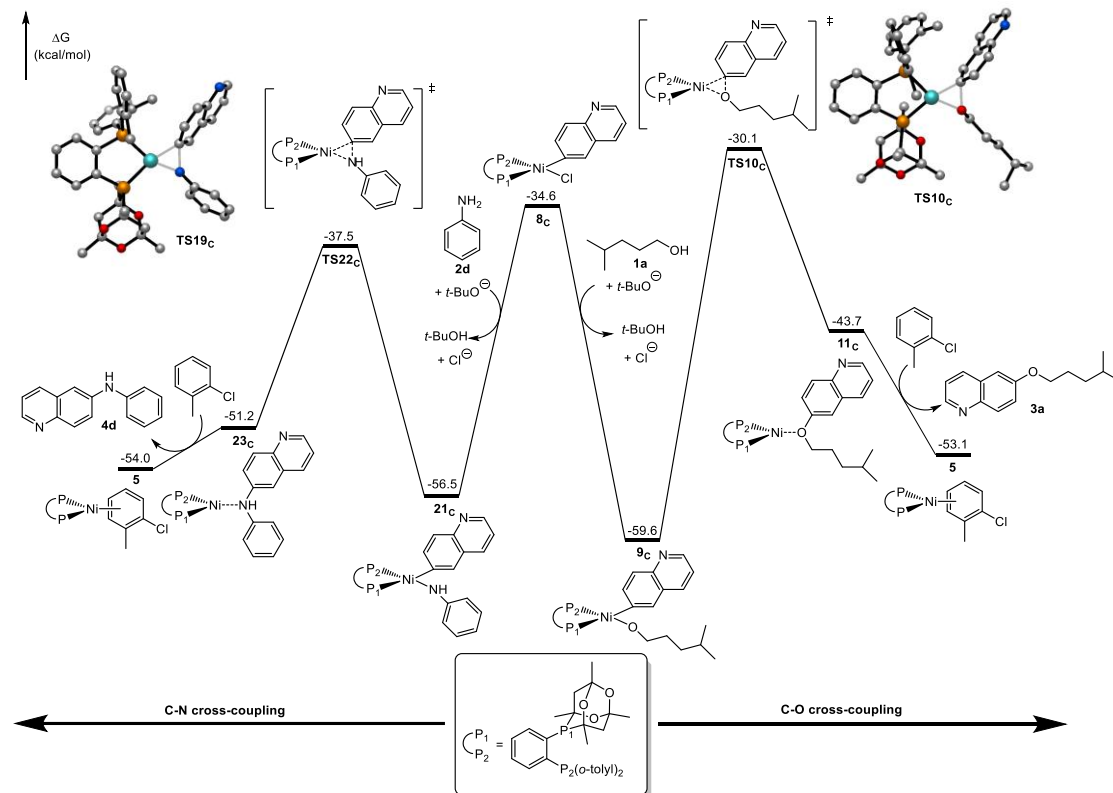
**Fig. S6** Free energy profiles of Ni-catalyzed competitive arylation of the alkyl alcohol and linear alkylamine from **8c**.



**Fig. S7** Free energy profiles of Ni-catalyzed competitive arylation of the alkyl alcohol and secondary dialkylamine from **8c**.



**Fig. S8** Free energy profiles of Ni-catalyzed competitive arylation of the alkyl alcohol and branched primary alkylamine from **8c**.



**Fig. S9** Free energy profiles of Ni-catalyzed competitive arylation of the alkyl alcohol and aniline from **8c**.

#### 4. The formation of the intermediate 24.

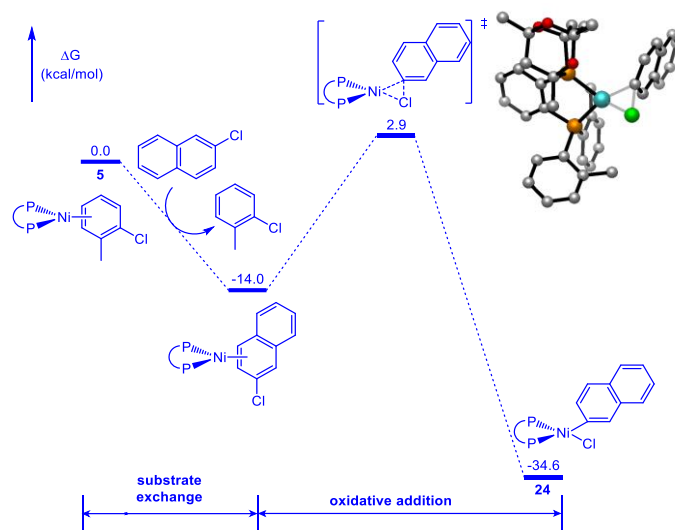


Fig. S10 Free energy profile for the formation of the intermediate 24.

#### 5. Cartesian coordinates of all the structures.

##### 5-Chloroquinoline

C	-3.24415300	0.29002100	0.00000900
C	-1.00251500	0.78251400	0.00000300
C	-0.64467000	-0.60278200	0.00000100
C	-1.69885800	-1.55124000	0.00000100
C	-2.99881000	-1.10685900	0.00000300
H	-0.26178900	2.80078300	0.00000200
H	-4.27090100	0.65316500	0.00000500
C	0.02994100	1.75632400	0.00000200
C	0.72394800	-0.97309200	-0.00000100
H	-1.46435200	-2.61214600	-0.00000100
H	-3.83285400	-1.80078700	0.00000100
C	1.68825400	0.00645100	-0.00000200
C	1.35294800	1.38187400	-0.00000100
H	1.00093700	-2.02190700	-0.00000300
H	2.14466700	2.12221900	-0.00000300
N	-2.29873700	1.20798500	0.00000500
Cl	3.38464300	-0.44097000	-0.00000600

##### *o*-Chlorotoluene

C	-1.88703200	-1.24539700	0.00000200
C	-0.51131500	-1.47113900	-0.00000400
C	0.35906400	-0.38332800	-0.00000600
C	-0.09667100	0.94302500	-0.00000600
C	-1.48454000	1.13365600	0.00000100
C	-2.37461100	0.06074000	0.00000200
H	-2.56933200	-2.08955500	0.00000700



H	-0.10997700	-2.47812300	-0.00000600
H	-1.86608500	2.15085800	0.00000300
H	-3.44416900	0.24537200	0.00000400
Cl	2.09142900	-0.70450200	0.00000300
C	0.85004700	2.11283600	0.00000000
H	1.50340600	2.09473800	0.87873600
H	1.50346600	2.09470100	-0.87868800
H	0.29874400	3.05618700	-0.00003700

***t*-BuO<sup>-</sup>**

C	-0.00011700	-0.00015100	0.16276200
C	0.72803300	1.26568800	-0.43672600
H	1.75829900	1.28482200	-0.05729800
H	0.76185000	1.32124400	-1.53965800
H	0.22538700	2.16621500	-0.05974800
C	0.73238400	-1.26254900	-0.43814500
H	1.76241700	-1.27936500	-0.05800400
H	0.23227100	-2.16494700	-0.06227300
H	0.76650800	-1.31641900	-1.54113800
C	-1.45973100	-0.00219000	-0.43836300
H	-1.98863800	-0.88773600	-0.06185500
H	-1.99173200	0.88039300	-0.05911300
O	-0.00081200	-0.00104800	1.48540900
H	-1.52327300	-0.00060900	-1.54135700

***t*-BuOH**

C	0.00539000	-0.00000100	0.01573700
C	-0.68815600	-1.26273900	-0.51151700
H	-1.74599500	-1.27388800	-0.22165300
H	-0.64354000	-1.31709200	-1.60422700
H	-0.21111800	-2.15568000	-0.09787100
C	-0.68798000	1.26283400	-0.51151500
H	-1.74581600	1.27413400	-0.22164300
H	-0.21081100	2.15570800	-0.09787500
H	-0.64336300	1.31717800	-1.60422500
C	1.48900200	-0.00010100	-0.35402200
H	1.98035600	0.88586400	0.05831000
H	1.98023600	-0.88613600	0.05830200
O	-0.01798900	-0.00000100	1.45170800
H	-0.94499500	0.00007000	1.72539800
H	1.61941200	-0.00010600	-1.44028300

**Cl<sup>-</sup>**

Cl	0.	0.	0.
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**1a**

C	-2.24276300	-0.48198900	0.22724400
H	-2.22452600	-0.63971700	1.31872400
H	-2.30013200	-1.47825200	-0.24224400
C	-0.96223400	0.21532400	-0.20781800
H	-0.99717800	0.35969100	-1.29506000
H	-0.95158900	1.21406200	0.24167000
C	0.29337800	-0.57094400	0.17900800
H	0.35338900	-0.65309800	1.27435600
H	0.20120400	-1.59915600	-0.19793500
C	1.61181900	0.02367100	-0.34543700
H	1.52837800	0.10236000	-1.43966600
C	2.78425900	-0.91199000	-0.02612400
H	2.90719200	-1.02371700	1.05806900
H	2.62535400	-1.91044700	-0.44752500
O	-3.34188000	0.33466300	-0.15816400
C	1.87707900	1.42840800	0.21126300
H	1.09262600	2.13640100	-0.07036600
H	1.93084000	1.40590100	1.30680500
H	2.82904600	1.82293100	-0.15941400
H	3.72537700	-0.52192900	-0.42782700
H	-4.15417100	-0.10721700	0.11690700

**1b**

C	2.58705400	-1.61540000	0.52258500
C	1.24782700	-1.24326300	0.37626000
C	0.89458500	-0.01165800	-0.18862000
C	1.93676900	0.83635100	-0.59785000
C	3.27271600	0.47399600	-0.45085300
C	3.60608700	-0.76006600	0.11166000
H	2.82834800	-2.57949700	0.96093800
H	0.47977700	-1.93157000	0.70732600
H	1.70424400	1.79987900	-1.04315300
H	4.05438200	1.15424200	-0.77671300
H	4.64660900	-1.04838500	0.22605600
C	-0.56525300	0.45120200	-0.37784000
C	-0.82325700	1.68822400	0.51898600
H	-0.09399300	2.46067200	0.24528800
H	-1.80656600	2.09436000	0.26104900
C	-0.73036000	1.42488300	2.02168100
H	0.23511600	0.98302700	2.28614000
H	-0.83938300	2.35767400	2.58309400
H	-1.51545200	0.74273800	2.36227900

C	-1.55800800	-0.68701500	-0.06880800
H	-1.41290500	-1.05475400	0.95048700
H	-1.35200600	-1.53250900	-0.73642100
C	-3.02585800	-0.31882100	-0.23451800
H	-3.31078700	0.45706600	0.49291100
H	-3.19022400	0.09103200	-1.23856600
O	-3.77434300	-1.51362200	-0.01538600
H	-4.70559700	-1.30766300	-0.16016300
N	-0.82754000	0.87922100	-1.77031600
H	-0.26243700	1.69413600	-1.99524900
H	-0.52541900	0.14338500	-2.40609400

**2a**

N	5.03114900	-0.40765300	-0.07863200
H	5.08187700	-0.99440400	0.75174300
C	3.84886000	0.45579500	0.00723700
H	3.82760400	1.10279200	0.90390300
H	3.86253100	1.13004500	-0.85858400
C	2.56959200	-0.37889200	-0.03011200
H	2.58584500	-1.00100900	-0.93304900
H	2.56873800	-1.07361700	0.82283300
C	1.29547000	0.46847300	0.00781800
H	1.29897300	1.09768300	0.90908000
H	1.29414400	1.16138200	-0.84530500
C	0.01234400	-0.36690300	-0.01916200
H	0.01224500	-1.05954800	0.83418800
H	0.00852300	-0.99664200	-0.91966600
C	-1.26448700	0.47754400	0.01436100
H	-1.26000200	1.10748300	0.91514000
H	-1.26414700	1.17027900	-0.83895700
C	-2.54739400	-0.35780800	-0.01265800
H	-2.54760800	-1.05178100	0.83984300
H	-2.55282100	-0.98691800	-0.91404200
C	-3.82569300	0.48540800	0.02263800
H	-3.81922700	1.11251700	0.92433300
H	-3.82396900	1.17901200	-0.82891000
C	-5.10148100	-0.35956900	-0.00613600
H	-5.99981900	0.26547800	0.02190400
H	-5.14838600	-0.97094000	-0.91442900
H	-5.14190600	-1.04088100	0.85128500
H	5.87610400	0.15835500	-0.07480700

**2b**

C	-0.44213700	-0.01088100	-0.32452200
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N	0.73149000	-0.66707200	0.26075400
C	-0.64711700	1.44877400	0.11655200
H	0.22031900	2.07209700	-0.11954200
H	-1.51821300	1.89162000	-0.37815600
H	-0.81592800	1.50015100	1.19944700
C	-1.67949100	-0.85500400	-0.01186600
H	-1.53419100	-1.88495100	-0.34721100
H	-1.86897200	-0.87340800	1.06895600
H	-2.57131800	-0.44477000	-0.49590800
C	2.01697900	-0.08870000	-0.10593100
H	2.14379200	-0.15670500	-1.19257300
H	2.16407400	0.96792500	0.17746100
H	2.82009100	-0.67190800	0.35536000
H	-0.28419600	-0.02040700	-1.41269400
H	0.63470200	-0.67528100	1.27417800

**2c**

N	0.00069400	0.15413300	-1.48443500
H	0.81479000	0.70061400	-1.76172500
C	-0.00003800	-0.00511900	-0.01698900
C	1.25459800	-0.80553600	0.35695000
H	2.16318300	-0.25721000	0.08127400
H	1.29265600	-0.99352700	1.43452300
H	1.26392800	-1.76367100	-0.16955700
C	0.00353800	1.34803800	0.72114300
H	0.89157500	1.93265900	0.45416900
H	-0.88143000	1.93730300	0.45417600
H	0.00318900	1.21828800	1.80946700
C	-1.25906800	-0.79885900	0.35656600
H	-2.16466700	-0.24568500	0.08078100
H	-1.27339200	-1.75684700	-0.17011400
H	-1.29841100	-0.98681300	1.43410300
H	-0.81045900	0.70480300	-1.76206800

**2d**

C	1.17083600	1.20235400	0.00334200
C	-0.22157500	1.20813100	-0.00525800
C	-0.93839400	-0.00001300	-0.01032900
C	-0.22155200	-1.20812300	-0.00529700
C	1.17091300	-1.20231700	0.00335700
C	1.88044300	0.00000000	0.00823100
H	1.70473500	2.14847900	0.00881500
H	-0.76406800	2.15031600	-0.01248100
H	-0.76389700	-2.15037100	-0.01318600

H	1.70468800	-2.14851700	0.00898700
H	2.96546900	0.00013800	0.01656500
N	-2.33426700	-0.00011900	-0.07647100
H	-2.77553800	-0.83577100	0.28208600
H	-2.77554400	0.83636700	0.28022900

**3a**

C	0.79111700	0.79829900	0.11410000
C	1.37148300	-0.45181700	0.02836800
C	1.60382700	1.96683700	0.14858900
C	2.96913800	1.86938500	0.09554000
H	1.10312300	2.92680800	0.21653300
C	3.60479900	0.60003500	0.00585300
H	0.77276100	-1.35446900	0.00221900
C	2.78532100	-0.57156000	-0.02690200
C	5.53731900	-0.63211300	-0.12696400
C	4.82245800	-1.85368300	-0.16501500
C	3.44818700	-1.82085600	-0.11490000
H	6.62567300	-0.64377900	-0.16625100
H	5.36140900	-2.79326300	-0.23267300
H	2.86241400	-2.73610100	-0.14171600
H	3.60289700	2.74926900	0.11962000
N	4.96519500	0.55389200	-0.04483600
C	-1.43514900	-0.07446000	0.11834800
H	-1.26784900	-0.64005400	-0.80982200
H	-1.23679800	-0.75104900	0.96214500
C	-2.85567300	0.46248300	0.17452600
H	-2.98579500	1.01928900	1.11046000
H	-2.98101700	1.18149800	-0.64153300
C	-3.89604500	-0.65746000	0.07879700
H	-3.79564400	-1.17094300	-0.88854800
H	-3.68232700	-1.41226200	0.84818400
C	-5.35276600	-0.19035300	0.24345800
H	-5.42936600	0.32209100	1.21388300
C	-6.29876400	-1.39722900	0.26851800
H	-6.25703000	-1.94255500	-0.68206500
H	-6.03183800	-2.09789900	1.06690000
O	-0.54614700	1.03892200	0.17108300
C	-5.77152500	0.80026400	-0.85073700
H	-5.16669500	1.71139300	-0.83602400
H	-5.66876200	0.34542600	-1.84372800
H	-6.81844900	1.09640300	-0.72838500
H	-7.33623900	-1.08505300	0.42651400

**3b**

C	2.04782600	0.84357000	0.27177100
C	2.69824000	-0.27730500	-0.20318300
C	2.79335100	1.95993600	0.74205800
C	4.16306400	1.93226300	0.72834400
H	2.24256000	2.82054900	1.10617600
C	4.87173100	0.79617800	0.24803800
H	2.14831600	-1.13656200	-0.56778200
C	4.11893200	-0.32526300	-0.22473100
C	6.94258900	-0.37676900	-0.24884700
C	6.20012600	-1.48651000	-0.71652900
C	4.82291400	-1.46073300	-0.70460000
H	8.02766300	-0.40904700	-0.26347800
H	6.72233400	-2.36368600	-1.08715300
H	4.25432800	-2.31423000	-1.06450100
H	4.72775400	2.78790300	1.08846000
C	-0.12211500	-0.08116500	-0.10790700
H	0.09055200	-0.28845500	-1.16515300
H	0.11428500	-0.98426600	0.47064800
C	-1.56822500	0.35332900	0.07786200
H	-1.72229900	0.63231600	1.12405300
H	-1.72700000	1.25331500	-0.51971400
C	-2.61605400	-0.71191100	-0.33366100
O	0.69623600	0.99640100	0.34042700
C	-4.01416400	-0.08441200	-0.22384400
C	-4.32227700	1.00594900	-1.05377900
C	-5.01329200	-0.55942800	0.63272200
C	-5.57451400	1.61292200	-1.01163300
H	-3.57419800	1.35828800	-1.75508800
C	-6.27076600	0.04873900	0.67925200
H	-4.83041500	-1.41470600	1.27060100
C	-6.55586000	1.13966300	-0.13779200
H	-5.78661800	2.45385800	-1.66552100
H	-7.02677300	-0.33892200	1.35589100
H	-7.53274600	1.61244800	-0.10119900
C	-2.45913200	-1.99978600	0.52032300
H	-1.58101000	-2.53740200	0.14108600
H	-3.31192400	-2.65498800	0.30675300
C	-2.29299200	-1.82090500	2.03562800
H	-2.32949900	-2.79123900	2.54082900
H	-1.33140600	-1.36155000	2.28194300
H	-3.07266900	-1.18913700	2.46806000
N	-2.42005500	-1.00650900	-1.77417600
H	-1.59484300	-1.58960700	-1.89748300

H	-3.20852000	-1.55545800	-2.10965200
C	6.28775800	0.73962800	0.22284600
H	6.84979600	1.59698800	0.58401300

**4a**

C	-2.16826600	-0.93458700	-0.07110000
C	-2.63445600	0.37233400	-0.10251500
C	-3.11484000	-2.00183300	0.03313300
C	-4.46029600	-1.75706800	0.09854900
H	-2.74422400	-3.02398400	0.05355100
C	-4.96302900	-0.42753300	0.05890100
H	-1.94500000	1.20617900	-0.17240300
C	-4.02314700	0.64618900	-0.04614300
C	-6.75458100	1.00702000	0.08682300
C	-5.91533600	2.14294700	-0.01466900
C	-4.55352000	1.96104600	-0.08034700
H	-7.83460700	1.13739200	0.13938900
H	-6.35204600	3.13637900	-0.03958800
H	-3.87652400	2.80790600	-0.15882000
H	-5.17966500	-2.56503400	0.17972500
N	-6.30916600	-0.23480000	0.12374900
C	0.21197100	-0.25358600	-0.02251500
H	0.10414000	0.48320600	-0.82899800
H	0.10506300	0.30200700	0.92553400
C	1.59917800	-0.88617900	-0.10154400
H	1.70073400	-1.63759500	0.69506000
H	1.69089700	-1.42422800	-1.05332400
C	2.72459800	0.14307600	0.02800300
H	2.61565600	0.90051000	-0.76033100
H	2.62097700	0.67857400	0.98169000
C	4.12235200	-0.47621300	-0.05658700
H	4.23148100	-1.23729300	0.72865200
C	5.24803700	0.55332300	0.07512000
H	5.13351900	1.31782800	-0.70612700
H	5.14591200	1.08196900	1.03326800
C	6.64782600	-0.05976200	-0.01870400
H	6.75031700	-0.58736000	-0.97754600
H	6.76329100	-0.82537800	0.76154200
C	7.77360400	0.97046600	0.11346600
H	7.65529900	1.73558400	-0.66557200
H	7.67112200	1.49577400	1.07249800
C	9.16872700	0.34918800	0.01468700
H	9.30767100	-0.15603200	-0.94780400
H	9.95394800	1.10585900	0.11033500

