

Ni(I)–Ni(III) vs Ni(II)–Ni(IV): Mechanistic Study of Ni-catalyzed Alkylation of
Benzamides with Alkyl Halides

Yingzi Li,^[a] Lufeng Zou,^[b] Ruopeng Bai^{*[a]} and Yu Lan^{*[a]}

[a] School of Chemistry and Chemical Engineering, Chongqing University,
Chongqing 400030 (P. R. China)

[b] 340 Quinnipiac St Bldg 40, Wallingford, CT 06492 (USA)

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1. Complete reference for Gaussian 09

Gaussian 09, Revision D.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, **2013**.

2. Absolute calculation energies, enthalpies, and Gibbs energy for manuscript

Geometry	$E_{(\text{elec-B3LYP})}^1$	$E_{(\text{solv, B3LYP})}^2$	$G_{(\text{corr-B3LYP})}^3$	$H_{(\text{corr-B3LYP})}^4$	IF ⁵	$\langle S2 \rangle$ values
1	-1469	-1471	0.316	0.2381	-	
2	-801	-802	0.26	0.2025	-	
3	-2271	-2273	0.579	0.4665	-	
4-ts	-2271	-2273	0.575	0.4645	-54.8	
5	-2271	-2273	0.579	0.4676	-	
6	-1235	-1237	0.285	0.2152	-	
7-ts	-1235	-1237	0.279	0.2131	-1312.4	
8	-970	-972	0.238	0.1808	-	
9	-1235	-1237	0.285	0.2152	-	
10-ts	-1235	-1237	0.279	0.2092	-482.5	
11-ts	-2271	-2273	0.56	0.4515	-1313.2	
12	-2006	-2008	0.532	0.4341	-	
13	-3699	-3704	0.372	0.2926	-	
14-ts	-3699	-3704	0.37	0.2933	-244.2	
15	-3699	-3704	0.371	0.2955	-	
16-ts	-3699	-3704	0.371	0.2948	-229.4	
17	-3699	-3704	0.373	0.2941	-	
18	-959	-959	0.38	0.3088	-	
19-ts	-4735	-4740	0.663	0.5414	-251.7	
20	-4735	-4740	0.666	0.5471	-	
21-ts	-3964	-3969	0.416	0.323	-157.0	
22	-3964	-3969	0.417	0.3272	-	
23-ts	-3964	-3969	0.412	0.3259	-1213.2	
BuBr	-2571	-2574	0.002	-0.016	-	
Br⁻	-76.4	-76.5	0.025	0.0035	-	
H₂O	-189	-189	0.015	-0.009	-	

CO₂	-264	-265	0.031	0.0005	-	
HCO₃⁻	-1036	-1037	0.291	0.2281	-	
PPh₃	-1469	-1472	0.315	0.2372	-	
1a	-2271	-2273	0.576	0.4622	-	0.76
3a	-2271	-2273	0.57	0.4544	-	0.76
4a-ts	-2271	-2273	0.576	0.4608	-951.8	0.76
5a	-1235	-1237	0.282	0.2075	-	0.77
6a	-1235	-1237	0.281	0.2093	-	0.78
7a	-1235	-1237	0.276	0.2044	-	0.98
8a-ts	-1235	-1237	0.278	0.2082	-1138.2	0.78
9a-ts	-970	-972	0.236	0.177	-49.9	0.77
10a	-3699	-3704	0.367	0.2846	-	0.78
11a-ts	-3699	-3704	0.369	0.2887	-563.5	0.79
12a	-3699	-3704	0.368	0.29	-	0.81
13a-ts	-3699	-3704	0.371	0.2884	-280.5	0.81
14a	-3700	-3704	0.383	0.2979	-	0.76
15a	-3700	-3704	0.382	0.2983	-	0.76
16a-ts	-3700	-3704	0.383	0.2995	-287.2	0.92
17a	-1393	-1395	0.413	0.3263	-	1.01
18a	-1393	-1395	0.408	0.3238	-	1.05
19a-ts	-1128	-1130	0.368	0.2945	-1126.4	0.91
20a	-3964	-3969	0.414	0.3188	-	0.78
21a-ts	-3964	-3969	0.415	0.321	-310.3	1.16
22a	-3964	-3969	0.41	0.321	-	1.25
23a-ts	-1469	-1471	0.316	0.2381	-1233.3	1.03