H	9.32542200	-0.39573300	0.80299600
H	4.22614400	-1.00876900	-1.01212700
N	-0.82479900	-1.25862300	-0.17104800
H	-0.58469500	-2.16677100	0.20213800

**4b**

C	0.84402600	-0.34090100	-0.43608500
C	-0.08476600	0.66867700	-0.62408000
C	0.38949300	-1.60129200	0.05366000
C	-0.93505300	-1.81953500	0.35026700
H	1.10736300	-2.40012600	0.20247900
C	-1.89387700	-0.78763700	0.18920900
H	0.23439100	1.61408100	-1.04788500
C	-1.45063300	0.47980600	-0.30558000
C	-4.06961800	-0.07154400	0.33559800
C	-3.74002600	1.21788900	-0.15461600
C	-2.43193900	1.49041500	-0.47477700
H	-5.10299600	-0.29776500	0.59567800
H	-4.51745000	1.96642800	-0.26878500
H	-2.13468800	2.46493100	-0.85331600
H	-1.28325600	-2.77647100	0.72474000
N	-3.19659300	-1.04433100	0.50436600
C	2.99490500	0.66268500	0.25406800
N	2.21425200	-0.10887400	-0.74704800
C	3.00833900	0.00382800	1.64257400
H	3.35580000	-1.03276900	1.59552900
H	3.67256900	0.54771100	2.32166000
H	2.00359700	0.00465700	2.07670000
C	2.55149400	2.12360100	0.34765000
H	2.51606100	2.58251300	-0.64425900
H	1.56452200	2.21313600	0.80944700
H	3.25965400	2.68494300	0.96556300
C	2.94295000	-1.26750200	-1.24905000
H	3.86495700	-0.92286800	-1.72811600
H	3.22590600	-2.00752500	-0.48132400
H	2.33920400	-1.77796200	-2.00329300
H	4.01897400	0.65858400	-0.13906700

**4c**

C	0.63641600	-0.70188600	-0.11971100
C	-0.09334700	0.48073900	-0.11160800
C	-0.08700800	-1.93859200	-0.06639700
C	-1.45363400	-1.97646400	-0.00808600
H	0.47891800	-2.86752700	-0.07688600



C	-2.21583000	-0.77713500	0.00209400
H	0.39764100	1.44320100	-0.15553900
C	-1.50834300	0.46437200	-0.05195300
C	-4.25788800	0.26729400	0.06973600
C	-3.66193600	1.55085700	0.01856000
C	-2.29118900	1.64728100	-0.04173000
H	-5.34218500	0.17730800	0.11799200
H	-4.28813100	2.43747700	0.02730300
H	-1.79750500	2.61497100	-0.08223400
H	-1.99188700	-2.91747500	0.03375000
N	-3.57293300	-0.86099200	0.06257900
C	3.01371900	0.25981300	0.02901100
C	4.37727700	-0.44917200	0.02228300
H	4.43994900	-1.18516300	0.83217000
H	4.54105000	-0.96327900	-0.93018900
N	2.01500700	-0.79558300	-0.21316000
H	2.36088700	-1.72365700	-0.01838600
C	2.81042400	0.94037200	1.39634500
H	2.88294300	0.20158600	2.20051700
H	3.57817300	1.70319100	1.55984900
H	1.83348900	1.42055600	1.47325400
C	3.00012200	1.28917600	-1.11656000
H	3.15348000	0.78375400	-2.07395100
H	2.05902400	1.83767500	-1.17660900
H	3.80291800	2.01947200	-0.97406700
H	5.18401900	0.27401600	0.16520000

**4d**

C	0.00066400	1.01897200	-0.01965400
C	0.51559300	-0.24892500	0.20013900
C	0.90099000	2.09851900	-0.27192700
C	2.25661700	1.90195400	-0.30513100
H	0.48858200	3.08879400	-0.44858100
C	2.80910000	0.60935600	-0.10038700
H	-0.14194600	-1.07817500	0.43197200
C	1.91201900	-0.47571200	0.15466000
C	4.65316100	-0.74766200	0.05147100
C	3.85854400	-1.88993200	0.31901900
C	2.49157800	-1.75276900	0.37001900
H	5.73698600	-0.84444700	0.00633600
H	4.33408800	-2.85239100	0.47867800
H	1.84721700	-2.60424400	0.57254700
H	2.94301800	2.71990600	-0.49581600
N	4.16181700	0.45975200	-0.15132600

N	-1.35823900	1.32570400	0.01592900
H	-1.57556600	2.28583700	0.23582300
C	-2.45408900	0.45585900	-0.00870600
C	-3.62909900	0.83202600	0.66254900
C	-2.44228000	-0.74749800	-0.73348200
C	-4.76082000	0.02315300	0.61549400
H	-3.64411200	1.76085000	1.22721500
C	-3.57571800	-1.55690100	-0.75872500
H	-1.55904600	-1.03044900	-1.29301400
C	-4.74063700	-1.18304100	-0.08688600
H	-5.65906900	0.33371600	1.14092600
H	-3.54925800	-2.48341400	-1.32490800
H	-5.61969300	-1.81856700	-0.11411400

**4e**

C	-0.61893700	-1.05730800	-0.47338200
C	-1.31024400	0.01529100	0.06897400
C	-1.36587400	-2.17978900	-0.94624100
C	-2.73365000	-2.21261300	-0.86719200
H	-0.82724100	-3.02060900	-1.37801800
C	-3.46297100	-1.12921800	-0.30960900
H	-0.78337700	0.89229300	0.41861200
C	-2.72448200	0.00244700	0.16212400
C	-5.54552000	-0.05882400	0.34130200
C	-4.81878000	1.06382900	0.80642400
C	-3.44503200	1.09369300	0.71910900
H	-6.62853900	-0.06965200	0.41685700
H	-5.35255800	1.90710600	1.23518000
H	-2.88871300	1.95676300	1.07517400
H	-3.27721400	-3.08055300	-1.23110900
C	1.73527900	-0.35426300	0.18325400
C	3.14836000	-0.79843600	-0.27987400
H	3.25204100	-0.54815100	-1.34243900
N	0.76749800	-1.10618400	-0.63916400
H	1.08420400	-2.04353000	-0.84007400
C	1.52824700	-0.67529900	1.69199900
H	1.31405000	-1.74767200	1.76190600
H	0.61511300	-0.17847400	2.03029500
H	3.89094700	-0.20092700	0.25499300
C	1.59807300	1.14163800	-0.15520600
C	1.52591300	1.51542500	-1.50474800
C	1.53736100	2.15076400	0.81182800
C	1.41318500	2.85186700	-1.87729500
H	1.52083300	0.73864600	-2.26188700

C	1.42320900	3.49336900	0.44195800
H	1.55165600	1.90452100	1.86556800
C	1.36563600	3.85107900	-0.90292700
H	1.35017500	3.11355700	-2.92949100
H	1.37290600	4.25693100	1.21264800
H	1.27329900	4.89408400	-1.19010100
C	-4.87641100	-1.13141900	-0.20551800
H	-5.42458300	-1.99797100	-0.56678200
C	3.50773400	-2.27602200	-0.08885100
C	2.68853200	-0.34984800	2.64376300
H	3.04255400	0.67884000	2.54636700
H	2.37083100	-0.49450800	3.68113400
H	3.55015200	-1.00141300	2.47529900
O	4.86912800	-2.52472000	-0.40819000
H	5.01112100	-2.24828500	-1.32304500
H	2.84859400	-2.92919900	-0.68515700
H	3.39048400	-2.57892600	0.95438000

## 5

Ni	0.19511600	1.06737600	-0.38488100
P	-1.38733500	-0.42291000	-0.32636600
P	1.70662200	-0.47281700	0.10324500
C	-0.57293500	-2.08510400	-0.34388000
C	0.82468500	-2.09038400	-0.14046900
C	-2.91019000	-0.60402300	-1.42940700
C	-2.42863300	-0.34229300	1.25892700
O	-3.76544300	-1.69565300	-1.02536900
O	-3.24982800	0.83406400	1.13589400
C	1.52865900	-3.30158900	-0.17756400
C	-1.22641800	-3.30397200	-0.59925600
C	-3.33867000	-1.56234700	1.38759800
C	-3.69460400	0.70270100	-1.26550600
C	-2.51702400	-0.87333500	-2.87197900
C	-1.54965100	-0.11568500	2.47390800
H	2.60380600	-3.29732700	-0.03202700
C	0.86613800	-4.50283900	-0.41640800
C	-0.51277700	-4.50019100	-0.63510000
H	-2.29128800	-3.30347800	-0.79294800
C	-4.38047900	-1.56566900	0.25944100
H	-2.75582200	-2.48571500	1.37877400
H	-3.87591200	-1.50174600	2.34033900
H	-4.52386700	0.70875600	-1.98091000
H	-3.05105100	1.56183200	-1.45658000
C	-4.27766300	0.78751800	0.15167300

H	-3.41484800	-0.94329700	-3.49408400
H	-1.96170000	-1.81083900	-2.95630300
H	-1.88623500	-0.06089400	-3.24340100
H	-2.17637500	0.00582300	3.36358000
H	-0.94513100	0.78415200	2.33798100
H	-0.87841100	-0.96334800	2.62831400
O	-5.11553800	-0.35173200	0.34269800
H	1.42420200	-5.43401400	-0.44520900
H	-1.03416000	-5.43055700	-0.84082700
C	-5.37693200	-2.70070200	0.36419900
C	-5.13602600	2.01345900	0.37994900
H	-6.08579300	-2.63460600	-0.46367300
H	-5.92039400	-2.63078000	1.30885400
H	-4.85855300	-3.66157900	0.31724500
H	-5.53928600	1.98296600	1.39417600
H	-5.96190200	2.03214400	-0.33447500
H	-4.53174900	2.91502300	0.26347600
C	-0.17280200	3.66263500	1.75943400
C	0.94292500	3.31466200	1.03423500
C	0.83745900	2.95816500	-0.35034700
H	-0.07283800	3.88671600	2.81732300
H	1.92066100	3.30529800	1.49849500
Cl	2.32240100	3.24591700	-1.35840600
C	-1.43766300	3.77521800	1.12613300
H	-2.30394000	4.09557400	1.69510800
C	-0.45578200	3.00947800	-0.99547600
C	-1.55493600	3.48073300	-0.20843900
H	-2.50761700	3.62187100	-0.71204600
C	-0.59244600	3.03051300	-2.50372100
H	-1.61055400	2.75888200	-2.79876100
H	-0.38728400	4.03417800	-2.89843700
H	0.09896100	2.34502900	-2.99505900
C	3.20094000	-0.79875000	-0.92257500
C	4.40977000	-1.21938700	-0.35185600
C	3.10697800	-0.64393100	-2.32400100
C	5.53138300	-1.46419600	-1.14264300
H	4.47001600	-1.35925500	0.72244800
C	4.24501000	-0.89033900	-3.09991700
C	5.44935900	-1.29173100	-2.52325600
H	6.45991800	-1.78744100	-0.68159600
H	4.17970900	-0.76662600	-4.17761100
H	6.31670900	-1.47256500	-3.15118400
C	2.30319000	-0.58209700	1.84091200
C	1.77401500	-1.55163400	2.70818200

C	3.18917300	0.39363300	2.35603400
C	2.09060500	-1.56036300	4.06452900
C	3.49418000	0.36520300	3.72260300
C	2.95267800	-0.59264800	4.57709200
H	1.66500400	-2.31964100	4.71375700
H	4.17422600	1.11539300	4.11807600
H	3.20474400	-0.58349700	5.63327800
C	1.81298300	-0.25924300	-2.99271800
H	1.07274000	-1.06465000	-2.91894800
H	1.37199200	0.62015600	-2.50980100
H	1.96842600	-0.03653900	-4.05138400
H	1.10826500	-2.31195300	2.31718900
C	3.85942900	1.42354800	1.48278700
H	3.25671000	1.69706000	0.61671700
H	4.07886100	2.33178100	2.05104000
H	4.80932000	1.04298600	1.09102100

## 6

Ni	0.19620100	-0.74108700	-0.59655900
Cl	-0.97364200	-3.02410600	-2.47530400
P	-1.63643000	-0.01089300	0.34438300
P	1.19646800	1.14546100	-0.04391400
C	0.20596000	-2.67400300	-1.14966100
C	0.13473500	-3.54668400	0.00077400
C	-1.09789300	1.27413400	1.55907300
C	0.20987900	1.77913500	1.38327800
C	-2.92948000	-1.05663700	1.22795700
C	-2.90612100	0.80547500	-0.79497000
C	1.22889600	-3.76850200	0.78145000
C	2.64448700	-2.42242100	-0.72817700
O	-4.01837100	-0.26221200	1.74495300
O	-3.46257800	-0.26157800	-1.58165700
C	0.74412000	2.67770900	2.31465400
C	-1.84713400	1.69866300	2.66847800
C	-4.02614600	1.46643000	0.00876400
C	-3.48133600	-1.99723800	0.15085800
C	-2.33078500	-1.80006100	2.41024600
C	-2.22947400	1.75378700	-1.76670900
H	1.17122700	-4.38600100	1.67151100
C	2.52026700	-3.22840600	0.43960900
H	1.76089300	3.03619000	2.18555300
C	-0.00992900	3.08942600	3.41223400
C	-1.30561200	2.59860700	3.58594700
H	-2.84140000	1.29704600	2.82045400

C	-4.82757400	0.40102200	0.76813300
H	-3.62483200	2.21442600	0.69660900
H	-4.70702700	1.96814400	-0.68731000
H	-4.15636100	-2.71660200	0.62640900
H	-2.67596100	-2.53790200	-0.34757500
C	-4.28505800	-1.19703000	-0.88213600
H	-3.09665800	-2.42933600	2.87449600
H	-1.95318000	-1.10134100	3.16077200
H	-1.50226400	-2.42981300	2.07597100
H	-2.96803600	2.15043700	-2.47062300
H	-1.45185200	1.22901600	-2.32699000
H	-1.76548900	2.58685700	-1.23287000
O	-5.33336700	-0.52349900	-0.18516500
H	0.41471800	3.78078200	4.13392800
C	-6.01491600	0.96239900	1.52157000
C	-4.92617000	-2.06531700	-1.94181100
H	-6.53757700	0.14739200	2.02626700
H	-6.69962000	1.45114600	0.82517800
H	-5.67860900	1.68857400	2.26580800
H	-5.49678300	-1.43456800	-2.62655900
H	-5.59795300	-2.78884600	-1.47476300
H	-4.14892400	-2.59360500	-2.49771500
H	-0.81710700	-4.01205400	0.23547100
C	3.93568900	-1.99130200	-1.08001800
H	4.07610000	-1.39622400	-1.97785100
C	4.77243300	-3.08880800	0.87998700
H	5.59784400	-3.34898400	1.54070700
C	5.00929200	-2.32232000	-0.27216400
H	6.01316900	-1.98506800	-0.50688000
C	1.46833400	-2.09389200	-1.50648900
H	1.62165300	-1.75697700	-2.52626800
N	3.57242100	-3.53693800	1.23387400
H	-1.89317400	2.90744100	4.44550400
C	2.88513900	1.02067000	0.65834600
C	3.95653000	1.72274400	0.08961700
C	3.11877000	0.12134500	1.72669900
C	5.25758500	1.54437900	0.55705400
H	3.76829600	2.42071900	-0.71926500
C	4.43103700	-0.03239300	2.18362000
C	5.49458800	0.66171400	1.60880200
H	6.07602800	2.09571700	0.10389200
H	4.61905700	-0.72838800	2.99568900
H	6.50348600	0.51018400	1.98097300
C	1.25665300	2.58312700	-1.19664900

C	0.77285800	3.84192600	-0.81086000
C	1.72678900	2.39926200	-2.51808900
C	0.75674500	4.91381700	-1.70173300
C	1.71339600	3.49152600	-3.39301600
C	1.23308300	4.73916200	-2.99878300
H	0.37585900	5.87805200	-1.37914600
H	2.07940600	3.35187000	-4.40644100
H	1.22838800	5.56578200	-3.70285000
C	2.01039500	-0.64631700	2.40234300
H	1.48541100	-0.02106100	3.13283500
H	1.26173900	-0.99414100	1.68170600
H	2.41011700	-1.52374500	2.91376200
H	0.39745900	3.98836800	0.19430600
C	2.21495300	1.06235600	-3.01159600
H	3.00688200	0.65541300	-2.37574600
H	1.39893700	0.33348700	-3.00348400
H	2.60152100	1.14129600	-4.03065300

**TS7**

Ni	0.19479900	0.59960900	0.71872900
Cl	0.26119700	0.99573300	3.04782100
P	-1.11112900	-0.86331400	-0.30720800
P	2.00252100	-0.42335700	-0.07132100
C	-0.74247200	2.00677000	1.53843000
C	-2.13078000	2.22169500	1.77784300
C	-0.00548900	-1.86587000	-1.41497300
C	1.38662800	-1.67162900	-1.27985100
C	-2.68660300	-0.61567200	-1.32797000
C	-1.95568000	-2.07804100	0.87806000
C	-2.74383900	3.29896200	1.19972700
C	-0.59313100	4.06916800	0.26533100
O	-3.25561500	-1.86417900	-1.78088400
O	-2.99083300	-1.30768500	1.52585800
C	2.27999000	-2.36442500	-2.10821600
C	-0.46209900	-2.74923000	-2.41059500
C	-2.60038600	-3.24653000	0.13477000
C	-3.69534800	0.04829000	-0.38986200
C	-2.41323200	0.21621900	-2.56893500
C	-0.99928400	-2.52312800	1.96777200
H	-3.81097400	3.46796900	1.30537400
C	-2.01065600	4.23015300	0.39462000
H	3.34623900	-2.19248400	-2.00067900
C	1.81116200	-3.25078600	-3.07354000
C	0.43592500	-3.43312400	-3.22786500

H	-1.52605400	-2.87112400	-2.56175200
C	-3.73949000	-2.74111100	-0.75870600
H	-1.85629700	-3.79026800	-0.45070600
H	-3.03123700	-3.93500900	0.86967600
H	-4.58954000	0.30777500	-0.96673400
H	-3.27921700	0.95784000	0.04140400
C	-4.10622700	-0.93554000	0.71228700
H	-3.34251100	0.35779100	-3.12918400
H	-1.68627200	-0.27641400	-3.21937100
H	-2.01967600	1.19456800	-2.27934600
H	-1.52387800	-3.17028800	2.67811500
H	-0.60250300	-1.65582300	2.49868000
H	-0.16189800	-3.07919100	1.53609000
O	-4.67745700	-2.07792400	0.07772600
H	2.51146500	-3.78211800	-3.71097200
C	-4.48296500	-3.84824100	-1.47588600
C	-5.15491000	-0.38333300	1.65415200
H	-5.27802100	-3.41176800	-2.08373700
H	-4.92260400	-4.53261600	-0.74725100
H	-3.79907500	-4.40265400	-2.12338000
H	-5.39835000	-1.13877900	2.40379700
H	-6.05692200	-0.12755000	1.09422300
H	-4.77811100	0.51057300	2.15528800
H	-2.67711000	1.49233300	2.36387800
C	0.10110300	5.03632300	-0.49862000
H	1.17924300	4.95484700	-0.61018300
C	-2.00523900	6.11448400	-0.91932200
H	-2.57866200	6.91201800	-1.38908900
C	-0.60599200	6.05617600	-1.09929100
H	-0.10590900	6.80758900	-1.70217000
C	0.04911600	2.97864100	0.92011200
H	1.13295000	2.92421500	0.95002000
N	-2.69224000	5.24345300	-0.19657300
H	0.05777500	-4.10386000	-3.99384200
C	3.30023600	0.40562200	-1.07383500
C	4.66003300	0.13423200	-0.86941100
C	2.91104900	1.33375500	-2.06817900
C	5.64197400	0.78438700	-1.61559800
H	4.94917100	-0.59389700	-0.11855500
C	3.91381200	1.97601000	-2.80336300
C	5.26591200	1.71475900	-2.58248000
H	6.69059100	0.56351800	-1.44087800
H	3.62309300	2.69172400	-3.56777400
H	6.01980700	2.23278700	-3.16769500



C	2.89835400	-1.39884300	1.19492800
C	2.79926500	-2.79819700	1.20995200
C	3.56621900	-0.73375800	2.25160100
C	3.35166500	-3.54711300	2.24688000
C	4.11763200	-1.50844000	3.27864300
C	4.01461300	-2.89838700	3.28657700
H	3.26195300	-4.62915300	2.23991700
H	4.63038600	-1.00297300	4.09242100
H	4.44655600	-3.46890000	4.10330800
C	1.46218000	1.61298500	-2.37878700
H	0.97887900	0.73173700	-2.81564800
H	0.89397800	1.86391200	-1.47613100
H	1.36660800	2.43705400	-3.08998300
H	2.28474900	-3.30722800	0.40330100
C	3.72284200	0.76524500	2.29046700
H	4.49940700	1.10285300	1.59562400
H	2.79184800	1.26540200	2.01366200
H	3.99611700	1.09840900	3.29406100

## 8

Ni	-0.09381500	-1.08178000	0.27215200
Cl	-0.66744600	-3.22350900	0.69339900
P	0.45760200	0.95997600	-0.39666500
P	-2.28883600	-0.37749400	0.02587700
C	1.72812500	-1.61277300	0.48448300
C	2.37970400	-1.36956900	1.72649400
C	-0.94991700	1.57575300	-1.43693300
C	-2.18897800	0.92180200	-1.26524800
C	2.02278000	1.42156000	-1.36660000
C	0.79901300	2.23075800	0.97194100
C	3.68942900	-1.74426400	1.93564600
C	3.77899300	-2.65597200	-0.33597400
O	1.99891300	2.83358900	-1.66686100
O	2.06791700	1.87483500	1.53522700
C	-3.28181000	1.25121400	-2.07557800
C	-0.84809200	2.57474700	-2.42044400
C	0.88173000	3.63145200	0.36426600
C	3.24345100	1.15668500	-0.48337900
C	2.09151200	0.68512600	-2.69286100
C	-0.20585900	2.13201300	2.10229900
H	4.19183100	-1.56284000	2.88110300
C	4.43373200	-2.37807000	0.90686100
H	-4.21881700	0.71962900	-1.94343700
C	-3.16245200	2.23718800	-3.05256000

C	-1.94498000	2.89848400	-3.21858900
H	0.09796800	3.07516000	-2.57407700
C	2.10771800	3.73113300	-0.55119600
H	-0.03439000	3.87655800	-0.17740700
H	1.00766500	4.35576000	1.17571700
H	4.13579800	1.38156700	-1.07648500
H	3.28653100	0.12009800	-0.16350700
C	3.22810700	2.09561900	0.72219200
H	2.97736400	1.01687100	-3.24253000
H	1.20816400	0.87926500	-3.30549000
H	2.16935000	-0.38843300	-2.50876400
H	0.11472000	2.78511100	2.91959900
H	-0.26498300	1.10674800	2.47420600
H	-1.19973000	2.43861200	1.77238900
O	3.25050600	3.43573600	0.23189100
H	-4.01108400	2.48293900	-3.68355600
C	2.30802700	5.10862400	-1.14625100
C	4.42175700	1.92556900	-1.63397800
H	3.19758800	5.10002200	-1.77909500
H	2.44359400	5.84037500	-0.34713500
H	1.44035400	5.38937500	-1.74833100
H	4.34830700	2.63564700	2.46024900
H	5.34151100	2.11592600	1.07679500
H	4.44107500	0.90716600	2.02458800
H	1.84375400	-0.86128700	2.52189900
C	4.54180900	-3.30150500	-1.34140200
H	4.07540900	-3.53554600	-2.29534200
C	6.40901000	-3.29008100	0.17097800
H	7.45049000	-3.53338800	0.37939100
C	5.85560900	-3.61996800	-1.09184300
H	6.46965500	-4.11454600	-1.83789300
C	2.42410500	-2.26854000	-0.51109300
H	1.93961600	-2.51526400	-1.45327500
N	5.74102300	-2.69589900	1.13978900
H	-1.84068900	3.66313500	-3.98243800
C	-3.53018300	-1.54941100	-0.62466900
C	-4.75782200	-1.71093500	0.02897300
C	-3.23198800	-2.30942000	-1.77978500
C	-5.70198200	-2.62093200	-0.44442100
H	-4.97564400	-1.12107500	0.91234500
C	-4.19872800	-3.20919600	-2.23819700
C	-5.41911800	-3.37210700	-1.58243000
H	-6.64788400	-2.73909600	0.07487900
H	-3.98210800	-3.80006200	-3.12366500

H	-6.14422600	-4.08612400	-1.96133700
C	-3.11821100	0.48067100	1.42649100
C	-3.73269200	1.72640300	1.23047100
C	-3.08443100	-0.08831900	2.72057700
C	-4.30626200	2.42053100	2.29386700
C	-3.67088500	0.62663200	3.77244700
C	-4.27151100	1.86815900	3.57252100
H	-4.77422600	3.38471900	2.12082800
H	-3.64670800	0.19525900	4.76910400
H	-4.71024500	2.39904500	4.41203100
C	-1.92370400	-2.17379800	-2.51494600
H	-1.78968100	-1.16643700	-2.92327000
H	-1.08803000	-2.38083600	-1.83801100
H	-1.87215200	-2.88297600	-3.34445400
H	-3.75575000	2.16683700	0.24125900
C	-2.43696300	-1.41818700	2.99264400
H	-2.85272800	-2.21622000	2.37090200
H	-1.36850800	-1.40271900	2.75798400
H	-2.55534300	-1.70115800	4.04107300

**9**

Ni	0.17330700	0.29109700	0.32394800
P	-1.71128700	-0.64897200	-0.37895500
P	1.13309200	-1.81912400	-0.01526100
C	-0.56494400	2.04480700	0.49646200
C	-0.53227100	2.97246400	-0.52787300
C	-1.13737600	2.43993400	1.74195000
C	-1.25273000	-2.11191800	-1.42384000
C	0.06767900	-2.59772700	-1.29018900
C	-3.12059300	0.20690200	-1.31302700
C	-2.84589800	-1.23516100	1.02178000
C	-1.67073500	3.69649400	1.92845500
H	-1.17141100	1.72386700	2.55731100
O	-4.18310600	-0.73482900	-1.57103300
O	-3.38840400	-0.04135200	1.60667500
C	0.52953300	-3.62452300	-2.12216200
C	-2.09175700	-2.69913500	-2.38628500
C	-3.98098400	-2.09087600	0.45815400
C	-3.68090800	1.30926100	-0.41188500
C	-2.65896000	0.73916800	-2.65894900
C	-2.06372700	-1.92844800	2.11948100
C	-1.67035700	4.64659400	0.87314500
H	1.55304400	-3.97109700	-2.01807100
C	-0.31129400	-4.18955700	-3.07865400

C	-1.62228300	-3.72708400	-3.20365800
H	-3.10114500	-2.32921200	-2.50677700
C	-4.89172000	-1.23066600	-0.42518900
H	-3.58611400	-2.94165200	-0.10226400
H	-4.57969700	-2.47215200	1.29195400
H	-4.45360500	1.84213500	-0.97574700
H	-2.90690200	2.01448700	-0.12267100
C	-4.33812500	0.69077200	0.82267300
H	-3.51194100	1.18175600	-3.18204000
H	-2.24147900	-0.05446100	-3.28292700
H	-1.89911000	1.50897400	-2.50520300
H	-2.73401300	-2.14425700	2.95719800
H	-1.25035300	-1.28961400	2.47222000
H	-1.63343700	-2.86466300	1.75950300
O	-5.38546100	-0.16770800	0.37158500
H	0.05458800	-4.98204400	-3.72436800
H	-2.28261600	-4.15914700	-3.94964500
C	-6.08831700	-1.98013200	-0.97190100
C	-4.95140600	1.71368500	1.75158300
H	-6.68735200	-1.30228700	-1.58316400
H	-6.69936900	-2.35400000	-0.14770100
H	-5.75762700	-2.82128100	-1.58609500
H	-5.40972200	1.20199600	2.60043000
H	-5.71562400	2.28515400	1.22038300
H	-4.17466300	2.39261700	2.10732800
H	-0.08368900	2.72140100	-1.48820100
C	-1.07747500	4.27635600	-0.37619700
C	-2.21930800	6.73639200	0.09321000
C	-1.65345300	6.47575200	-1.17965000
C	-1.08449300	5.24516600	-1.41014100
H	-2.67623500	7.70619800	0.28820200
H	-1.67608300	7.24199100	-1.94818200
H	-0.63939300	5.00088200	-2.37186500
H	-2.10749500	3.99864800	2.87579200
N	-2.23519000	5.87069100	1.08769900
C	2.47063100	2.09193200	0.70167000
H	2.18379500	2.54608100	-0.26423300
H	2.19510000	2.83275300	1.47378900
C	3.98722600	1.87436200	0.69443400
H	4.29893300	1.50572000	1.68107400
H	4.19141500	1.06706100	-0.01619600
C	4.78248100	3.12793800	0.32771300
H	4.46827700	3.48042600	-0.66667100
H	4.52966000	3.93597400	1.02805300

C	6.30969400	2.93984600	0.32014500
H	6.60588300	2.57800500	1.31620100
C	7.01603800	4.27856900	0.07250700
H	6.74943900	4.67902200	-0.91336500
H	6.73020500	5.02480100	0.82163900
O	1.85277000	0.85643800	0.91045400
C	6.75797900	1.89659500	-0.71287800
H	6.33206600	0.90975500	-0.51360900
H	6.44368300	2.19573000	-1.72116200
H	7.84915100	1.79691200	-0.72193900
H	8.10575800	4.16930300	0.10274400
C	2.80367400	-1.82244400	-0.76246000
C	3.79654200	-2.68208200	-0.27681500
C	3.10298700	-0.91872400	-1.80832700
C	5.09181900	-2.64403200	-0.79227500
H	3.55544100	-3.38299100	0.51479000
C	4.40700100	-0.90156600	-2.31274600
C	5.39902600	-1.74371100	-1.80932400
H	5.85135800	-3.31180700	-0.39776200
H	4.64906100	-0.20359700	-3.10922400
H	6.40513900	-1.69522300	-2.21459600
C	1.18955900	-3.06384000	1.33518000
C	1.84445800	-2.75275300	2.55084100
C	0.50232000	-4.28136900	1.20530500
C	1.76453000	-3.68291700	3.59631600
C	0.44007000	-5.18855900	2.26050300
C	1.07074500	-4.88373300	3.46537200
H	2.26070300	-3.44885800	4.53414100
H	-0.10071500	-6.12225600	2.14005100
H	1.02437300	-5.57690700	4.30001900
C	2.06911700	0.01325600	-2.38456500
H	1.21056400	-0.53430100	-2.78829000
H	1.69447100	0.68544000	-1.60571900
H	2.49614800	0.61552700	-3.18988700
C	2.65319500	-1.49649300	2.73978400
H	3.65418500	-1.62230500	2.30875600
H	2.22464200	-0.61512900	2.24793100
H	2.77902400	-1.28005600	3.80418500
H	0.00080300	-4.52058300	0.27519700

**TS10**

Ni	0.08559100	0.39356600	0.34019400
P	-1.49672500	-0.93483600	-0.32655600
P	1.56679500	-1.32603800	-0.04681700

C	-0.71299500	2.12917000	0.63677000
C	-1.06182800	2.93462100	-0.45964100
C	-1.42448300	2.31696000	1.87622500
C	-0.71490200	-2.23118000	-1.38778800
C	0.68507300	-2.38607400	-1.26418700
C	-3.05393400	-0.38277200	-1.23141000
C	-2.45839200	-1.82079700	1.03944200
C	-2.46615500	3.19506000	1.96680700
H	-1.12380100	1.72939800	2.73760300
O	-3.91246100	-1.50408800	-1.53256800
O	-3.23281800	-0.80319500	1.69256300
C	1.36784200	-3.28470400	-2.09334000
C	-1.39812300	-2.99863800	-2.34606500
C	-3.40035400	-2.86631400	0.44180600
C	-3.78926100	0.55233900	-0.26821700
C	-2.71812700	0.29420900	-2.54836400
C	-1.52397600	-2.39185300	2.08899400
C	-2.88528600	3.97496400	0.84305600
H	2.44570700	-3.37805000	-2.00179100
C	0.67597700	-4.03983200	-3.03842700
C	-0.70698800	-3.89346000	-3.16232100
H	-2.46661500	-2.86822200	-2.46267700
C	-4.48198300	-2.17789600	-0.40271600
H	-2.84501900	-3.59506000	-0.15302800
H	-3.89892000	-3.39648100	1.26033200
H	-4.64753800	0.98368800	-0.79335300
H	-3.14050600	1.36187500	0.05943200
C	-4.31036400	-0.23864100	0.93387000
H	-3.64339500	0.59964600	-3.04624000
H	-2.16823600	-0.37661100	-3.21333700
H	-2.11148100	1.18154900	-2.34999100
H	-2.11181500	-2.79574000	2.91912700
H	-0.85907300	-1.61321100	2.47074700
H	-0.90940700	-3.19083200	1.66857300
O	-5.16934100	-1.26823200	0.44077900
H	1.21329100	-4.73213000	-3.67959200
H	-1.25032900	-4.47074600	-3.90451300
C	-5.50971100	-3.13729700	-0.96448100
C	-5.11795200	0.59841800	1.89924900
H	-6.24503500	-2.57527000	-1.54362900
H	-6.01656000	-3.65711500	-0.14871100
H	-5.02512800	-3.87090600	-1.61371100
H	-5.46323200	-0.03164000	2.72175400
H	-5.98151200	1.02485500	1.38472900

H	-4.49886500	1.40723100	2.28872700
H	-0.53980400	2.83185600	-1.40716300
C	-2.14820700	3.83793700	-0.38171100
C	-4.34241200	5.49733000	-0.07276900
C	-3.69268900	5.44139500	-1.32609900
C	-2.60011000	4.61626500	-1.47954600
H	-5.20843500	6.14322000	0.06327200
H	-4.05929600	6.04370100	-2.15218400
H	-2.07871400	4.54748500	-2.43156400
H	-3.01480500	3.32480700	2.89496700
N	-3.95764600	4.79178000	0.98059700
C	1.81548100	2.73412800	0.18465700
H	1.77836000	2.38229100	-0.85325100
H	1.48218900	3.78213300	0.18151800
C	3.23785100	2.60940300	0.70983200
H	3.27170400	2.99432100	1.73692100
H	3.49615600	1.54829100	0.75394300
C	4.24374700	3.35285100	-0.17449900
H	4.33397200	2.82563500	-1.13469400
H	3.85540300	4.35443300	-0.40582500
C	5.64246300	3.50631900	0.44689400
H	5.53056700	4.09822500	1.36753200
C	6.56668100	4.27723800	-0.50326300
H	6.71489900	3.71846400	-1.43552400
H	6.14696700	5.25473600	-0.76436800
O	0.94313200	1.98769900	1.02727300
C	6.26332500	2.15599300	0.82534200
H	5.66485700	1.62589300	1.57213100
H	6.34268500	1.50697000	-0.05300900
H	7.26835200	2.29098600	1.23957700
H	7.55220100	4.44220000	-0.05484800
C	3.16369400	-0.98838900	-0.87912600
C	4.37558500	-1.45155100	-0.34853300
C	3.16776200	-0.17571600	-2.03857500
C	5.59089400	-1.11646800	-0.94345600
H	4.36374700	-2.08366800	0.53314200
C	4.39935100	0.15001400	-2.61629500
C	5.60247500	-0.31004900	-2.08029900
H	6.52070500	-1.48148500	-0.51836200
H	4.41105500	0.77521100	-3.50508500
H	6.54305300	-0.03674700	-2.54875700
C	1.96844800	-2.46350500	1.33737800
C	2.43289200	-1.92219300	2.55982300
C	1.72317200	-3.84113200	1.23866100

C	2.63272900	-2.79209700	3.63829000
C	1.92523700	-4.68718300	2.32744200
C	2.38005400	-4.15898800	3.53402100
H	2.98733400	-2.38119300	4.57950300
H	1.72497200	-5.74993100	2.23126600
H	2.53583800	-4.80552200	4.39237900
C	1.89118300	0.30007700	-2.68720100
H	1.43052200	-0.49952700	-3.27804700
H	1.14435500	0.60514500	-1.94341700
H	2.08186700	1.14678200	-3.35109300
C	2.73997500	-0.45562700	2.71953400
H	3.64022400	-0.18267700	2.15719800
H	1.93438700	0.18433900	2.34680700
H	2.91882900	-0.20769000	3.76856900
H	1.35919100	-4.25559300	0.30602900

## 11

Ni	0.22650500	0.37602400	0.34203400
P	-1.15030800	-1.06672600	-0.34507000
P	1.92523000	-0.88636400	0.12987300
C	-1.24208000	2.73563400	0.66601900
C	-1.94041200	3.34396000	-0.35350400
C	-1.87944400	2.36601600	1.87931400
C	-0.07356700	-2.22411800	-1.33647200
C	1.31881800	-2.14710300	-1.09099400
C	-2.70217400	-0.83081300	-1.41102200
C	-2.08301600	-2.17179700	0.89200600
C	-3.21423100	2.61634400	2.05607300
H	-1.28057100	1.88664400	2.64530800
O	-3.31881700	-2.07454100	-1.81640600
O	-3.11544200	-1.34806500	1.47464400
C	2.20246900	-2.95475300	-1.81879500
C	-0.53044300	-3.10246500	-2.33397000
C	-2.74292300	-3.36146100	0.19414100
C	-3.69513800	-0.07107600	-0.52281300
C	-2.37824200	-0.07058800	-2.68550800
C	-1.17780900	-2.59172600	2.03332800
C	-3.98577900	3.21828800	1.02144000
H	3.26851400	-2.88129000	-1.62757300
C	1.73045200	-3.82893700	-2.79659900
C	0.36174300	-3.89347500	-3.05825100
H	-1.58909600	-3.14462500	-2.55518200
C	-3.84433500	-2.87599800	-0.75748800
H	-2.00073200	-3.95719400	-0.34098200



H	-3.21477000	-3.99722900	0.95175300
H	-4.55675200	0.23185000	-1.12765900
H	-3.22775100	0.81980600	-0.10535900
C	-4.18877600	-0.98157700	0.60706200
H	-3.28980500	0.07320500	-3.27474900
H	-1.64973700	-0.61336100	-3.29345600
H	-1.96052200	0.90703300	-2.42842200
H	-1.76015700	-3.12997100	2.78852600
H	-0.71374200	-1.71624800	2.49414200
H	-0.37963700	-3.24309200	1.67050000
O	-4.78112100	-2.13698500	0.01283200
H	2.42728200	-4.44508800	-3.35750800
H	-0.01542700	-4.55727200	-3.83112700
C	-4.60397700	-4.00431900	-1.42403400
C	-5.25488800	-0.35213700	1.47714100
H	-5.37348600	-3.58340300	-2.07449300
H	-5.07803900	-4.63197900	-0.66637500
H	-3.92232000	-4.61423300	-2.02219700
H	-5.56335300	-1.07229600	2.23804000
H	-6.11896100	-0.08229200	0.86648100
H	-4.87055900	0.54584300	1.95890900
H	-1.45581100	3.61354800	-1.28505200
C	-3.33265900	3.58172300	-0.19916800
C	-6.02818600	3.92685200	0.24789700
C	-5.48371100	4.32038200	-0.99726000
C	-4.13579900	4.14953400	-1.21792300
H	-7.09291800	4.05550400	0.43589800
H	-6.12871800	4.74734000	-1.75833000
H	-3.67951200	4.43568800	-2.16188300
H	-3.72067200	2.35577500	2.97850800
N	-5.31852100	3.39741600	1.22777500
C	0.94985600	3.26793000	-0.23135500
H	0.88729800	2.89873000	-1.26090200
H	0.57069000	4.29550200	-0.20287800
C	2.36264300	3.17953200	0.31037100
H	2.39397000	3.68327600	1.28435600
H	2.58886600	2.12370300	0.48255000
C	3.38869400	3.78997600	-0.64921900
H	3.55000100	3.09447800	-1.48209200
H	2.99033100	4.71587000	-1.08821600
C	4.74423200	4.11034100	0.00570200
H	4.58075500	4.93891300	0.71116000
C	5.74392400	4.57738200	-1.05881900
H	5.95973100	3.76351600	-1.76112000

H	5.35290200	5.42362900	-1.63460600
O	0.10655600	2.45192500	0.61499400
C	5.30905400	2.92227100	0.79361700
H	4.66535100	2.64970800	1.63494600
H	5.41560900	2.04271200	0.15371500
H	6.29687300	3.16359200	1.20067900
H	6.69160400	4.88681300	-0.60591400
C	3.57680100	-0.49623800	-0.60864300
C	4.77913200	-0.84635000	0.02302100
C	3.62192900	0.22133600	-1.82901700
C	6.01278300	-0.50497100	-0.53127700
H	4.74713000	-1.40437000	0.95288300
C	4.86880600	0.56037100	-2.36581600
C	6.05918900	0.20171700	-1.73220700
H	6.93061400	-0.79063500	-0.02593100
H	4.90303400	1.11040200	-3.30307300
H	7.01292200	0.47736900	-2.17205900
C	2.37234200	-1.88601600	1.61268400
C	2.67370200	-1.22019500	2.82472100
C	2.33470200	-3.28729900	1.59211600
C	2.92605900	-1.98741100	3.96730900
C	2.58371200	-4.03422700	2.74283500
C	2.87954700	-3.38102400	3.93728700
H	3.15835800	-1.47756600	4.89865200
H	2.54616200	-5.11885400	2.70278100
H	3.07283400	-3.94959700	4.84211000
C	2.36454400	0.58164900	-2.58014700
H	1.99120000	-0.27519400	-3.15219900
H	1.55777300	0.86008900	-1.89071900
H	2.54351700	1.40444100	-3.27794300
C	2.73707600	0.28420500	2.90851200
H	3.54183600	0.68367500	2.28154500
H	1.80660900	0.73698900	2.54653100
H	2.91627800	0.61133100	3.93617800
H	2.10154000	-3.80028700	0.66614500

**12**

Ni	-0.37735100	0.40374900	0.59683300
P	-2.11263800	-0.62714900	-0.43201600
P	0.77898700	-1.67064800	0.11462700
C	-1.19824400	2.11992100	0.74449600
C	-1.08503800	3.06942700	-0.25747900
C	-1.96477700	2.46352900	1.90110700
C	-1.47100000	-1.96982800	-1.53129400