Table S1 ¹The $E_{\text{(elec-B3LYP)}}$ is the electronic energy calculated by B3LYP in gas phase. ²The $E_{\text{(solv, B3LYP)}}$ is the electronic energy calculated by M11-L in 1,4-dioxane solvent. ³The $G_{\text{(corr-B3LYP)}}$ is the thermal correction to Gibbs free energy calculated by B3LYP in gas phase. ⁴The $H_{\text{(corr-B3LYP)}}$ is the thermal correction to enthalpy calculated by B3LYP in gas phase. ⁵The IF is the B3LYP calculated imaginary frequencies for the transition states. ⁶The calculated $\langle S2 \rangle$ value.

3. B3LYP geometries for all the compounds and transition states

1

Ni	-1.63101600	-0.37322200	-0.65494200
O	-2.29107700	0.54609800	-2.08436500
C	-3.55165800	0.19676900	-1.75390400
O	-3.44635000	-0.55888700	-0.65317200
O	-4.56045100	0.51260900	-2.33964200
P	0.54008500	0.01096500	-0.22668000
C	1.02805100	1.72138200	0.16801600
C	0.13683500	2.74226500	-0.20533200
C	2.23481600	2.04693100	0.80815600
C	0.44589700	4.07295000	0.08153900
H	-0.78361000	2.49195700	-0.72770400
C	2.53631400	3.37902600	1.08907100
H	2.93829900	1.26434100	1.07791500
C	1.64137600	4.39096400	0.72884900
H	-0.24440300	4.85918500	-0.21004000
H	3.47019000	3.62811600	1.58536500
H	1.88161600	5.42814500	0.94618300
C	2.04959300	-0.94879500	-0.59643000
C	2.48732900	-1.00254200	-1.92989500
C	2.77580000	-1.62300000	0.39813500
C	3.64533100	-1.70726800	-2.25873500
H	1.91889800	-0.50028000	-2.70847000
C	3.92994600	-2.33191500	0.06180600
H	2.43572100	-1.60188200	1.42966800
C	4.36678700	-2.37181700	-1.26416000
H	3.97771900	-1.74500600	-3.29218000
H	4.48626400	-2.85396100	0.83538300
H	5.26461000	-2.92599000	-1.52330600
C	-0.25974700	-0.72766500	1.25387500
C	-0.53465200	-0.01832000	2.44133000
C	-0.87255900	-1.98867000	1.04813400
C	-1.37943100	-0.56538000	3.39969600
H	-0.08635300	0.95738400	2.60135000
C	-1.73374500	-2.52079700	2.01968300
H	-0.62934800	-2.58408000	0.16975300
C	-1.98669900	-1.81209700	3.18853900
H	-1.57888700	-0.01578100	4.31542000
H	-2.19914600	-3.48669300	1.84900700
H	-2.65888100	-2.22039500	3.93740900