C	-0.14758700	-2.40210500	-1.29703200
C	-3.48276800	0.22070800	-1.42260200
C	-3.32958400	-1.41071900	0.79070900
C	-2.61157400	3.67481000	2.01404700
H	-2.06301800	1.73677500	2.70299200
O	-4.46324500	-0.74170600	-1.86674400
O	-3.99932800	-0.31227500	1.42996200
C	0.44660400	-3.33912300	-2.15290500
C	-2.17526500	-2.51105300	-2.62173500
C	-4.35425000	-2.26859800	0.04867100
C	-4.18042600	1.20375000	-0.48097200
C	-2.93115000	0.90341200	-2.66227300
C	-2.60045300	-2.16607400	1.88484100
C	-2.53405600	4.63646700	0.97201300
H	1.47165200	-3.64751700	-1.97247300
C	-0.26056000	-3.86069200	-3.23328600
C	-1.57360800	-3.44577700	-3.46263500
H	-3.18570100	-2.17740200	-2.81851300
C	-5.23487300	-1.38101400	-0.84046000
H	-3.85849900	-3.04262400	-0.54162800
H	-5.00224600	-2.75581700	0.78496200
H	-4.92343400	1.75998900	-1.06172300
H	-3.47134400	1.90529000	-0.05001400
C	-4.91346900	0.44010500	0.62290900
H	-3.75492400	1.35474000	-3.22342600
H	-2.41228000	0.19542200	-3.31285900
H	-2.23381900	1.68893200	-2.36126500
H	-3.32197900	-2.50104700	2.63651400
H	-1.85923700	-1.52228900	2.36507200
H	-2.08494000	-3.03815900	1.47704700
O	-5.86245000	-0.42435800	-0.00148400
H	0.21079500	-4.58156300	-3.89444900
H	-2.13081200	-3.84274900	-4.30596500
C	-6.33003000	-2.14149400	-1.55751300
C	-5.67168300	1.33977700	1.57238700
H	-6.91461800	-1.44445500	-2.16114800
H	-6.98593900	-2.62208900	-0.82861400
H	-5.89461000	-2.90374200	-2.20831100
H	-6.16851400	0.72932600	2.32929300
H	-6.42165200	1.91109300	1.02109200
H	-4.97643000	2.02931700	2.05395400
H	-0.48284400	2.86693200	-1.14229200
C	-1.74404800	4.32600800	-0.18108700
C	-3.12022400	6.69130400	0.12931100

C	-2.36296700	6.48876400	-1.05137800
C	-1.67666200	5.30669500	-1.20238400
H	-3.67043100	7.62257800	0.26051500
H	-2.33444400	7.26101100	-1.81375000
H	-1.08314600	5.10883700	-2.09192500
H	-3.20103500	3.93013100	2.88983100
N	-3.21153400	5.81321800	1.10897800
C	2.07183400	1.88160000	0.85183100
H	2.00926500	1.61877800	-0.21019900
H	1.93123200	2.97395400	0.89244700
C	3.49216100	1.52371400	1.30924300
H	3.62741800	1.80761000	2.36154800
H	3.59208200	0.43411200	1.26465500
C	4.57608500	2.15968700	0.43573800
H	4.33268100	1.96532300	-0.61786800
H	4.56864900	3.25223800	0.55432700
C	5.97778700	1.61439300	0.71955200
H	6.28227800	1.88252300	1.74088000
C	7.03267600	2.10117500	-0.27668200
H	6.70467000	1.84546000	-1.29480700
H	7.09322600	3.19815100	-0.24586300
C	2.47262800	-1.52426200	-0.57270200
C	3.54189200	-2.24272300	-0.02159700
C	2.70555300	-0.61975000	-1.63561000
C	4.84336900	-2.05597600	-0.48453900
H	3.35165600	-2.95447100	0.77369100
C	4.02025900	-0.44764200	-2.08215300
C	5.08430300	-1.14667900	-1.51292200
H	5.66138700	-2.61485600	-0.04075900
H	4.20984000	0.25278600	-2.89085000
H	6.09504100	-0.97977300	-1.87249400
C	0.84363700	-3.04402500	1.34078200
C	1.39490600	-2.82284300	2.62501800
C	0.25723700	-4.28514100	1.04219400
C	1.32686000	-3.86543900	3.56021400
C	0.19857600	-5.30242100	1.99163400
C	0.73494600	-5.08960200	3.26022000
H	1.74692800	-3.69933200	4.54840500
H	-0.26589400	-6.25083400	1.73951100
H	0.69148500	-5.87072700	4.01342400
C	1.58474200	0.11797900	-2.32591400
H	1.06929800	-0.53398100	-3.03980900
H	0.82793300	0.46803900	-1.61340400
H	1.96689900	0.98515300	-2.86977700

C	2.07778600	-1.53636000	3.00514700
H	3.12889100	-1.55301800	2.69060100
H	1.62735600	-0.64262500	2.54685500
H	2.07018900	-1.40678200	4.09134800
H	-0.16943900	-4.45745800	0.06197300
C	8.42190400	1.50654600	-0.03285400
H	8.35536200	0.40912900	-0.06262300
H	8.75459900	1.75983600	0.98366300
C	9.47479200	1.97580200	-1.04131000
H	9.13914500	1.72387600	-2.05658900
H	9.54224100	3.07148600	-1.00861700
C	10.85751800	1.36860600	-0.79276900
H	10.82362000	0.27465000	-0.85137300
H	11.59058000	1.71926800	-1.52647600
H	11.22992100	1.63266500	0.20347400
H	5.94011100	0.51753800	0.68937200
N	1.04600000	1.15769200	1.61333800
H	0.65176000	1.81365100	2.28397900

### TS13

Ni	0.40387800	0.37321100	-0.62719400
P	1.97344500	-0.75604400	0.41471400
P	-1.01300700	-1.52694500	-0.11960200
C	1.12449400	2.12936900	-0.90246500
C	1.18209900	3.02308100	0.17722500
C	2.00483900	2.38056900	-2.01653900
C	1.20173000	-2.00420100	1.53735300
C	-0.15575700	-2.32036200	1.30329600
C	3.37678300	0.02740500	1.40379000
C	3.15032100	-1.67894600	-0.74399800
C	2.88750500	3.42716000	-2.01964800
H	1.97959500	1.70092600	-2.86496300
O	4.29140700	-0.97298000	1.90168200
O	3.89882000	-0.65926900	-1.42579300
C	-0.83136400	-3.18980300	2.17028600
C	1.84949600	-2.58344500	2.64238900
C	4.11302000	-2.56451000	0.04747600
C	4.13147800	0.92942500	0.42468700
C	2.85369200	0.79403800	2.60610400
C	2.38567700	-2.43998800	-1.81017500
C	2.98267200	4.31774300	-0.90822200
H	-1.87843300	-3.41171400	1.98951300
C	-0.17580500	-3.75502900	3.26170500
C	1.16612500	-3.44914500	3.49484300

H	2.88288500	-2.33024100	2.84122000
C	5.03525000	-1.69396600	0.91159100
H	3.56570100	-3.28266100	0.66276500
H	4.73848700	-3.12003400	-0.65950200
H	4.89360700	1.48217600	0.98338700
H	3.45737700	1.64178100	-0.04497500
C	4.83800400	0.07892300	-0.63315100
H	3.69739300	1.21862500	3.15865700
H	2.28685900	0.14544800	3.27877400
H	2.20993700	1.60728500	2.26196300
H	3.09087100	-2.86710300	-2.53014800
H	1.70015900	-1.77157900	-2.33713700
H	1.80080800	-3.24839300	-1.36557100
O	5.72725400	-0.80921300	0.04531900
H	-0.71030300	-4.42410200	3.92934000
H	1.68229500	-3.87769000	4.34880600
C	6.07709400	-2.48802800	1.67102000
C	5.66181800	0.89256300	-1.60516000
H	6.69495200	-1.80225000	2.25409500
H	6.71132900	-3.03444100	0.96979300
H	5.59107400	-3.19678100	2.34602800
H	6.14566000	0.22165400	-2.31821400
H	6.42519200	1.45522200	-1.06374200
H	5.01256100	1.58976900	-2.13645300
H	0.53226900	2.88455900	1.03811400
C	2.09838700	4.10156400	0.20158800
C	3.98641700	6.12143500	0.09954800
C	3.16645300	6.00256600	1.24557900
C	2.22651900	4.99774900	1.29563900
H	4.73479000	6.91081000	0.04690700
H	3.28582800	6.70002100	2.06942800
H	1.57973800	4.87649800	2.16156800
H	3.55495200	3.60261500	-2.85835000
N	3.90464200	5.31265200	-0.94493800
C	-1.65714300	2.48523800	-1.01621500
H	-1.51274000	2.51724100	0.06915400
H	-1.58775900	3.53066500	-1.35685000
C	-3.05327700	1.92198300	-1.29909400
H	-3.27810200	2.00871900	-2.37098100
H	-3.03842100	0.85327200	-1.06878700
C	-4.15617400	2.58259300	-0.47072700
H	-3.90937900	2.46409500	0.59343500
H	-4.18615300	3.66435800	-0.66106000
C	-5.53310000	1.96548700	-0.72992200

H	-5.86132600	2.20899100	-1.74995600
C	-6.59995700	2.40561300	0.27436900
H	-6.24651300	2.17469300	1.28913000
H	-6.72154500	3.49721500	0.23635500
C	-2.71320400	-1.30764300	0.53907200
C	-3.80185200	-2.01693200	0.01315700
C	-2.92479800	-0.35403900	1.56345000
C	-5.09579100	-1.79287400	0.48277500
H	-3.63180500	-2.75243600	-0.76594500
C	-4.23029300	-0.14835200	2.02094800
C	-5.31037700	-0.85461200	1.49105600
H	-5.92825800	-2.34897900	0.06273000
H	-4.40062400	0.58348900	2.80573400
H	-6.31362000	-0.66561500	1.86022900
C	-1.15566800	-2.88008800	-1.35424200
C	-1.61398700	-2.56971400	-2.65635500
C	-0.73235200	-4.18523100	-1.06201700
C	-1.62373800	-3.58643100	-3.61859300
C	-0.74639700	-5.18043900	-2.03763300
C	-1.19173900	-4.87841200	-3.32301900
H	-1.97316700	-3.35195000	-4.62037400
H	-0.40915000	-6.18290600	-1.79231300
H	-1.20230300	-5.64298200	-4.09402200
C	-1.78344000	0.40718500	2.18972400
H	-1.23582800	-0.22177300	2.90066700
H	-1.05476200	0.73385800	1.43789200
H	-2.14642800	1.28867200	2.72364200
C	-2.11252900	-1.19361600	-3.01378300
H	-3.10025000	-1.00926000	-2.57541700
H	-1.45451900	-0.40431100	-2.63448400
H	-2.20548100	-1.08226000	-4.09717800
H	-0.37971600	-4.42541000	-0.06592800
C	-7.95521500	1.73032000	0.05118300
H	-7.81941100	0.63926300	0.06935000
H	-8.32318700	1.97090400	-0.95610300
C	-9.01341100	2.12470900	1.08547400
H	-8.64326900	1.88021600	2.09062200
H	-9.14566600	3.21480000	1.06947800
C	-10.36294200	1.44045700	0.85528500
H	-10.26432100	0.34964800	0.89817100
H	-11.10024500	1.73826000	1.60775200
H	-10.76989400	1.69484000	-0.12982500
H	-5.44149300	0.87329800	-0.68851600
N	-0.60001800	1.67309300	-1.59402800

H	-0.38499600	1.92916500	-2.54798200
<b>14</b>			
Ni	-0.16932700	0.27847000	0.49407700
P	-1.74588300	-0.87511600	-0.32870900
P	1.29366500	-1.23957000	0.10136300
C	-1.21389000	2.79844500	0.96611600
C	-1.65642000	3.45366100	-0.16879200
C	-2.07618500	2.68311100	2.09458100
C	-0.88097200	-2.05360500	-1.48190700
C	0.50946900	-2.21443000	-1.27138000
C	-3.26673400	-0.28353700	-1.29640600
C	-2.80574500	-1.96122700	0.81730800
C	-3.34188700	3.20650200	2.06973300
H	-1.71654300	2.15785000	2.97520300
O	-4.09118000	-1.36065400	-1.79805900
O	-3.66475900	-1.05419700	1.53900100
C	1.25469600	-3.03738100	-2.12520500
C	-1.48011500	-2.72186800	-2.56279500
C	-3.67764900	-2.93921700	0.02896200
C	-4.08878300	0.52118600	-0.28453800
C	-2.86638300	0.55202300	-2.50027100
C	-1.94966900	-2.65675900	1.85698500
C	-3.84325500	3.84688500	0.90159600
H	2.32234000	-3.14533400	-1.96026500
C	0.64359400	-3.69780600	-3.19028000
C	-0.72471000	-3.53316000	-3.40993600
H	-2.53787500	-2.58262600	-2.74793100
C	-4.71323600	-2.17518200	-0.80373200
H	-3.06372500	-3.57981300	-0.60808600
H	-4.22052500	-3.57580300	0.73674200
H	-4.91003900	1.02421200	-0.80622900
H	-3.46544100	1.27305400	0.19472400
C	-4.68575600	-0.41623400	0.77010500
H	-3.76332100	0.90194100	-3.02157000
H	-2.25882500	-0.02864900	-3.19916600
H	-2.28924500	1.41806800	-2.16624000
H	-2.59212500	-3.17682000	2.57533900
H	-1.32840700	-1.93247600	2.38925500
H	-1.28752100	-3.38360300	1.38219000
O	-5.48594900	-1.38337500	0.08956900
H	1.23348300	-4.32844600	-3.84920900
H	-1.20651100	-4.03254700	-4.24582100
C	-5.67699500	-3.07867100	-1.54482300



C	-5.58769600	0.28640800	1.76138000
H	-6.38335500	-2.46449700	-2.10719900
H	-6.22702800	-3.69877700	-0.83367000
H	-5.13029100	-3.72307300	-2.23793200
H	-6.01420300	-0.45195900	2.44378500
H	-6.39384800	0.80233600	1.23592700
H	-5.01044200	1.01659200	2.32970100
H	-1.01517800	3.55125000	-1.03771100
C	-2.97718600	3.96297800	-0.23229500
C	-5.58459200	4.85618700	-0.20074600
C	-4.81542700	5.02285400	-1.37729900
C	-3.51291100	4.57970000	-1.39084000
H	-6.61675100	5.20202100	-0.17747100
H	-5.25845000	5.49263900	-2.24959600
H	-2.89127800	4.68536000	-2.27609400
H	-4.00182100	3.13346400	2.92703000
N	-5.12726500	4.29420400	0.90385200
C	1.18882600	2.94748400	0.36071900
H	1.08515800	2.75763300	-0.70978100
H	1.09448300	4.03161500	0.51789000
C	2.53546600	2.43281700	0.84722200
H	2.66122300	2.68861800	1.90973800
H	2.51796700	1.34167000	0.78035800
C	3.72376200	2.96364400	0.04668800
H	3.58641400	2.69947400	-1.00945800
H	3.76238800	4.06072600	0.09492700
C	5.04466700	2.36733700	0.53850100
H	5.22003400	2.67569300	1.57897500
C	6.25040700	2.75013000	-0.32061700
H	6.05303100	2.45189000	-1.35871800
H	6.37200400	3.84256300	-0.33149200
C	2.99703500	-1.00929400	-0.58655700
C	4.12893400	-1.57713600	0.01760900
C	3.16693500	-0.17222800	-1.71707100
C	5.41062300	-1.34023900	-0.48001600
H	4.00261900	-2.22512900	0.87835400
C	4.45959200	0.04966800	-2.20305600
C	5.57765000	-0.52705000	-1.59977300
H	6.27101300	-1.79531000	0.00189800
H	4.58878700	0.68804600	-3.07356900
H	6.56936900	-0.33466400	-1.99767200
C	1.57394200	-2.50648700	1.41620600
C	1.93843400	-2.08628400	2.71714700
C	1.35575800	-3.87081700	1.17713100

C	2.07021100	-3.04853100	3.72446600
C	1.48679900	-4.81479800	2.19470800
C	1.84474600	-4.40196600	3.47616300
H	2.35009200	-2.72490700	4.72359200
H	1.30915400	-5.86525400	1.98399600
H	1.94731400	-5.12545200	4.27947300
C	1.98898600	0.45038500	-2.42463500
H	1.51526800	-0.26464700	-3.10642400
H	1.21164300	0.75084000	-1.71082800
H	2.29743900	1.32250900	-3.00809500
C	2.18932600	-0.63521400	3.04015500
H	3.05231500	-0.24374000	2.49033500
H	1.32729000	-0.02601400	2.74368200
H	2.37690500	-0.49823300	4.10849100
H	1.07076100	-4.19880800	0.18430900
C	7.54962600	2.09227100	0.15052200
H	7.39812500	1.00578700	0.20542900
H	7.77619700	2.41939300	1.17514700
C	8.74815300	2.38892200	-0.75484100
H	8.51536400	2.05977400	-1.77698300
H	8.89925400	3.47515600	-0.81447000
C	10.03783800	1.71487300	-0.28099100
H	9.92141600	0.62565800	-0.24382900
H	10.87842500	1.93780300	-0.94600500
H	10.31089900	2.05018500	0.72593200
H	4.95149700	1.27522300	0.54889500
N	0.09225700	2.23973700	1.06514800
H	0.34199400	2.14879000	2.04790100

**15**

Ni	0.03709200	-0.85147400	0.43956400
P	0.47030800	1.26535600	-0.32052600
P	-2.33028200	-0.16695200	-0.08245900
C	1.85025500	-1.38421000	0.45664100
C	2.42156000	-1.89014600	-0.70042300
C	2.67989100	-1.27751100	1.61075000
C	-0.94939600	1.98390000	-1.26476200
C	-2.19793000	1.34048800	-1.13474400
C	2.03052400	1.90505800	-1.18816700
C	0.72738200	2.39050300	1.18508300
C	4.00222400	-1.66357600	1.59728900
H	2.26538200	-0.86474700	2.52388500
O	1.98804200	3.34156600	-1.32407300
O	1.98887500	2.01134200	1.75580800

C	-3.30355100	1.80122400	-1.86423300
C	-0.84661600	3.08432800	-2.13709200
C	0.78655000	3.85564300	0.75144400
C	3.23129400	1.56094400	-0.30419600
C	2.16344900	1.32765800	-2.58727300
C	-0.32296500	2.13020400	2.24816100
C	4.59584900	-2.17949000	0.41608100
H	-4.25327300	1.28514700	-1.76823900
C	-3.18886400	2.89511500	-2.71599700
C	-1.95408000	3.53207300	-2.85309300
H	0.10738600	3.57943500	-2.25532300
C	2.03503400	4.09784800	-0.10581800
H	-0.11915000	4.13873400	0.21101600
H	0.86705700	4.48131000	1.64654300
H	4.13688700	1.86936700	-0.83679800
H	3.28397100	0.49432600	-0.10790900
C	3.16102200	2.34997400	1.00476400
H	3.04640500	1.75522000	-3.07181300
H	1.28653500	1.55157600	-3.19954400
H	2.28586700	0.24381200	-2.52096000
H	-0.09921100	2.72820500	3.13709500
H	-0.32921700	1.07339300	2.52473200
H	-1.31838500	2.39630400	1.88546200
O	3.16338200	3.73881800	0.67377000
H	-4.05195900	3.24159900	-3.27628800
H	-1.84877900	4.37907600	-3.52459000
C	2.21273500	5.54256500	-0.52182500
C	4.33814200	2.10298300	1.92096100
H	3.12106000	5.63423000	-1.12066900
H	2.30246500	6.17475900	0.36406600
H	1.35598600	5.87193200	-1.11486000
H	4.22116300	2.70052900	2.82742200
H	5.26356500	2.39090800	1.41749900
H	4.38372100	1.04471800	2.18091900
H	1.83183100	-1.99578500	-1.60946800
C	3.78159200	-2.29510300	-0.75550900
C	6.43857400	-3.01042100	-0.67413500
C	5.72233600	-3.17115300	-1.88708700
C	4.39565000	-2.81257200	-1.92394000
H	7.49109300	-3.28912200	-0.63254700
H	6.22495800	-3.57148800	-2.76196300
H	3.80700400	-2.91907300	-2.83223600
H	4.62990200	-1.58328600	2.47997200
N	5.91321700	-2.53638700	0.43828200

C	-0.29267700	-3.76733600	1.14735800
C	-3.29670200	-1.23574500	-1.22349100
C	-4.65281800	-1.50831000	-1.00054300
C	-2.65393800	-1.76548500	-2.36600400
C	-5.37253100	-2.32385700	-1.87220200
H	-5.15046400	-1.07208100	-0.14165000
C	-3.39350800	-2.58684400	-3.22393000
C	-4.73659400	-2.87331900	-2.98384100
H	-6.42171100	-2.52709700	-1.68062100
H	-2.90190600	-3.00463000	-4.09826200
H	-5.28310300	-3.51795500	-3.66556800
C	-3.50008900	0.31431800	1.25068300
C	-3.92959900	-0.65229500	2.19171900
C	-3.88405700	1.65553100	1.40819600
C	-4.73547400	-0.22491400	3.25497500
C	-4.67667100	2.05611000	2.48193200
C	-5.10466700	1.10983300	3.41066500
H	-5.06961900	-0.96311100	3.97892800
H	-4.95574500	3.09999500	2.58793500
H	-5.72089800	1.40745700	4.25383700
C	-1.22555300	-1.42800700	-2.70959000
H	-1.15304300	-0.41828900	-3.13005800
H	-0.58119200	-1.45279700	-1.82337300
H	-0.82252500	-2.13135800	-3.44214500
C	-3.57076500	-2.11069600	2.06838500
H	-4.25531400	-2.62597300	1.38492300
H	-2.54579900	-2.24731200	1.68994100
H	-3.64310400	-2.60438600	3.04123200
H	-3.56022900	2.39631500	0.68672900
N	-0.47762000	-2.35981300	1.49167300
C	1.07030400	-4.40679500	1.48200700
H	1.36266300	-4.21720900	2.51830600
H	1.01479100	-5.49366200	1.34830500
H	1.85944600	-4.02142500	0.83442800
C	-0.64711400	-4.00522900	-0.31972700
H	-1.62687800	-3.58190800	-0.55471000
H	0.09787000	-3.53841300	-0.97066700
H	-0.66629900	-5.07622400	-0.54847900
C	-0.27489500	-2.10995100	2.90686500
H	-0.88713400	-2.80786200	3.50500900
H	0.76091700	-2.21479800	3.27070800
H	-0.61164100	-1.09688700	3.16141800
H	-1.04175900	-4.31667000	1.75365700

**TS16**

Ni	-0.05593100	-0.70642700	0.45162800
P	0.46518200	1.31661400	-0.24308700
P	-2.33584300	-0.10513500	-0.09463800
C	1.63205100	-1.62691700	0.67911000
C	2.11705600	-2.17104000	-0.52807400
C	2.61205300	-1.37827300	1.70753300
C	-0.92611600	2.06137700	-1.20867900
C	-2.18391700	1.42999500	-1.10223100
C	2.03821500	1.78379100	-1.17579100
C	0.82158600	2.50760500	1.18452600
C	3.93375500	-1.70356900	1.54960500
H	2.30623900	-0.89675100	2.62779200
O	2.11539500	3.20952900	-1.39434700
O	2.05526600	2.06131000	1.77065300
C	-3.27711700	1.91541000	-1.83403200
C	-0.79759800	3.16436000	-2.07258600
C	1.00017100	3.93587900	0.67102500
C	3.20774000	1.37156700	-0.28003300
C	2.08846100	1.11267600	-2.53732600
C	-0.24336900	2.38325300	2.25799500
C	4.42459100	-2.26698800	0.33725900
H	-4.23452900	1.41025300	-1.75630400
C	-3.13794700	3.01850100	-2.67136600
C	-1.89179000	3.63579900	-2.79482700
H	0.17072500	3.63192000	-2.19090300
C	2.24834000	4.02004300	-0.21910000
H	0.11090400	4.27295900	0.13420100
H	1.15692200	4.59865600	1.52878000
H	4.13836400	1.53967500	-0.83163600
H	3.14252100	0.31872100	-0.01522500
C	3.23672100	2.24402400	0.97801000
H	3.00772500	1.40412700	-3.05445300
H	1.23406800	1.40041900	-3.15562300
H	2.08480600	0.02732700	-2.40370500
H	0.02203700	3.00462700	3.11912200
H	-0.33096200	1.34203400	2.58000700
H	-1.21564300	2.70403900	1.87497900
O	3.35589600	3.60489500	0.56208000
H	-3.99085900	3.38439400	-3.23500200
H	-1.76728500	4.48378500	-3.46181000
C	2.54280400	5.42106400	-0.71217400
C	4.40735600	1.95500800	1.89018700
H	3.44715600	5.40298500	-1.32358500

H	2.69762500	6.08842600	0.13829900
H	1.70922800	5.79175000	-1.31397400
H	4.36887400	2.62888800	2.74869900
H	5.34354600	2.11262700	1.35056400
H	4.36043100	0.92065300	2.23045500
H	1.44141200	-2.35066600	-1.35866500
C	3.48052500	-2.48496300	-0.72055500
C	6.18384800	-3.03574200	-0.92255800
C	5.34404000	-3.28921400	-2.03344500
C	3.99932000	-3.01542200	-1.93301100
H	7.24990900	-3.24803300	-0.98938100
H	5.76688300	-3.69534400	-2.94761200
H	3.32435300	-3.19925500	-2.76592300
H	4.65571300	-1.51220400	2.33834500
N	5.74957100	-2.54098100	0.22492200
C	-0.22516700	-3.76454500	1.06154100
C	-3.38172900	-1.11944300	-1.21264400
C	-4.71627600	-1.42009900	-0.90872100
C	-2.79980500	-1.62634800	-2.39889800
C	-5.47651900	-2.23148800	-1.74956600
H	-5.16376500	-1.00967200	-0.00966100
C	-3.58025500	-2.44091600	-3.22577200
C	-4.90336300	-2.74882700	-2.91008300
H	-6.50873500	-2.45532600	-1.49788200
H	-3.13780100	-2.83855700	-4.13519000
H	-5.48256000	-3.38777100	-3.56981600
C	-3.42702800	0.36224700	1.30251700
C	-3.74876100	-0.61449700	2.27499700
C	-3.84705500	1.68809200	1.48660400
C	-4.49036400	-0.22030700	3.39440300
C	-4.57767100	2.05907400	2.61397200
C	-4.90135700	1.10011200	3.57191600
H	-4.74114200	-0.96728200	4.14274500
H	-4.89035300	3.09115600	2.73999600
H	-5.46824100	1.37694400	4.45569100
C	-1.38955100	-1.27999500	-2.80528100
H	-1.33688300	-0.26465400	-3.21448300
H	-0.70364700	-1.30931000	-1.95033300
H	-1.01955800	-1.97180900	-3.56588400
C	-3.32991000	-2.05364000	2.11852100
H	-3.98028100	-2.58282500	1.41317700
H	-2.30895100	-2.12680800	1.73362100
H	-3.37784100	-2.57937100	3.07552200
H	-3.59973000	2.43705000	0.74329100

N	0.06300600	-2.37689500	1.45861200
C	0.97291500	-4.71776700	1.21994400
H	1.41567300	-4.63587300	2.21642400
H	0.64668600	-5.75446300	1.08258500
H	1.75172800	-4.49871200	0.48788700
C	-0.84596500	-3.86236500	-0.33059100
H	-1.70215400	-3.19227600	-0.42487900
H	-0.12441800	-3.61410700	-1.11051900
H	-1.19054700	-4.88560500	-0.51397900
C	0.14149800	-2.22123800	2.90379200
H	-0.77784400	-2.59919000	3.37193100
H	0.99231400	-2.75427300	3.35663100
H	0.22680200	-1.16468400	3.16888100
H	-0.99991600	-4.10919400	1.76857400

**17**

Ni	-0.37356700	-0.62371300	0.50376700
P	0.45776500	1.19269800	-0.23902400
P	-2.31526800	-0.16615700	-0.18572800
C	1.97656600	-2.12026400	1.16125000
C	2.05523800	-2.35468900	-0.19889000
C	3.17697800	-2.02927900	1.91550000
C	-0.81276200	1.88036500	-1.40765700
C	-2.06821000	1.23065500	-1.39504600
C	2.12423300	1.62180400	-1.04356600
C	0.69502700	2.49849900	1.11883800
C	4.40863800	-2.13670800	1.30652500
H	3.12831800	-1.85737200	2.98341300
O	2.30618200	3.03136300	-1.31954700
O	1.84367200	2.04876400	1.88001200
C	-3.06182000	1.61518600	-2.30365600
C	-0.59252200	2.91074900	-2.33752500
C	0.99278200	3.88647300	0.55495400
C	3.17174300	1.20319100	-0.00633700
C	2.29985200	0.90413100	-2.36973800
C	-0.48043400	2.51197300	2.07752500
C	4.51136300	-2.36338400	-0.08700900
H	-4.01809400	1.10087400	-2.29406900
C	-2.82892200	2.63828300	-3.22177200
C	-1.59155800	3.28440900	-3.23662900
H	0.37375600	3.39928500	-2.37006100
C	2.33720300	3.88514600	-0.17881600
H	0.19037400	4.20568100	-0.11423400
H	1.05906300	4.60151400	1.38275000

H	4.17026400	1.28922800	-0.44825200
H	3.01311000	0.17121400	0.30278200
C	3.10495700	2.13695900	1.20846700
H	3.28559900	1.13168200	-2.78794400
H	1.53460700	1.21438200	-3.08549600
H	2.22252500	-0.17414100	-2.21907300
H	-0.26327300	3.17356800	2.92297900
H	-0.68891200	1.50675000	2.44913800
H	-1.37894600	2.87068100	1.56995000
O	3.33508900	3.46520900	0.74842000
H	-3.60505500	2.92425600	-3.92588800
H	-1.39894600	4.07607300	-3.95530700
C	2.75139700	5.25143300	-0.68430300
C	4.15884700	1.83249600	2.25204000
H	3.71861700	5.17066700	-1.18464600
H	2.83659400	5.94767100	0.15287200
H	2.01088400	5.62905300	-1.39371100
H	4.05498700	2.53065100	3.08528100
H	5.15422100	1.93768300	1.81531600
H	4.03449800	0.80990600	2.61489300
H	1.14450800	-2.37448900	-0.78571800
C	3.30401600	-2.48847500	-0.84576100
C	5.81550400	-2.63592300	-1.95536600
C	4.68226400	-2.77249800	-2.80018900
C	3.42917700	-2.69996900	-2.24397700
H	6.81385000	-2.69227500	-2.38721500
H	4.81986600	-2.92982100	-3.86489600
H	2.53276200	-2.79460900	-2.85114400
H	5.32901400	-2.04805400	1.87352200
N	5.75083800	-2.44036900	-0.65443200
C	-0.02278400	-3.26708200	2.04935400
C	-3.36677900	-1.28679800	-1.21141900
C	-4.73114100	-1.48230800	-0.95358100
C	-2.74926500	-2.01884900	-2.25442100
C	-5.48092400	-2.40036100	-1.68842900
H	-5.21111000	-0.90291200	-0.17164300
C	-3.51709000	-2.93680700	-2.97844000
C	-4.86989700	-3.13596900	-2.70250600
H	-6.53639000	-2.53541000	-1.47028500
H	-3.04225700	-3.50207500	-3.77669800
H	-5.44095000	-3.85774900	-3.27902700
C	-3.50906000	0.55240300	1.02571300
C	-3.94448300	-0.22522800	2.12767700
C	-3.89686600	1.89938400	0.95161100



C	-4.75151900	0.37541000	3.10058100
C	-4.69655400	2.48063500	1.93414200
C	-5.12802600	1.71509800	3.01543100
H	-5.08550000	-0.22415600	3.94368500
H	-4.98072000	3.52559400	1.85091400
H	-5.75068900	2.15481000	3.78894800
C	-1.30267500	-1.80069100	-2.61903200
H	-1.17661900	-0.87938600	-3.19960500
H	-0.68957600	-1.67388400	-1.71620300
H	-0.91243900	-2.63402400	-3.21027000
C	-3.56702800	-1.67654100	2.27048100
H	-4.11919500	-2.30716100	1.56472900
H	-2.50609100	-1.81156000	2.03625100
H	-3.76862400	-2.03966800	3.28189700
H	-3.56869800	2.50176400	0.11292100
N	0.67439500	-1.95442400	1.77118500
C	0.85081200	-4.25683700	2.82812900
H	1.25880100	-3.81939200	3.74384200
H	0.25382500	-5.12748400	3.11543100
H	1.68682400	-4.60807100	2.21634900
C	-0.58576200	-3.90106100	0.78074800
H	-1.17766700	-3.16776500	0.22569300
H	0.20953800	-4.28288700	0.13442700
H	-1.22908500	-4.74475100	1.04993100
C	0.70452700	-1.11721000	2.99294500
H	-0.32700100	-0.87961700	3.25974800
H	1.17449300	-1.61758800	3.85135300
H	1.23124300	-0.18725600	2.77435000
H	-0.87031100	-2.97922400	2.67841600

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Ni	0.01382300	-0.84685200	0.40487600
P	0.53307800	1.25391900	-0.31698300
P	-2.29351800	-0.07507000	-0.08299900
C	1.81136800	-1.41295500	0.43621000
C	2.41759300	-1.89568100	-0.71135500
C	2.59415000	-1.35828900	1.62777100
C	-0.83093700	1.97427800	-1.33561000
C	-2.08303200	1.33104900	-1.25459100
C	2.13134800	1.85371200	-1.14586700
C	0.77655500	2.37817200	1.19186200
C	3.91360000	-1.75163500	1.65196800
H	2.14329000	-0.97898100	2.54041200
O	2.11464800	3.29100200	-1.28838800

O	2.01846600	1.97370700	1.78934900
C	-3.14186100	1.75101500	-2.07192700
C	-0.67987300	3.04582700	-2.23548600
C	0.87239400	3.83946900	0.75294100
C	3.30584400	1.49632600	-0.23315100
C	2.29163600	1.27106900	-2.54006400
C	-0.29410500	2.14176800	2.23982500
C	4.54806000	-2.23216200	0.47587600
H	-4.09547300	1.23711800	-2.00917900
C	-2.97580800	2.80738800	-2.96280400
C	-1.74138500	3.45470500	-3.03978200
H	0.27642500	3.54501400	-2.30984500
C	2.14609400	4.05383300	-0.07416900
H	-0.01438000	4.13261500	0.18631300
H	0.93943600	4.47085500	1.64522000
H	4.22792000	1.78903300	-0.74599500
H	3.33963000	0.43043000	-0.02978600
C	3.21493000	2.29172000	1.06980800
H	3.19549400	1.68219500	-2.99965400
H	1.43698500	1.50870600	-3.17759400
H	2.39304500	0.18585000	-2.46852600
H	-0.04456800	2.70720500	3.14303700
H	-0.35564000	1.07958000	2.49073800
H	-1.27207400	2.46625300	1.87957900
O	3.24844300	3.67915000	0.73537800
H	-3.80143000	3.12083100	-3.59452700
H	-1.59932000	4.27771000	-3.73393300
C	2.36049500	5.49243900	-0.49399300
C	4.36326100	2.02678200	2.01721200
H	3.28535600	5.56404500	-1.06982900
H	2.43872200	6.12866100	0.39011600
H	1.52522500	5.83299800	-1.11085400
H	4.23386400	2.62901300	2.91887100
H	5.30667900	2.29585800	1.53725700
H	4.38270300	0.96844400	2.28130600
H	1.85700600	-1.97376700	-1.64148000
C	3.77643000	-2.31011800	-0.72742800
C	6.42637600	-3.04068700	-0.56966800
C	5.75426300	-3.16366900	-1.81147300
C	4.43089400	-2.79785000	-1.88645000
H	7.47566900	-3.32499300	-0.49740300
H	6.28687100	-3.54113600	-2.67873200
H	3.87607900	-2.87507100	-2.81863400
H	4.50773500	-1.70803800	2.55999400

N	5.86178800	-2.59605300	0.53604000
C	-0.41414200	-3.78012000	1.08111300
C	-1.45042400	-4.51070700	1.96644300
H	-1.22069300	-4.36259000	3.02732900
H	-2.45598100	-4.12579100	1.78003500
C	-3.39518900	-1.15728400	-1.07522800
C	-4.71897900	-1.40546000	-0.69047800
C	-2.87831500	-1.75681800	-2.24771300
C	-5.53181200	-2.25868400	-1.43543800
H	-5.11822200	-0.91799400	0.19189500
C	-3.71123700	-2.61080900	-2.97788500
C	-5.02261800	-2.86888800	-2.58004400
H	-6.55443900	-2.44296700	-1.12090100
H	-3.31890600	-3.08179500	-3.87515400
H	-5.64283000	-3.54160100	-3.16468700
C	-3.37180200	0.65341600	1.22497400
C	-3.73394900	-0.12696300	2.34773700
C	-3.76305300	2.00043000	1.16377300
C	-4.47595600	0.48326500	3.36798600
C	-4.49409100	2.58656300	2.19521800
C	-4.85098200	1.82349200	3.30499400
H	-4.75520900	-0.11397800	4.23158800
H	-4.77838900	3.63232900	2.12885500
H	-5.41663400	2.26785700	4.11860300
C	-1.48421000	-1.46965100	-2.74727900
H	-1.44673000	-0.51024500	-3.27540100
H	-0.76337100	-1.41079400	-1.92339000
H	-1.14862100	-2.25069600	-3.43372700
C	-3.36579600	-1.58046400	2.45555100
H	-4.02213500	-2.19539600	1.82743200
H	-2.33138900	-1.77936600	2.13012100
H	-3.47616300	-1.93317100	3.48462800
H	-3.48689800	2.60431600	0.30851500
N	-0.42670600	-2.35427500	1.46719700
H	0.18024400	-2.28285700	2.28574700
C	0.95482200	-4.45976200	1.29085000
H	1.29121300	-4.33327200	2.32657500
H	0.89078500	-5.53600300	1.09055700
H	1.71493200	-4.03363600	0.63613100
C	-0.83183100	-3.92440900	-0.38429800
H	-1.79640700	-3.44255900	-0.55830100
H	-0.08644800	-3.46247000	-1.03703600
H	-0.92274600	-4.98003400	-0.66306200
H	-1.45105200	-5.58907700	1.76702000

**TS19**

Ni	0.07158600	0.76448600	0.36707800
P	-0.51733300	-1.26316700	-0.29183600
P	2.32488300	0.01095300	-0.06830700
C	-1.58872500	1.68641100	0.57913800
C	-2.23097200	2.13485600	-0.58772400
C	-2.41468500	1.50285000	1.74838100
C	0.82583600	-1.99854900	-1.32760700
C	2.10000200	-1.39782300	-1.23071100
C	-2.13231700	-1.70202500	-1.17171900
C	-0.84141300	-2.46430300	1.13732600
C	-3.75558500	1.77168300	1.74209100
H	-1.95479400	1.12599400	2.65879100
O	-2.23081900	-3.12498100	-1.40064100
O	-2.04936500	-2.00843400	1.76665900
C	3.15039000	-1.84513300	-2.04380700
C	0.64275500	-3.04652100	-2.24739100
C	-1.05066500	-3.88398300	0.61076800
C	-3.26609200	-1.28914000	-0.23099800
C	-2.23175600	-1.02300300	-2.52617600
C	0.25067100	-2.37295000	2.18532300
C	-4.41599600	2.22333600	0.55924500
H	4.12020200	-1.36304300	-1.97098900
C	2.95340500	-2.88423100	-2.94970800
C	1.69592000	-3.48227800	-3.04954500
H	-0.33462000	-3.50067200	-2.34388900
C	-2.33201000	-3.94686300	-0.23078800
H	-0.18601000	-4.21599000	0.03159300
H	-1.17551700	-4.55927400	1.46400800
H	-4.21655600	-1.44105500	-0.75265900
H	-3.18122600	-0.24036400	0.04152600
C	-3.25991100	-2.17337900	1.01735100
H	-3.16632300	-1.32024000	-3.01151800
H	-1.39752400	-1.29992800	-3.17551600
H	-2.23412400	0.06043700	-2.38483100
H	-0.02649900	-2.97719400	3.05483000
H	0.38797700	-1.33511400	2.49996400
H	1.20038800	-2.73798200	1.78871800
O	-3.40674100	-3.52925400	0.59420600
H	3.77274200	-3.21977400	-3.57834800
H	1.52980000	-4.28644600	-3.76024700
C	-2.65882200	-5.33932000	-0.72771500
C	-4.39346300	-1.87674500	1.97276500

H	-3.58433600	-5.30537200	-1.30589000
H	-2.79030600	-6.01412100	0.12083400
H	-1.85121200	-5.71178100	-1.36286100
H	-4.33023800	-2.55326700	2.82774700
H	-5.35039200	-2.02302400	1.46747700
H	-4.32270800	-0.84345100	2.31365000
H	-1.66627800	2.27554900	-1.50465000
C	-3.62077600	2.40002400	-0.62191800
C	-6.35061200	2.83907200	-0.51453900
C	-5.66771300	3.04507500	-1.73515600
C	-4.30890600	2.82723500	-1.78841100
H	-7.42509300	3.00663700	-0.45801800
H	-6.21773300	3.37079900	-2.61312800
H	-3.75226300	2.97549900	-2.71096900
H	-4.36402100	1.63335000	2.63106800
N	-5.75383400	2.44146500	0.59870300
C	0.28155400	3.89182400	0.77862500
C	1.41334000	4.43823500	1.67196700
H	1.15434200	4.34640000	2.73291200
H	2.34354600	3.89444300	1.49554600
C	3.52634800	1.05370400	-0.98072300
C	4.80812000	1.31071500	-0.47478900
C	3.11253600	1.66272300	-2.18980700
C	5.67933100	2.17318800	-1.13859700
H	5.12818000	0.82358100	0.44008500
C	4.00373100	2.52441500	-2.83775500
C	5.27320300	2.78579800	-2.32283900
H	6.66822900	2.36191300	-0.73199100
H	3.69045400	2.99941600	-3.76365000
H	5.94026600	3.46421400	-2.84605300
C	3.29256700	-0.73114000	1.31180600
C	3.50485200	0.02233100	2.48948600
C	3.74519800	-2.05793000	1.25279000
C	4.15986600	-0.58812400	3.56569500
C	4.39171100	-2.64748000	2.33758800
C	4.59757500	-1.90964800	3.50155700
H	4.32224800	-0.01001900	4.47133200
H	4.72865300	-3.67746700	2.27081300
H	5.09473600	-2.35862900	4.35615500
C	1.76505300	1.38157800	-2.80898300
H	1.77368700	0.43295900	-3.35700000
H	0.97854300	1.30390500	-2.04948800
H	1.48521200	2.17553000	-3.50560900
C	3.07501700	1.46071200	2.59371200