2

N	0.26066200	-0.29749100	0.01263000
H	0.30657400	0.71197200	-0.08362100
C	-1.05632100	-0.75946700	0.03369300
C	-2.05966600	0.26879000	-0.02637700
C	-1.44440000	-2.08781700	0.10985700
C	-3.44080900	-0.09241900	-0.00714200
C	-2.81869400	-2.42278100	0.12923500
H	-0.68652400	-2.85723500	0.14974900
C	-2.54676200	2.51583200	-0.15942500
C	-4.38046200	0.96792400	-0.07090300
C	-3.80355400	-1.46192200	0.07263000
H	-3.09182900	-3.47281100	0.18952300
C	-3.94010400	2.26981600	-0.14723900
H	-2.17515400	3.53785000	-0.21922300
H	-5.44303000	0.73645400	-0.05890100
H	-4.85547300	-1.73466500	0.08702000
H	-4.63669900	3.10102600	-0.19741900
C	1.42568500	-1.02930000	0.03329800
O	1.45165100	-2.25726800	0.03853600
C	2.69299200	-0.21898100	0.03195500
C	2.76034000	1.13375800	0.39871300
C	3.86992300	-0.88454700	-0.33933900
C	3.98086200	1.80917700	0.37668300
H	1.87450100	1.66559000	0.73545300
C	5.08649600	-0.20726700	-0.36765600
H	3.80386200	-1.93541500	-0.60045500
C	5.14469400	1.14294600	-0.01205500
H	4.02251500	2.85452600	0.67008800
H	5.99049000	-0.73185300	-0.66497300
H	6.09378600	1.67196700	-0.03089400
N	-1.63745400	1.56153300	-0.10123200

3

N	2.67870100	0.79402100	-0.17729300
C	2.50509900	2.17507000	0.03025800
C	1.29663600	2.83272800	-0.37792900
C	3.51442900	2.92573700	0.61590100
C	1.21970700	4.26242600	-0.24861100
C	3.40427400	4.31918800	0.78164500
H	4.41073500	2.41507200	0.94304600
C	-0.85976400	2.79280000	-1.27944000
C	0.05460500	4.92212100	-0.70895400
C	2.28623800	4.98562900	0.33830100
H	4.22454900	4.86429000	1.23903000

C	-0.98123700	4.19388800	-1.23938600
H	-1.67745300	2.18893700	-1.65783700
H	-0.00154900	6.00488700	-0.63148300
H	2.19920800	6.06453900	0.43100900
H	-1.88798900	4.66178500	-1.60675900
C	3.22364500	-0.05388800	0.77552200
O	3.46997200	0.32726200	1.91729200
C	3.45139100	-1.47466400	0.35335000
C	3.48487100	-1.90268300	-0.98220100
C	3.64622800	-2.41265600	1.37999200
C	3.67931500	-3.25134000	-1.28335000
H	3.36520000	-1.20666200	-1.80473200
C	3.84656900	-3.75684400	1.07707300
H	3.63585100	-2.06198400	2.40644300
C	3.85810300	-4.17988900	-0.25661900
H	3.67450600	-3.56451300	-2.32256000
H	3.99292200	-4.47573900	1.87905300
H	4.00881700	-5.23002100	-0.49359200
N	0.21521900	2.12890700	-0.86390000
Ni	0.05412000	0.18786900	-1.25900500
O	1.34794900	0.19668600	-2.61848700
C	1.01729800	-1.07165200	-2.93966400
O	0.03314700	-1.44323600	-2.11115900
O	1.53849000	-1.75120300	-3.79745600
H	2.39781800	0.43392800	-1.09628500
P	-1.56772600	-0.42100100	0.23779200
C	-1.45023000	0.17033300	1.97499500
C	-0.26819700	0.79551800	2.39616400
C	-2.46735700	-0.07015400	2.91612200
C	-0.10804800	1.18756800	3.72731300
H	0.53955600	0.95977200	1.69293800
C	-2.31090100	0.33398800	4.24088500
H	-3.37740000	-0.58228300	2.61696000
C	-1.13091100	0.96473000	4.64822900
H	0.82230000	1.65504200	4.03573400
H	-3.10506300	0.14632600	4.95864600
H	-1.00846200	1.26972800	5.68401100
C	-1.77027000	-2.23926500	0.40539600
C	-0.61829700	-3.03983500	0.41859300
C	-3.02759800	-2.83831500	0.57857500
C	-0.72415400	-4.41613600	0.61920000
H	0.35595000	-2.59617700	0.24821000
C	-3.12815400	-4.21667700	0.77196400
H	-3.93043400	-2.23532700	0.54899300