H	3.74035100	2.10799500	2.01021500
H	2.06596100	1.61763400	2.20001600
H	3.10372600	1.80622600	3.63015300
H	3.58371900	-2.64176400	0.35481600
N	0.01632000	2.50061000	1.19038400
H	-0.24167400	2.48724200	2.17134400
C	-0.96624500	4.77918800	0.96731100
H	-1.30347400	4.74538500	2.00930100
H	-0.73964600	5.82196300	0.72003800
H	-1.78952400	4.44252600	0.33670100
C	0.75520400	3.92953900	-0.67542600
H	1.65026100	3.31629400	-0.79519500
H	-0.01612800	3.56540300	-1.35567700
H	1.00201500	4.95610900	-0.96531200
H	1.58819300	5.49947800	1.46182900

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Ni	-0.38004100	-0.71609300	0.33529400
P	0.46969400	1.13913200	-0.25288300
P	-2.37162400	-0.01935000	-0.04296600
C	1.72371300	-2.47944500	0.75820300
C	2.38485800	-2.61156200	-0.45125900
C	2.48424800	-2.21566300	1.93437700
C	-0.81372800	1.88823200	-1.37583900
C	-2.11773200	1.34880700	-1.26954200
C	2.11168900	1.38572600	-1.16789800
C	0.89369800	2.49388600	1.01765100
C	3.84789100	-2.07591000	1.88783400
H	1.96055200	-2.11091400	2.88118200
O	2.37331800	2.75457500	-1.55290300
O	2.05526200	2.01896600	1.73011300
C	-3.13155500	1.80244700	-2.12253300
C	-0.56816400	2.86869300	-2.35171800
C	1.24647500	3.81910900	0.33995700
C	3.18251900	0.95398100	-0.16048200
C	2.15585100	0.56682800	-2.44628600
C	-0.20409300	2.65383900	2.05063700
C	4.54721600	-2.18809300	0.65603300
H	-4.12124500	1.35998300	-2.05342700
C	-2.87329900	2.78193300	-3.08055900
C	-1.58743800	3.31111000	-3.19561900
H	0.43447200	3.26136700	-2.46609200
C	2.53655500	3.67611700	-0.47615000
H	0.42434500	4.16222000	-0.29131900

H	1.42352500	4.57190900	1.11626400
H	4.15509700	0.90725600	-0.66171700
H	2.94574600	-0.02896800	0.24116300
C	3.27016900	1.97146000	0.98032400
H	3.13248000	0.68091100	-2.92763400
H	1.37962600	0.89021500	-3.14469700
H	1.99717500	-0.48718500	-2.20847600
H	0.08818200	3.41076100	2.78611300
H	-0.37636000	1.70987400	2.56880500
H	-1.14045300	2.96041300	1.57747500
O	3.56333600	3.24622800	0.40977600
H	-3.66697800	3.11894800	-3.74122300
H	-1.37216300	4.06240000	-3.95014200
C	3.00337000	4.97446000	-1.10112600
C	4.36838700	1.66189700	1.97490200
H	3.92350000	4.79212200	-1.66025100
H	3.19767800	5.71438200	-0.32170700
H	2.24034100	5.35977600	-1.78213000
H	4.39918500	2.44754000	2.73288200
H	5.33296300	1.61126500	1.46562100
H	4.16820800	0.70170100	2.45325700
H	1.82985100	-2.76606100	-1.36641200
C	3.78994000	-2.46469400	-0.52681000
C	6.51713000	-2.06780000	-0.51412200
C	5.86619500	-2.33144800	-1.74484300
C	4.50611200	-2.53220100	-1.74967300
H	7.59411700	-1.90840300	-0.49783600
H	6.44382200	-2.36971900	-2.66281500
H	3.96858700	-2.72992100	-2.67323500
H	4.42756900	-1.87118500	2.78132300
N	5.89449500	-1.99752200	0.64789900
C	-0.39124700	-3.86841300	0.46214300
C	-1.78958200	-3.81413300	1.08690200
H	-1.73044800	-3.76527000	2.18059100
H	-2.33695600	-2.94236700	0.72292100
C	-3.78020600	-0.96216300	-0.77143900
C	-4.92771700	-1.22893300	-0.00656700
C	-3.62550000	-1.60411500	-2.02632600
C	-5.91100700	-2.10770000	-0.45729300
H	-5.04963700	-0.73839500	0.95335500
C	-4.62589400	-2.47989600	-2.46038800
C	-5.76123100	-2.73747100	-1.69190400
H	-6.79022700	-2.29437100	0.15267600
H	-4.50758800	-2.97024400	-3.42375600

H	-6.51875200	-3.42577500	-2.05489200
C	-3.17645300	0.87875500	1.36880200
C	-2.90862300	0.50533600	2.70473800
C	-4.01669500	1.97533400	1.12596000
C	-3.49102600	1.24554800	3.74165500
C	-4.58789900	2.70166600	2.16871500
C	-4.32183100	2.33423000	3.48639800
H	-3.27723900	0.96363400	4.76920100
H	-5.23027100	3.54974000	1.95098300
H	-4.75225200	2.89362600	4.31177200
C	-2.43235700	-1.35335500	-2.91678800
H	-2.57106700	-0.45125800	-3.52214500
H	-1.51903600	-1.19302000	-2.33433900
H	-2.27067300	-2.19532200	-3.59585300
C	-2.00154000	-0.64639000	3.05632800
H	-2.44698100	-1.60718600	2.78336400
H	-1.05055600	-0.56397700	2.50673700
H	-1.78961800	-0.65917500	4.12925900
H	-4.21712500	2.27613500	0.10462300
N	0.30296000	-2.58868100	0.89007000
H	0.09179100	-2.48577800	1.88131600
C	0.37889400	-5.08610700	0.99080500
H	0.45418300	-5.05942600	2.08354200
H	-0.13790200	-6.00880300	0.71075800
H	1.39102400	-5.12406800	0.58036900
C	-0.53389800	-3.92646700	-1.06124500
H	-0.89647600	-2.96723800	-1.43099400
H	0.40816500	-4.17113700	-1.55529000
H	-1.25779500	-4.70048400	-1.33240700
H	-2.34895900	-4.71601900	0.82533200

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Ni	-0.00360600	0.54664200	-0.49929600
P	0.50836800	-1.46490700	0.35820300
P	-2.26580900	-0.08516300	-0.07238600
C	1.82552300	1.09926200	-0.59649400
C	2.37863100	1.82903100	0.44041600
C	2.62134700	0.87782200	-1.75964200
C	-0.92126200	-2.12346700	1.32851800
C	-2.16322000	-1.49128200	1.11666800
C	2.05123200	-1.94686800	1.34825400
C	0.87075200	-2.71655000	-1.01990200
C	3.90850400	1.35984800	-1.86063200
H	2.20889700	0.29937400	-2.58127000



O	2.03566000	-3.36414300	1.62620300
O	2.14733400	-2.35327500	-1.56515900
C	-3.28997400	-1.89536200	1.84614500
C	-0.84133700	-3.15381100	2.28356000
C	0.95133500	-4.12844400	-0.44040300
C	3.28378700	-1.65899000	0.48835300
C	2.09447400	-1.22752000	2.68515700
C	-0.13107500	-2.58582000	-2.15084400
C	4.49200800	2.09454500	-0.79455700
H	-4.23666400	-1.39087000	1.68389600
C	-3.19784300	-2.91992500	2.78338800
C	-1.96864500	-3.54439100	3.00265600
H	0.11066600	-3.63192800	2.46833600
C	2.16228900	-4.23960400	0.49509900
H	0.02786900	-4.39139300	0.07958700
H	1.09788100	-4.83560000	-1.26354000
H	4.16939800	-1.88889200	1.08973300
H	3.32345400	-0.61613800	0.18654600
C	3.29328400	-2.57817000	-0.73412800
H	2.97185900	-1.55989400	3.24804400
H	1.20088000	-1.43276900	3.27976400
H	2.16920000	-0.15071400	2.51471000
H	0.16401500	-3.24143300	-2.97597600
H	-0.16464600	-1.55393000	-2.51031500
H	-1.13301800	-2.86560100	-1.81869700
O	3.31693300	-3.92550300	-0.26402800
H	-4.07578200	-3.22183200	3.34630500
H	-1.88312100	-4.33528900	3.74185600
C	2.35854200	-5.62768800	1.06654700
C	4.50332200	-2.38816000	-1.62070900
H	3.23822300	-5.62854900	1.71315700
H	2.50866900	-6.34350500	0.25565800
H	1.48266300	-5.92257600	1.64969500
H	4.44557300	-3.08092900	-2.46278000
H	5.41281400	-2.59020500	-1.05085700
H	4.52974900	-1.36191300	-1.98965900
H	1.79557600	2.05562100	1.33107900
C	3.70410500	2.33591700	0.37545200
C	6.28657600	3.23733400	0.07000000
C	5.59092300	3.54323900	1.26637300
C	4.30108000	3.09080800	1.41569700
H	7.31053000	3.58668000	-0.05905400
H	6.07923500	4.12622500	2.04092200
H	3.72735100	3.30547100	2.31390700

H	4.51352100	1.19568500	-2.74751000
N	5.77353000	2.54486000	-0.92817500
C	-3.36263500	1.03311400	0.88397700
C	-4.70666800	1.20894600	0.53311400
C	-2.82697500	1.71438900	2.00184700
C	-5.52780600	2.06729600	1.26350300
H	-5.11094400	0.66960300	-0.31679000
C	-3.66952800	2.56889800	2.71946200
C	-5.00415100	2.75279000	2.35765400
H	-6.56633700	2.19830600	0.97585300
H	-3.26453100	3.10530100	3.57284100
H	-5.63064100	3.42998000	2.93026800
C	-3.29644600	-0.74533100	-1.44489300
C	-3.64592700	0.09047800	-2.53345900
C	-3.66337300	-2.10008500	-1.46198400
C	-4.35221500	-0.48178700	-3.60002300
C	-4.35827800	-2.64515100	-2.53975300
C	-4.70262800	-1.83037500	-3.61588800
H	-4.62451400	0.15381300	-4.43793700
H	-4.62593600	-3.69729700	-2.53417900
H	-5.24191600	-2.24030400	-4.46466100
C	-1.39056300	1.54602200	2.42562200
H	-1.19274100	0.52776100	2.77855300
H	-0.71047500	1.74444100	1.58881500
H	-1.13973200	2.24094400	3.22988900
C	-3.30493400	1.55607400	-2.56766700
H	-3.92470900	2.12046800	-1.86140000
H	-2.25336400	1.74469700	-2.30259200
H	-3.48731900	1.96712100	-3.56398200
H	-3.40094900	-2.73982600	-0.62797900
N	-0.32619800	2.16001900	-1.57934200
H	0.45398800	2.17159200	-2.23303900
C	-0.31969300	3.38912600	-0.91352800
C	0.76308600	4.29340200	-0.99835600
C	-1.42935400	3.77850000	-0.13466500
C	0.73764100	5.51130300	-0.32423100
H	1.63222300	4.01659600	-1.58868400
C	-1.44338800	4.98993900	0.54830700
H	-2.28723100	3.12222800	-0.08754200
C	-0.35871600	5.86797400	0.46557500
H	1.58899500	6.18216800	-0.40673600
H	-2.31602100	5.25286300	1.14134200
H	-0.37162100	6.81508900	0.99643500

**TS22**

Ni	-0.12045000	0.45622100	-0.53489000
P	0.97476600	-1.30851300	0.17440700
P	-2.09786700	-0.68722600	0.07752000
C	1.18679300	1.89241300	-0.74116000
C	1.48638500	2.58018500	0.44388400
C	2.16095300	1.91931800	-1.80094000
C	-0.13813400	-2.36443800	1.20512100
C	-1.51983300	-2.08881200	1.12762300
C	2.62985600	-1.27688400	1.07653700
C	1.62173000	-2.40318100	-1.22393200
C	3.36198600	2.55810200	-1.65465300
H	1.94145600	1.39177600	-2.72605400
O	3.11824900	-2.61206200	1.33070100
O	2.66082300	-1.64035700	-1.86131100
C	-2.42375600	-2.81065700	1.91949200
C	0.30387200	-3.35915700	2.09563900
C	2.21690300	-3.69977600	-0.67585400
C	3.61137600	-0.57626900	0.13551400
C	2.51489300	-0.57552300	2.41858400
C	0.54366500	-2.63279100	-2.26741700
C	3.70778200	3.21096500	-0.43349500
H	-3.48187700	-2.57448600	1.86695400
C	-1.97287300	-3.80228700	2.78653700
C	-0.60533000	-4.06937400	2.87715800
H	1.36486100	-3.54969600	2.19017500
C	3.45656500	-3.38832700	0.17480700
H	1.47534100	-4.25568100	-0.09809100
H	2.53611300	-4.32251300	-1.51839700
H	4.56360400	-0.45253900	0.66140700
H	3.24237000	0.40573400	-0.15206400
C	3.86112100	-1.44536700	-1.10126300
H	3.48932800	-0.58069300	2.91631500
H	1.78923200	-1.07424500	3.06630200
H	2.20251500	0.46032900	2.25955400
H	0.95600900	-3.19870600	-3.10872900
H	0.16476300	-1.67465500	-2.63301600
H	-0.29386000	-3.19157000	-1.84058700
O	4.37903900	-2.69759700	-0.65265400
H	-2.68145200	-4.35250600	3.39825500
H	-0.24267200	-4.82693900	3.56559200
C	4.15721600	-4.62559600	0.69492900
C	4.87461600	-0.85716900	-2.05686900
H	5.02932500	-4.32439900	1.27862900

H	4.48267600	-5.24725900	-0.14193700
H	3.48099700	-5.20253000	1.33074900
H	5.01741800	-1.54100100	-2.89620800
H	5.82721200	-0.71255700	-1.54308100
H	4.51628500	0.10540800	-2.42313400
H	0.75959300	2.62844600	1.24928000
C	2.73721400	3.21650800	0.62348600
C	5.23845600	4.38037000	0.81704400
C	4.35894500	4.45082900	1.92244400
C	3.11345200	3.87265600	1.82543700
H	6.22747400	4.83157100	0.88075900
H	4.67281000	4.95712100	2.83038400
H	2.41043100	3.90908800	2.65408000
H	4.09923400	2.56759700	-2.45182800
N	4.93231400	3.78517800	-0.32474500
C	-3.34768300	0.06407800	1.19868200
C	-4.70613000	0.10663900	0.85851200
C	-2.90729000	0.67210300	2.39966700
C	-5.62813800	0.76813100	1.66876000
H	-5.04561600	-0.38304000	-0.04777800
C	-3.84957000	1.33185400	3.19483500
C	-5.19688500	1.39097700	2.83765500
H	-6.67553000	0.79533100	1.38418600
H	-3.51562400	1.80678900	4.11360200
H	-5.90311300	1.91715300	3.47264000
C	-3.06676200	-1.49110900	-1.26165800
C	-3.62411000	-0.69078400	-2.28871400
C	-3.18460100	-2.88687600	-1.33111000
C	-4.30402400	-1.32972200	-3.33200900
C	-3.85332400	-3.50105700	-2.38907000
C	-4.42051800	-2.71799700	-3.39145000
H	-4.74104500	-0.71948800	-4.11763200
H	-3.93059100	-4.58347600	-2.42400600
H	-4.94725100	-3.18242700	-4.21972200
C	-1.47109900	0.60541700	2.86147900
H	-1.24517300	-0.36895000	3.30823900
H	-0.76377000	0.73873800	2.03409800
H	-1.26739100	1.37656000	3.60851800
C	-3.49128500	0.80961700	-2.28977400
H	-3.97985700	1.27075700	-1.42600000
H	-2.44004400	1.10468400	-2.23990800
H	-3.93211800	1.23942200	-3.19231500
H	-2.74963700	-3.50191200	-0.55247600
N	-0.46613900	2.10794400	-1.47679900

H	-0.18641200	2.19386000	-2.44536500
C	-1.28004200	3.15977700	-1.06638400
C	-1.54793400	4.24739600	-1.91901500
C	-1.86776600	3.14708200	0.20902000
C	-2.40368900	5.26638500	-1.51285600
H	-1.08809900	4.27791500	-2.90400000
C	-2.72066400	4.17115700	0.60917000
H	-1.67526300	2.30703600	0.85972600
C	-2.99891700	5.23750800	-0.24749600
H	-2.60597700	6.09217700	-2.18921600
H	-3.17980800	4.12112600	1.59243900
H	-3.66641200	6.03492700	0.06321500

### 23

Ni	-0.24565600	0.16135900	-0.67876700
P	1.57300000	-0.65316800	0.03575400
P	-1.43172100	-1.18683000	0.50474700
C	-0.18510200	2.68132300	-1.24661600
C	-0.62166400	3.34291300	-0.11456900
C	1.08714600	2.99654200	-1.80364400
C	1.10806100	-1.44721400	1.65841200
C	-0.27353600	-1.67356800	1.86290000
C	3.23088400	0.19663200	0.39170100
C	2.40440900	-2.02005800	-0.99009300
C	1.91075600	3.91568300	-1.20824000
H	1.40083300	2.48479600	-2.70981400
O	4.22786200	-0.69158900	0.95123500
O	3.00391000	-1.35452100	-2.12373900
C	-0.72553800	-2.19461100	3.08197200
C	1.99980400	-1.75602200	2.69929100
C	3.50470100	-2.73020400	-0.20110800
C	3.74175900	0.67454800	-0.97120500
C	3.05730900	1.33968400	1.37659300
C	1.38230500	-2.98685000	-1.55452600
C	1.51567600	4.57483100	-0.01011600
H	-1.79034000	-2.34786500	3.23109600
C	0.17278100	-2.49162400	4.10588400
C	1.53649200	-2.26903100	3.91115900
H	3.05699600	-1.56769800	2.56235200
C	4.65160200	-1.75956500	0.10548800
H	3.10321900	-3.15815400	0.71993000
H	3.90883000	-3.54423600	-0.81308900
H	4.63183600	1.29445000	-0.81773900
H	2.97907300	1.27039600	-1.47132500

C	4.13171000	-0.52826100	-1.83711100
H	4.01379200	1.84904400	1.53117400
H	2.69583000	0.97367500	2.34077300
H	2.33511700	2.05847800	0.98309500
H	1.87629700	-3.69007700	-2.23319400
H	0.60506500	-2.44742700	-2.10048400
H	0.90094900	-3.54867100	-0.75094800
O	5.13522700	-1.26072600	-1.13782000
H	-0.19004400	-2.88592600	5.05069900
H	2.24334500	-2.48714300	4.70668500
C	5.82346500	-2.41332500	0.80772600
C	4.72021800	-0.13907200	-3.17711000
H	6.60018500	-1.66575000	0.98157900
H	6.22843700	-3.21533500	0.18686900
H	5.50238200	-2.82694700	1.76690100
H	4.98992300	-1.04309800	-3.72702100
H	5.61329900	0.47202100	-3.02933100
H	3.98570600	0.42647300	-3.75563600
H	-1.59780800	3.14367500	0.30443800
C	0.22295400	4.28161500	0.52994300
C	1.99444300	6.04809900	1.68334300
C	0.74027700	5.83270500	2.30162900
C	-0.14499100	4.95179300	1.72273700
H	2.70391100	6.74262000	2.13055100
H	0.49204600	6.35968900	3.21732500
H	-1.11851400	4.75743800	2.16494700
H	2.88447300	4.15580600	-1.62059100
N	2.37973300	5.45065300	0.56942700
C	-2.96717500	-0.74662900	1.42684100
C	-4.18523200	-1.38170400	1.14130500
C	-2.96286200	0.38377100	2.28427900
C	-5.38613500	-0.91999600	1.67810200
H	-4.19095500	-2.24824100	0.48918100
C	-4.17873400	0.82940900	2.81316400
C	-5.38538300	0.19310100	2.51723500
H	-6.31537600	-1.43011500	1.44159100
H	-4.17592900	1.69647000	3.46907300
H	-6.31358200	0.56473900	2.94115200
C	-1.87011300	-2.80902400	-0.26796400
C	-2.44897000	-2.83164600	-1.55861000
C	-1.57616900	-4.02257100	0.36995100
C	-2.71333200	-4.07054500	-2.15418000
C	-1.84213800	-5.24675000	-0.24194300
C	-2.41366100	-5.27101600	-1.51205900

H	-3.15699600	-4.08833800	-3.14616000
H	-1.60235000	-6.17236200	0.27295100
H	-2.62384100	-6.21649800	-2.00331900
C	-1.68990800	1.11665200	2.63001400
H	-1.09828400	0.56395100	3.36685900
H	-1.04660300	1.24034600	1.75034300
H	-1.90800200	2.10534300	3.04316400
C	-2.77797700	-1.56580200	-2.30638900
H	-3.51504700	-0.95504600	-1.77638200
H	-1.88341900	-0.94207500	-2.41364700
H	-3.17487600	-1.79022600	-3.29977500
H	-1.12496800	-4.01316600	1.35487100
N	-0.96213100	1.66996300	-1.90766600
H	-0.53980500	1.46393200	-2.80800800
C	-2.38709100	1.82208500	-2.06569300
C	-2.91457300	2.03501500	-3.34040400
C	-3.24431200	1.68641700	-0.97258200
C	-4.29741600	2.09943300	-3.52078400
H	-2.24592800	2.14212700	-4.19106300
C	-4.62250800	1.77310100	-1.15197100
H	-2.83842300	1.44604100	-0.00254500
C	-5.15508900	1.97367900	-2.42768200
H	-4.70055700	2.25133200	-4.51736900
H	-5.27271400	1.64778200	-0.29213600
H	-6.23007000	2.02242300	-2.57020800

**24**

Ni	-0.09243100	1.07173100	-0.32208200
Cl	-0.65349200	3.19626600	-0.84046400
P	0.45952700	-0.95240200	0.39437300
P	-2.28885300	0.38527100	-0.02454400
C	1.73229600	1.59182600	-0.53645300
C	2.38640800	1.34527700	-1.77488600
C	-0.93711500	-1.54051200	1.46520800
C	-2.17435700	-0.88195100	1.29807000
C	2.03443700	-1.41147000	1.35045700
C	0.77292900	-2.24589500	-0.95853600
C	3.69887600	1.71669800	-1.97131000
C	3.78755700	2.62304400	0.30348200
O	2.00453900	-2.81980400	1.67012900
O	2.03662900	-1.90684400	-1.54454100
C	-3.25664700	-1.18609200	2.13214000
C	-0.82710300	-2.51999300	2.46732600
C	0.85458600	-3.63858100	-0.33306100

C	3.24512400	-1.16799400	0.44824100
C	2.12796800	-0.65900900	2.66611300
C	-0.24585100	-2.15462200	-2.07701900
H	4.18580500	1.52625500	-2.92545400
C	4.44440400	2.34587700	-0.93912800
H	-4.19248500	-0.65198000	2.00217700
C	-3.12890200	-2.15214400	3.12772200
C	-1.91384100	-2.81919500	3.28854100
H	0.11752000	-3.02464200	2.61615700
C	2.09253700	-3.73335400	0.56667700
H	-0.05511700	-3.86882000	0.22576700
H	0.96335700	-4.37558900	-1.13555800
H	4.14302800	-1.39307200	1.03285200
H	3.29317100	-0.13572700	0.11522600
C	3.20580800	-2.12305200	-0.74417100
H	3.01729800	-0.99394800	3.20813000
H	1.25084300	-0.83579300	3.29264700
H	2.21625300	0.41092800	2.46728700
H	0.06005200	-2.81935100	-2.89061000
H	-0.30279400	-1.13303300	-2.45960900
H	-1.23726600	-2.45103600	-1.73092700
O	3.22683000	-3.45688500	-0.23661200
H	-3.96938100	-2.37859400	3.77662300
C	2.29245000	-5.10369500	1.17825900
C	4.38724000	-1.97208300	-1.67515700
H	3.19115000	-5.09211500	1.79802500
H	2.41144100	-5.84773400	0.38786000
H	1.43181100	-5.36977600	1.79685300
H	4.30058300	-2.69544100	-2.48857100
H	5.31435900	-2.15488200	-1.12765600
H	4.40031300	-0.95984400	-2.08191700
H	1.85288100	0.84192000	-2.57497600
C	4.52681300	3.25571000	1.33864200
H	4.02509000	3.47087700	2.27880900
C	6.49896500	3.31332100	-0.06800700
H	7.54259700	3.58415200	-0.19769500
C	5.84948800	3.59161100	1.16001900
H	6.40142100	4.07447800	1.96132100
C	2.42715500	2.24228700	0.46266900
H	1.93729500	2.48816200	1.40230800
H	-1.80340500	-3.56901600	4.06613800
C	-3.50390700	1.58334000	0.62974300
C	-4.75683000	1.72346200	0.02068200
C	-3.16242300	2.37752400	1.74937900



C	-5.68383000	2.64640900	0.50292900
H	-5.00833300	1.10591100	-0.83446300
C	-4.11302100	3.28915500	2.21840900
C	-5.35832400	3.43149900	1.60611300
H	-6.64983400	2.74750100	0.01812200
H	-3.86385000	3.90553100	3.07756000
H	-6.06985900	4.15528400	1.99219700
C	-3.16092800	-0.50240900	-1.38125700
C	-3.74907500	-1.75448600	-1.14761400
C	-3.18454700	0.04955100	-2.68319500
C	-4.35074300	-2.47102700	-2.18027600
C	-3.79846600	-0.68770600	-3.70344400
C	-4.37203900	-1.93539000	-3.46623200
H	-4.79727600	-3.43958500	-1.97742800
H	-3.81827900	-0.26844700	-4.70535200
H	-4.83356600	-2.48363200	-4.28205000
C	-1.82410600	2.27064700	2.43379900
H	-1.63792400	1.25971300	2.81130800
H	-1.02287400	2.52317600	1.73087100
H	-1.76693400	2.96087800	3.27888200
H	-3.73022600	-2.18225300	-0.15289800
C	-2.57101100	1.38637700	-2.99514000
H	-2.97504000	2.18278200	-2.36358200
H	-1.49389900	1.39172200	-2.80522400
H	-2.73893100	1.65738600	-4.04002600
C	5.80870800	2.70607500	-1.09262700
H	6.30027000	2.49371700	-2.03879700

**25**

Ni	-0.34623100	0.09209600	0.63312400
P	-2.26983700	-0.23099100	-0.42837500
P	0.10715100	-2.16750500	0.12617400
C	-0.53971500	1.98611800	0.66271800
C	-0.08389400	2.75198900	-0.39460600
C	-1.02979800	2.65522200	1.82052800
C	-2.17127100	-1.75819200	-1.46283600
C	-1.06679200	-2.60221500	-1.22682400
C	-3.29933000	1.00125300	-1.43283600
C	-3.62659800	-0.48270200	0.87075900
C	-1.06577300	4.03035100	1.88893900
H	-1.38089200	2.06382000	2.65920200
O	-4.56277700	0.40314000	-1.79541300
O	-3.85561800	0.80935800	1.45492000
C	-0.86738200	-3.73511900	-2.02659900

C	-3.06668300	-2.08356500	-2.49759500
C	-4.91026800	-0.97412400	0.20158600
C	-3.59403900	2.20759900	-0.54027200
C	-2.60337400	1.38931200	-2.72573100
C	-3.15150800	-1.38504500	1.99375600
C	-0.60147200	4.83235400	0.81027000
H	-0.00321900	-4.36655800	-1.84748200
C	-1.76027200	-4.04568400	-3.04847500
C	-2.86030500	-3.21759500	-3.28033800
H	-3.90948300	-1.43414200	-2.69254800
C	-5.46877300	0.11686000	-0.71976700
H	-4.73197900	-1.89879400	-0.35224300
H	-5.65525200	-1.17395300	0.97885700
H	-4.14148200	2.94083800	-1.14152400
H	-2.67800300	2.66348200	-0.17493600
C	-4.49199300	1.78835700	0.62532300
H	-3.24896100	2.06621000	-3.29324600
H	-2.38756300	0.51389100	-3.34255800
H	-1.66731300	1.90275600	-2.49519600
H	-3.92331300	-1.43727600	2.76806000
H	-2.23179600	-0.99225700	2.43522700
H	-2.95392300	-2.39412700	1.62495700
O	-5.70243800	1.26934800	0.07380000
H	-1.59563600	-4.92407600	-3.66509000
H	-3.55698800	-3.44883800	-4.08060600
C	-6.78241500	-0.25708800	-1.37278100
C	-4.85809700	2.93744600	1.53723900
H	-7.11826800	0.56876900	-2.00294700
H	-7.53490100	-0.45184200	-0.60572300
H	-6.65571900	-1.15098700	-1.98845900
H	-5.50415500	2.57276800	2.33845200
H	-5.38686600	3.70601300	0.96926800
H	-3.94797500	3.36329900	1.96371600
H	0.31269700	2.27778500	-1.28959100
C	-0.09072100	4.17533500	-0.35462900
C	-0.14942500	6.99156800	-0.21516000
C	0.36212400	6.34208800	-1.36496200
C	0.39002700	4.96683100	-1.43138600
H	-0.16725700	8.07658100	-0.17389400
H	0.73286100	6.93514300	-2.19608500
H	0.78205700	4.46305400	-2.31167100
H	-1.44390800	4.52674300	2.78036800
C	2.03255100	1.10185300	1.99936800
H	1.74282700	2.10868200	1.66049700

H	2.37569300	1.23351900	3.03947500
C	3.20016300	0.55563500	1.14734900
H	3.81773700	-0.09691400	1.77169600
H	2.76463700	-0.07604500	0.37233600
C	4.08195300	1.61279900	0.45876700
O	0.94306300	0.22844900	2.00558700
C	1.70827500	-2.54879400	-0.69722500
C	2.38651200	-3.74012000	-0.39570200
C	2.21979800	-1.67813500	-1.68486300
C	3.57029500	-4.07632500	-1.04750100
H	1.97575200	-4.41166000	0.35003400
C	3.41319900	-2.03838400	-2.32520100
C	4.08491200	-3.21786100	-2.01852300
H	4.08120000	-5.00175400	-0.79989800
H	3.82573200	-1.36439100	-3.07008400
H	5.00956400	-3.46091500	-2.53283100
C	-0.14541000	-3.50291600	1.36704900
C	0.66085400	-3.54898400	2.53032200
C	-1.19579100	-4.42033000	1.21118300
C	0.37489200	-4.52963200	3.48886300
C	-1.46567800	-5.37866600	2.18649800
C	-0.67450100	-5.43326500	3.33156200
H	0.99178000	-4.57292800	4.38210300
H	-2.28729400	-6.07467100	2.04766400
H	-0.87228900	-6.17357100	4.10111400
C	1.56484000	-0.38131400	-2.09404800
H	1.41415500	-0.35815900	-3.17893200
H	0.59189500	-0.23017800	-1.62061900
H	2.19449300	0.47477300	-1.81510800
C	1.80701800	-2.59864000	2.74991100
H	2.65420600	-2.85066000	2.10147600
H	1.51985200	-1.55952100	2.52821100
H	2.15458000	-2.65206800	3.78512400
H	-1.81281300	-4.38602300	0.32142400
C	5.26741500	0.97955700	-0.28743300
C	5.50689400	-0.39821100	-0.31032400
C	6.15542100	1.80559800	-0.99563700
C	6.59290000	-0.93150800	-1.00888800
H	4.83897700	-1.07571500	0.20534500
C	7.23701600	1.28006800	-1.69814800
H	6.00613500	2.88168900	-0.99909100
C	7.46383900	-0.09781400	-1.70569300
H	6.74796800	-2.00638700	-1.00735100
H	7.90482600	1.94628700	-2.23705500

H	8.30861800	-0.51233400	-2.24805700
C	4.60979300	2.64203800	1.49620100
H	3.74481600	3.14287300	1.94605200
H	5.16603100	3.42225100	0.96211900
C	5.49710600	2.05350700	2.59551200
H	5.87226700	2.84125600	3.25655400
H	4.94603600	1.33831200	3.21365700
H	6.35913500	1.53227800	2.16785900
N	3.23754300	2.26726600	-0.57324600
H	2.42800500	2.69233100	-0.12552400
H	3.75307200	3.02980500	-1.00680100
C	-0.61939100	6.25058800	0.84663400
H	-1.00900200	6.74450000	1.73328000

### TS26

Ni	-0.34029200	0.23783600	0.25406300
P	-2.15247200	-0.82892800	-0.28403800
P	0.81334900	-1.76104600	-0.02961900
C	-0.85774600	2.08841100	0.52857500
C	-1.12733400	2.91061900	-0.57752400
C	-1.47898800	2.41579000	1.78624700
C	-1.65116600	-2.32014400	-1.25383600
C	-0.30274700	-2.72875400	-1.13211800
C	-3.59627100	-0.05946000	-1.22241400
C	-3.25225000	-1.42177200	1.14328000
C	-2.35401200	3.45936800	1.88616200
H	-1.24489600	1.80823000	2.65416300
O	-4.64851900	-1.02255900	-1.44834600
O	-3.82591500	-0.23860100	1.72040200
C	0.16844300	-3.81462800	-1.88193800
C	-2.49169400	-3.01626700	-2.13935200
C	-4.37407100	-2.31762500	0.61637500
C	-4.14132300	1.05641400	-0.32712000
C	-3.16017800	0.45622000	-2.58231500
C	-2.43493800	-2.07813500	2.23824200
C	-2.68878100	4.27454600	0.76001200
H	1.20786400	-4.11281400	-1.79045800
C	-0.67942300	-4.49873300	-2.75043000
C	-2.00856900	-4.09353000	-2.88071300
H	-3.51639300	-2.68972000	-2.26081700
C	-5.31987100	-1.50448100	-0.27818500
H	-3.96698900	-3.17565700	0.07690500
H	-4.95374300	-2.68844600	1.46857200
H	-4.90701900	1.60450000	-0.88542100

H	-3.35062700	1.75022800	-0.05146700
C	-4.78965300	0.45699100	0.92113200
H	-4.02519000	0.87452100	-3.10585100
H	-2.73297800	-0.34253300	-3.19398700
H	-2.41445200	1.24329900	-2.44477900
H	-3.08425100	-2.30275400	3.09032800
H	-1.63327700	-1.41316100	2.56845700
H	-1.98421300	-3.00646000	1.88233500
O	-5.82554000	-0.43072200	0.49739700
H	-0.30195100	-5.33657400	-3.32898200
H	-2.67164000	-4.61168600	-3.56720900
C	-6.50853400	-2.29869500	-0.77758600
C	-5.42725700	1.48767600	1.82487900
H	-7.13548800	-1.65367200	-1.39640700
H	-7.09396300	-2.66232500	0.06958200
H	-6.16987800	-3.14978900	-1.37369900
H	-5.88444500	0.98341900	2.67899900
H	-6.19562800	2.03562600	1.27543100
H	-4.66578500	2.18594100	2.17268200
H	-0.67483700	2.69932100	-1.54245800
C	-2.04651600	3.98517400	-0.49073000
C	-3.94495200	6.08396700	-0.27465100
C	-3.31898600	5.80180200	-1.50977500
C	-2.39549800	4.78299900	-1.61579200
H	-4.67055900	6.88823400	-0.20331600
H	-3.56981300	6.39415500	-2.38580400
H	-1.92048200	4.57123700	-2.57099900
H	-2.82049500	3.68156000	2.84373100
C	1.69131300	2.33795100	-0.01379300
H	1.47422000	2.12034600	-1.06499200
H	1.59261200	3.42298500	0.12196500
C	3.07668800	1.82019300	0.34263900
H	3.25833900	1.99109100	1.40762500
H	3.06981200	0.74117600	0.18583800
C	4.23828600	2.42811800	-0.48068700
O	0.75797500	1.70522300	0.85418000
C	2.42987900	-1.97617700	-0.87719700
C	3.42219200	-2.82238600	-0.35904100
C	2.66040100	-1.28068700	-2.08519600
C	4.63035300	-2.99980900	-1.03058800
H	3.23915400	-3.35347200	0.56872500
C	3.88573900	-1.46392000	-2.73549900
C	4.86145900	-2.31782300	-2.22537900
H	5.38486700	-3.66446600	-0.62065400

H	4.07659900	-0.91310500	-3.65129200
H	5.80487000	-2.43577200	-2.74933900
C	0.96986700	-2.79891000	1.47688600
C	1.61327400	-2.25561800	2.61361600
C	0.41178800	-4.08317600	1.54151300
C	1.65659600	-3.02476600	3.78219100
C	0.46505700	-4.83059900	2.71694100
C	1.08605000	-4.29570900	3.84389700
H	2.14702900	-2.61221600	4.65959100
H	0.02208600	-5.82137400	2.74938300
H	1.12953600	-4.86421300	4.76806200
C	1.61610100	-0.38968000	-2.70664900
H	0.91572700	-0.97414900	-3.31541400
H	1.01744100	0.12291700	-1.94544000
H	2.08682000	0.36505800	-3.33892200
C	2.27040200	-0.89945100	2.58148500
H	3.15181800	-0.90462500	1.92983700
H	1.60008200	-0.12402900	2.19768400
H	2.60098500	-0.60400200	3.58029700
H	-0.07647900	-4.49927000	0.66762300
C	5.54728900	1.74967400	-0.05038100
C	5.62971000	0.34985700	-0.11499800
C	6.68347300	2.45407600	0.36434800
C	6.79493200	-0.32163300	0.24363100
H	4.78078800	-0.21637700	-0.47169500
C	7.85491900	1.78319100	0.72707900
H	6.67399200	3.53613200	0.40957800
C	7.91515100	0.39272300	0.67376900
H	6.82390900	-1.40506100	0.17985600
H	8.71988700	2.35532100	1.05022300
H	8.82476600	-0.12847800	0.95761500
C	4.27247600	3.96954000	-0.32154100
H	3.41850000	4.37425800	-0.87826600
H	5.16122000	4.35056200	-0.83909000
C	4.21598000	4.51455100	1.11114900
H	4.37376000	5.59767300	1.11580200
H	3.24201200	4.32410200	1.57048800
H	4.97550800	4.06147600	1.75358900
N	4.03338300	2.05408600	-1.90528100
H	3.29079200	2.62993400	-2.29780200
H	4.87587000	2.28662400	-2.42709900
C	-3.62649700	5.32631400	0.83666000
H	-4.10144500	5.52957000	1.79401700

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Ni	-0.14356700	0.03006900	0.21560200
P	-1.91682600	-1.01016700	-0.24970300
P	1.11881700	-1.66827900	-0.00871900
C	-0.91653600	2.72654400	0.45279900
C	-1.49625200	3.41965400	-0.58553600
C	-1.52682300	2.66547200	1.73036000
C	-1.29517400	-2.47753200	-1.21896200
C	0.08147700	-2.77948700	-1.07835000
C	-3.43194300	-0.40091100	-1.21712600
C	-3.00771100	-1.74213300	1.12702200
C	-2.71805600	3.30963900	1.94356700
H	-1.03020900	2.10206100	2.51190200
O	-4.40804600	-1.43608900	-1.48345800
O	-3.71292000	-0.63170700	1.72303400
C	0.63852700	-3.84478800	-1.79759100
C	-2.06451100	-3.24928500	-2.10593600
C	-4.03599000	-2.72714900	0.57188700
C	-4.08510300	0.65543500	-0.31734100
C	-3.02556800	0.16826200	-2.56505000
C	-2.15587000	-2.34576700	2.22594300
C	-3.37163400	4.01763900	0.89540600
H	1.69600800	-4.06333000	-1.68789200
C	-0.14269100	-4.60804200	-2.66404700
C	-1.49409200	-4.30142500	-2.82293700
H	-3.10912700	-3.00479700	-2.24825700
C	-5.03808600	-1.99762700	-0.33294600
H	-3.54349400	-3.53874700	0.03255800
H	-4.59677400	-3.15932900	1.40831700
H	-4.87609500	1.16569900	-0.87741000
H	-3.34687800	1.39133200	-0.00271100
C	-4.71052300	-0.01776400	0.90857600
H	-3.90958400	0.53597400	-3.09622100
H	-2.53608100	-0.59086900	-3.18079700
H	-2.32966100	0.99782200	-2.41251700
H	-2.79182600	-2.65089600	3.06369200
H	-1.41730400	-1.62154100	2.57862100
H	-1.61687500	-3.21963900	1.85374700
O	-5.65704400	-0.98147300	0.44609600
H	0.30415000	-5.42757800	-3.21963500
H	-2.10763300	-4.87754600	-3.50996200
C	-6.14176500	-2.89472600	-0.85378900
C	-5.46864700	0.93307000	1.80997500
H	-6.81893700	-2.30602700	-1.47614300

H	-6.70046000	-3.32065500	-0.01754900
H	-5.71637800	-3.70424500	-1.45228200
H	-5.93979600	0.36175200	2.61270400
H	-6.23793400	1.45811700	1.23971900
H	-4.77928300	1.66024700	2.23813700
H	-1.02904000	3.45088800	-1.56366400
C	-2.74698500	4.06736000	-0.39232100
C	-5.25290800	5.29279400	0.03337300
C	-4.63764900	5.34087700	-1.23918400
C	-3.41249100	4.74522600	-1.44609300
H	-6.21863700	5.76529400	0.18320500
H	-5.13710800	5.85060000	-2.05762900
H	-2.94196800	4.77948300	-2.42502200
H	-3.18388000	3.27605100	2.92395000
C	1.30187400	2.64976900	-0.50500500
H	1.13637000	2.32671000	-1.53791400
H	1.18258300	3.73524900	-0.44791100
C	2.64570200	2.18134300	0.02116000
H	2.69967300	2.42392900	1.08636300
H	2.67289100	1.09464400	-0.06588700
C	3.87281600	2.78695800	-0.70427400
O	0.28998700	2.06013300	0.34384600
C	2.74849000	-1.83930700	-0.86802900
C	3.82080100	-2.54450300	-0.29882000
C	2.92664800	-1.20263100	-2.11904000
C	5.05171000	-2.63089000	-0.94731900
H	3.68399100	-3.03914900	0.65664200
C	4.17453700	-1.28827300	-2.74610500
C	5.23137400	-1.99526000	-2.17595000
H	5.86422900	-3.19196400	-0.49424900
H	4.31577200	-0.78030900	-3.69588100
H	6.19009200	-2.04249300	-2.68358700
C	1.39022200	-2.64995200	1.52736400
C	1.98885700	-2.02094900	2.64541400
C	0.95596900	-3.97806700	1.63855500
C	2.12317800	-2.75050200	3.83194700
C	1.09486400	-4.68669800	2.83135700
C	1.67978200	-4.06896900	3.93464600
H	2.58261400	-2.26967100	4.69169500
H	0.74814100	-5.71400400	2.89468600
H	1.79212400	-4.60745500	4.87110000
C	1.80325700	-0.46540200	-2.80046400
H	1.14399200	-1.16043900	-3.33399600
H	1.17332600	0.05460400	-2.06852300



H	2.19709700	0.26362100	-3.51131900
C	2.49129400	-0.60021500	2.58358800
H	3.32721900	-0.49833400	1.88264200
H	1.70531600	0.07736700	2.23055000
H	2.83633200	-0.26529400	3.56552600
H	0.49955900	-4.46193000	0.78240000
C	5.14221200	2.21854700	-0.05213700
C	5.29945200	0.82515200	0.01197200
C	6.17324300	3.02065700	0.45160300
C	6.43166700	0.25623600	0.58970700
H	4.54131700	0.18062000	-0.41153800
C	7.31111000	2.45202100	1.03000600
H	6.10805100	4.10046100	0.40051800
C	7.44197000	1.06765400	1.10901700
H	6.51994500	-0.82438100	0.62259600
H	8.09323600	3.09850300	1.41754900
H	8.32403800	0.62500700	1.56238000
C	3.81817900	4.33720600	-0.66810700
H	3.03065000	4.65419800	-1.36394900
H	4.74934900	4.72373700	-1.09809700
C	3.55284000	4.98881000	0.69564200
H	3.65343100	6.07653000	0.62724500
H	2.54067200	4.77697200	1.05227600
H	4.24692900	4.63444300	1.46155100
N	3.86729900	2.29464000	-2.10380500
H	3.18114700	2.81298500	-2.64900600
H	4.77270200	2.48527700	-2.52616300
C	-4.62812800	4.64613700	1.07761900
H	-5.09638500	4.60054300	2.05711500

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Ni	0.01969500	-0.29377100	0.30306400
P	0.96592100	1.70873800	-0.24170500
P	-2.07852800	0.94840600	-0.10375500
C	1.69481200	-1.16232500	0.36532900
C	2.20420300	-1.74189700	-0.78226700
C	2.45748400	-1.27007500	1.56391600
C	-0.22418200	2.80914200	-1.13231000
C	-1.58657800	2.46182700	-1.04197700
C	2.64866400	2.03580100	-1.05576100
C	1.44638100	2.62949800	1.34665700
C	3.65753100	-1.94464600	1.59558300
H	2.09110700	-0.80191300	2.47211400
O	2.92194700	3.45431900	-1.08966300

O	2.59075500	1.94861600	1.88535000
C	-2.54934900	3.22100200	-1.72345400
C	0.13958200	3.91595300	-1.92338400
C	1.82652300	4.07377400	1.01995800
C	3.73783800	1.38445600	-0.20096900
C	2.66597800	1.53997000	-2.49122700
C	0.35386100	2.51979900	2.39307500
C	4.18435100	-2.55783700	0.42673800
H	-3.59359300	2.93464000	-1.65736400
C	-2.17703100	4.31774000	-2.49337500
C	-0.82705300	4.65834300	-2.59651600
H	1.18296600	4.18398800	-2.01278800
C	3.10870500	4.09899000	0.17747000
H	1.01070700	4.58558200	0.50564000
H	2.03208900	4.60204700	1.95688800
H	4.69360100	1.53351900	-0.71414500
H	3.56639900	0.31933600	-0.07981800
C	3.81923300	2.07971900	-1.15965600
H	3.63348500	1.77379500	-2.94564500
H	1.87837400	2.00809300	-3.08660300
H	2.52187100	0.45688800	-2.49921300
H	0.70013100	2.96777600	3.32976300
H	0.10216500	1.47068500	2.57062700
H	-0.55094100	3.03767200	2.06852300
O	4.12373300	3.45491100	0.92914700
H	-2.93206900	4.89497000	-3.01841700
H	-0.52215600	5.50307300	-3.20717500
C	3.59478200	5.49779300	-0.13748600
C	4.90442500	1.52789300	2.05642600
H	4.51078000	5.43530600	-0.72828300
H	3.80223300	6.03562800	0.79007900
H	2.83567100	6.04011300	-0.70654500
H	4.90766000	2.07993000	2.99867700
H	5.87582600	1.64156700	1.57024900
H	4.71744300	0.47104100	2.24866100
H	1.64516500	-1.69884100	-1.71383400
C	3.43684700	-2.45047900	-0.79041200
C	5.88537800	-3.85157100	-0.73480400
C	5.14331400	-3.75266400	-1.93740600
C	3.94886500	-3.06840200	-1.96285400
H	6.82645500	-4.39332800	-0.72677900
H	5.52166300	-4.22150400	-2.84121200
H	3.37422300	-2.99205200	-2.88266400
H	4.21875000	-2.02565500	2.52420600

C	-0.80095600	-3.20266800	1.02667900
C	-2.04417200	-3.76572400	1.79051400
H	-2.94164500	-3.26049300	1.43648500
C	-3.29302500	0.29235300	-1.31753600
C	-4.67397600	0.38926200	-1.10273000
C	-2.80130100	-0.22640000	-2.53617200
C	-5.57902700	-0.02656000	-2.07806300
H	-5.04218500	0.80982500	-0.17344800
C	-3.72865400	-0.61616200	-3.50856600
C	-5.10238300	-0.52540100	-3.28933100
H	-6.64633000	0.04956700	-1.89426100
H	-3.35870100	-1.01431000	-4.44912900
H	-5.79600500	-0.84496500	-4.06136000
C	-3.08602300	1.62976000	1.28175700
C	-3.73742000	0.74580300	2.17462900
C	-3.14532800	3.01328800	1.51109900
C	-4.42721600	1.29285200	3.26418700
C	-3.82933000	3.53268000	2.60892200
C	-4.47414300	2.66725000	3.49005400
H	-4.93087000	0.61564300	3.94847600
H	-3.85584100	4.60609500	2.77002700
H	-5.01007700	3.05811600	4.34999000
C	-1.32567900	-0.35206300	-2.81703100
H	-0.86489700	0.62866100	-2.97899600
H	-0.80498400	-0.82835700	-1.97755500
H	-1.15143900	-0.96739700	-3.70121900
C	-3.71238700	-0.74183500	1.96668900
H	-4.41428300	-1.03941700	1.17824500
H	-2.70865400	-1.08237500	1.66773700
H	-3.99411500	-1.28381600	2.87298800
H	-2.65171600	3.69526400	0.82923100
N	-0.75875500	-1.74085100	1.27465700
H	-0.29242600	-1.63202400	2.17802700
C	0.46514300	-3.92949100	1.56019300
H	0.64323700	-3.56351200	2.57895300
H	1.33260400	-3.60173100	0.99089400
H	-2.17602200	-4.82941100	1.56652900
C	-1.01345900	-3.45839500	-0.47410700
C	-2.25428700	-3.18990600	-1.06933800
C	-0.00491800	-3.97866200	-1.29889700
C	-2.49439800	-3.47123800	-2.41373100
H	-3.05038300	-2.75148600	-0.48053100
C	-0.22859400	-4.23223800	-2.65264100
H	0.97431700	-4.18917700	-0.89189600

C	-1.48121200	-3.99290400	-3.21688500
H	-3.47368600	-3.26614400	-2.83195700
H	0.57794000	-4.63557800	-3.25907100
H	-1.66595800	-4.21343600	-4.26455100
C	5.41341800	-3.26677300	0.41924400
H	5.97710300	-3.34334100	1.34575100
C	-2.00630300	-3.56501900	3.29848300
C	0.41909700	-5.46223200	1.58660500
H	0.14398900	-5.87516200	0.61177200
H	1.40187100	-5.86528300	1.85329900
H	-0.30057000	-5.84143800	2.31815900
O	-3.32783300	-3.79772800	3.79373200
H	-3.30132200	-3.70191400	4.75370800
H	-1.68813900	-2.53767700	3.52413700
H	-1.28887600	-4.25193700	3.77177500

## TS29

Ni	-0.02850200	-0.18019600	0.30535900
P	0.46369900	1.92055100	-0.18432800
P	-2.31123500	0.45884000	-0.10517600
C	1.69691900	-0.97308500	0.54603600
C	2.29911500	-1.40161200	-0.64684300
C	2.56164800	-0.74065000	1.67365300
C	-0.94223200	2.71940600	-1.08196600
C	-2.18949800	2.06698700	-1.00081600
C	2.02184300	2.50672800	-1.07872700
C	0.80116200	3.00471600	1.33402300
C	3.90447500	-0.99859000	1.61175400
H	2.13359800	-0.35652500	2.59569800
O	2.04508300	3.94682400	-1.19165400
O	2.05836500	2.56384900	1.87259700
C	-3.30164600	2.59382400	-1.67388500
C	-0.84000200	3.88138000	-1.86960700
C	0.91818100	4.47421600	0.92860100
C	3.21788400	2.07955500	-0.22623700
C	2.08831300	1.94151700	-2.48674600
C	-0.23793300	2.76182700	2.41195700
C	4.52166100	-1.47524700	0.41626200
H	-4.25344500	2.07667000	-1.61250400
C	-3.18852700	3.75235200	-2.43598500
C	-1.95019000	4.38853800	-2.54054400
H	0.11992000	4.36922200	-1.96822200
C	2.15281200	4.67479400	0.03748100
H	0.01079600	4.81409800	0.42524100

H	1.05876300	5.07666900	1.83247500
H	4.13225900	2.32876900	-0.77451900
H	3.20076900	1.00804000	-0.04300800
C	3.22390600	2.85771400	1.09166400
H	2.98358500	2.32025500	-2.98915100
H	1.21119800	2.22673900	-3.07337300
H	2.14540100	0.85097200	-2.43309100
H	0.01787500	3.33566300	3.30838300
H	-0.27329300	1.69911800	2.66593700
H	-1.23054500	3.06314800	2.06904800
O	3.28324600	4.25020800	0.77974900
H	-4.05577200	4.14754200	-2.95637500
H	-1.84494000	5.28091600	-3.15053200
C	2.38480700	6.11899000	-0.35406600
C	4.41495100	2.55745000	1.97328700
H	3.28150900	6.18251500	-0.97373000
H	2.52359800	6.72858800	0.54138700
H	1.52973600	6.49832600	-0.91918600
H	4.35255600	3.16454300	2.87901700
H	5.33697200	2.80051500	1.44075100
H	4.41792500	1.50033500	2.23643100
H	1.68996700	-1.58557700	-1.52473000
C	3.68661400	-1.66512200	-0.73554100
C	6.46680900	-2.20504200	-0.84965500
C	5.64711500	-2.40034400	-1.98606600
C	4.29515700	-2.13783900	-1.93256100
H	7.53066800	-2.41404100	-0.90556100
H	6.09029300	-2.76268500	-2.90987300
H	3.66641000	-2.29589600	-2.80521500
H	4.52853000	-0.83752800	2.48851200
C	0.28753900	-3.37094500	0.94094700
C	-0.90170000	-4.07022800	1.66533200
H	-1.84023600	-3.69385600	1.26067500
C	-3.44293200	-0.41881100	-1.26008800
C	-4.75673200	-0.75327300	-0.90495600
C	-2.96140500	-0.73500900	-2.55204500
C	-5.59722100	-1.40763200	-1.80444300
H	-5.12931900	-0.48524300	0.07780300
C	-3.82863100	-1.37742200	-3.44297600
C	-5.13123700	-1.71940800	-3.08033100
H	-6.61063600	-1.66299500	-1.51019700
H	-3.46749700	-1.61571700	-4.44007200
H	-5.77667900	-2.22505300	-3.79212700
C	-3.35200500	0.86753300	1.35659900

C	-3.64466000	-0.15112400	2.29316700
C	-3.78360400	2.17875600	1.60522100
C	-4.36881300	0.18420200	3.44269500
C	-4.49521400	2.49307000	2.76215700
C	-4.79030400	1.49107000	3.68451100
H	-4.59793800	-0.59942800	4.15973400
H	-4.81651200	3.51532200	2.93746200
H	-5.34393300	1.72395200	4.58926600
C	-1.56781900	-0.36972400	-2.99984200
H	-1.50626900	0.69058900	-3.26822100
H	-0.83201300	-0.54741600	-2.20740900
H	-1.27003700	-0.96244800	-3.86691100
C	-3.20018700	-1.56747400	2.06088800
H	-3.78049900	-2.03847800	1.25888700
H	-2.15056000	-1.59659400	1.75154400
H	-3.31269300	-2.19058900	2.95012200
H	-3.56194600	2.96256300	0.89077400
N	0.18771300	-1.90917100	1.17980400
H	0.36283600	-1.73899600	2.16457400
C	1.62327900	-3.90897700	1.52886900
H	1.74096200	-3.46895500	2.52607000
H	2.45297800	-3.50744600	0.94679000
H	-0.87726600	-5.14118000	1.44050900
C	0.14336600	-3.65906400	-0.55878100
C	-1.05484600	-3.34145900	-1.21196900
C	1.16333500	-4.24890000	-1.31736800
C	-1.24342200	-3.64162300	-2.56081900
H	-1.85084300	-2.84708800	-0.66736600
C	0.98830200	-4.52939000	-2.67227200
H	2.12250400	-4.46529600	-0.86710900
C	-0.22219400	-4.23748600	-3.29986000
H	-2.19132200	-3.40198900	-3.02894900
H	1.80285300	-4.97872100	-3.23301100
H	-0.36786800	-4.46999500	-4.35087000
C	5.90454600	-1.75047700	0.32717900
H	6.52330500	-1.59804200	1.20877600
C	-0.94524400	-3.88891000	3.17707300
C	1.76000400	-5.43280600	1.64804600
H	1.53758100	-5.94226900	0.70695200
H	2.78427000	-5.69399800	1.93318300
H	1.09374600	-5.85045600	2.40855700
O	-2.19696300	-4.40771600	3.62794600
H	-2.20603300	-4.36027900	4.59187600
H	-0.85946800	-2.82297800	3.43595400

H	-0.10978800	-4.41551200	3.65923600
<b>30</b>			
Ni	-0.31943400	-0.17261700	0.26124700
P	0.49655900	1.75721300	-0.19274500
P	-2.24506600	0.31190100	-0.47915600
C	2.16802600	-1.56829200	0.78831200
C	2.28831500	-1.81308000	-0.56280600
C	3.33471000	-1.38563500	1.57391100
C	-0.78316400	2.61491000	-1.23672700
C	-2.01558600	1.94014700	-1.37037800
C	2.14738800	2.39488700	-0.88594600
C	0.68154900	2.79622000	1.38801400
C	4.58428900	-1.41997600	0.99645100
H	3.22896500	-1.19837900	2.63811100
O	2.24631400	3.83996400	-0.90926600
O	1.85865900	2.27566200	2.05132200
C	-3.02089700	2.47503300	-2.18580600
C	-0.59236800	3.81742300	-1.94114000
C	0.89486400	4.27774200	1.08810100
C	3.22796300	1.86856900	0.06201100
C	2.36185800	1.91973000	-2.31312900
C	-0.47889100	2.55235900	2.33382200
C	4.73562400	-1.64830000	-0.39483500
H	-3.96224500	1.94425800	-2.28775500
C	-2.81993800	3.66947300	-2.87371000
C	-1.59998900	4.33731100	-2.75226600
H	0.35854500	4.32917900	-1.86772400
C	2.23021300	4.48308500	0.36354800
H	0.06767100	4.66974400	0.49211100
H	0.93542300	4.83312100	2.03205800
H	4.21222400	2.10128300	-0.35868000
H	3.14480300	0.79003000	0.17794600
C	3.10964400	2.56619400	1.42170500
H	3.32536300	2.28378100	-2.68414200
H	1.57214500	2.28598100	-2.97397600
H	2.36442400	0.82663400	-2.34055500
H	-0.28358700	3.03352400	3.29804300
H	-0.62551700	1.47878000	2.48400800
H	-1.40337900	2.95607600	1.91577900
O	3.25541000	3.96757700	1.20645600
H	-3.60508500	4.07119200	-3.50780400
H	-1.42848200	5.26262700	-3.29513000
C	2.55858700	5.93857200	0.10351800

C	4.18457900	2.16334700	2.40899600
H	3.52253900	6.00311500	-0.40537500
H	2.61349100	6.48249900	1.04896000
H	1.78880300	6.38954500	-0.52760300
H	4.04650200	2.72266600	3.33670100
H	5.17019900	2.38940900	1.99612400
H	4.11830900	1.09418900	2.61372500
H	1.39714000	-1.95597000	-1.16017600
C	3.55806600	-1.85897500	-1.18412800
C	6.10411800	-1.87779200	-2.38970200
C	4.93936400	-2.08801600	-3.17019000
C	3.69653300	-2.08082100	-2.58108400
H	7.07852100	-1.88588000	-2.86847200
H	5.03417600	-2.25590800	-4.23870700
H	2.79942900	-2.24364300	-3.17192800
H	5.47062900	-1.25980100	1.60371300
C	0.26175500	-2.79053300	1.87856300
C	-1.12682600	-2.42832000	2.43591100
H	-1.62700600	-1.84349000	1.66076300
C	-3.08373900	-0.60669300	-1.84964500
C	-4.47284400	-0.79122200	-1.89795000
C	-2.28074400	-1.14711300	-2.88241900
C	-5.07038200	-1.53400600	-2.91504300
H	-5.09437600	-0.34319100	-1.13032700
C	-2.89772600	-1.89548600	-3.89202900
C	-4.27714600	-2.09995200	-3.91178800
H	-6.14831900	-1.66639700	-2.92784600
H	-2.27969000	-2.31753100	-4.68070300
H	-4.72770200	-2.68817700	-4.70571200
C	-3.60930700	0.73338100	0.70452500
C	-4.32344000	-0.25898200	1.42155600
C	-3.81619400	2.08331700	1.04474700
C	-5.18961300	0.14132100	2.45037300
C	-4.67999100	2.45862700	2.06980600
C	-5.36958200	1.48093300	2.78477000
H	-5.72664900	-0.62681900	3.00079500
H	-4.81071500	3.51036800	2.30689000
H	-6.04050200	1.75522100	3.59296600
C	-0.79621700	-0.89951400	-2.94111000
H	-0.58193600	0.11844300	-3.28745600
H	-0.34713000	-0.98028900	-1.94241800
H	-0.30206300	-1.60520400	-3.61420200
C	-4.24138200	-1.73951200	1.12547200
H	-5.15208200	-2.08246700	0.62266800



H	-3.40864300	-1.99115200	0.47240500
H	-4.13557700	-2.30398000	2.05531100
H	-3.29186300	2.85393600	0.49295300
N	0.86080300	-1.46878000	1.38770900
H	0.95387000	-0.86319500	2.20272800
C	1.15644800	-3.38849300	2.98602400
H	1.30914700	-2.61450300	3.74817400
H	2.15166900	-3.59583100	2.58341700
H	-1.70872200	-3.33925600	2.59989500
C	0.13988500	-3.69381500	0.64724500
C	-0.83782800	-3.42536500	-0.32250800
C	1.05434900	-4.72114700	0.38536400
C	-0.90103000	-4.15480600	-1.50876100
H	-1.51734300	-2.59577200	-0.18227500
C	0.99464000	-5.45748700	-0.79900900
H	1.84172000	-4.94582600	1.09397800
C	0.01720100	-5.17669400	-1.75243700
H	-1.66363500	-3.90903900	-2.24088200
H	1.72130000	-6.24479700	-0.97613900
H	-0.02768200	-5.74679700	-2.67578500
C	6.00319500	-1.66480500	-1.03407000
H	6.89380300	-1.50348800	-0.43269000
C	-1.15579800	-1.57636600	3.70784000
C	0.59549300	-4.64552900	3.65899500
H	0.38928400	-5.43294800	2.92967800
H	1.31066700	-5.03915900	4.38789100
H	-0.33686900	-4.43646300	4.19075600
O	-2.47178500	-1.13486300	4.00097600
H	-2.77041600	-0.56860900	3.27426300
H	-0.47147100	-0.71733400	3.61680200
H	-0.83291300	-2.14811300	4.58279900