C	-1.97667800	-5.00650800	0.79595100
H	0.17571200	-5.02441800	0.62085200
H	-4.10646100	-4.67250000	0.90019700
H	-2.05716000	-6.08028100	0.94335800
C	-3.17598800	0.17235600	-0.43380200
C	-3.97822600	1.13743200	0.19161400
C	-3.54316600	-0.30236500	-1.70827500
C	-5.13835800	1.60309400	-0.43470700
H	-3.70306300	1.52658800	1.16675100
C	-4.70344200	0.16263900	-2.32514800
H	-2.91437700	-1.03068000	-2.21448900
C	-5.50513800	1.11550700	-1.68905600
H	-5.75437000	2.34729400	0.06328100
H	-4.97828300	-0.21653200	-3.30546700
H	-6.40821800	1.47776200	-2.17261700

4-ts

N	1.98607900	0.13964800	-1.26099300
C	2.47159800	1.32172800	-0.76831900
C	1.51003400	2.37761300	-0.53863300
C	3.82177900	1.64750400	-0.57199400
C	1.94324500	3.68605800	-0.13882500
C	4.22996900	2.92424700	-0.15182300
H	4.57177400	0.89032000	-0.76925900
C	-0.72281500	3.09278100	-0.56470800
C	0.95701200	4.69031000	0.02133800
C	3.31988500	3.93942800	0.06585200
H	5.29184900	3.11334500	-0.01611800
C	-0.37018900	4.40350500	-0.19850100
H	-1.76198500	2.82556300	-0.72293500
H	1.26890700	5.69004000	0.31365400
H	3.63897200	4.93172700	0.37057900
H	-1.14483200	5.15497400	-0.08990600
C	2.57814700	-1.09118200	-1.18312100
O	2.31274900	-1.96131400	-2.02330900
C	3.48035100	-1.47628700	-0.02937200
C	4.46508000	-2.44625900	-0.26663000
C	3.32234700	-0.97688100	1.27091300
C	5.29480300	-2.88390900	0.76477800
H	4.55677100	-2.85204100	-1.26892900
C	4.13786100	-1.42933100	2.30876100
H	2.55294100	-0.23843700	1.47325600
C	5.13251700	-2.37706200	2.05683100
H	6.06238400	-3.62682300	0.56333800
H	3.99639600	-1.04261200	3.31493700

H	5.77340500	-2.72273400	2.86400700
N	0.17100200	2.12064700	-0.72295900
Ni	-0.44129000	0.41289100	-1.42210700
O	0.35806600	0.47460500	-3.30250400
C	-0.34471300	-0.76329600	-3.53154800
O	-0.99231000	-1.03902200	-2.42929700
O	-0.32895600	-1.32468400	-4.58772200
H	1.23698600	0.25998400	-2.82333700
P	-1.70428800	-0.30645600	0.30400000
C	-1.92448700	0.87018500	1.69860500
C	-3.16743200	1.44049900	2.00808000
C	-0.79300000	1.25462300	2.43930000
C	-3.27709500	2.37307200	3.04324300
H	-4.05182700	1.15402800	1.44808300
C	-0.90733500	2.18087100	3.47375500
H	0.17774900	0.82503500	2.20744700
C	-2.15066600	2.74359800	3.77759000
H	-4.24699100	2.80431600	3.27584900
H	-0.02564100	2.46513600	4.04143800
H	-2.23847700	3.46681100	4.58373600
C	-3.40152400	-0.75241800	-0.23457900
C	-4.17142000	-1.69673700	0.46249000
C	-3.94513400	-0.12228500	-1.36386700
C	-5.46821300	-1.99207400	0.04213900
H	-3.75511100	-2.21127500	1.32312500
C	-5.24419200	-0.41739500	-1.77904200
H	-3.34234700	0.57942800	-1.93304000
C	-6.00688200	-1.35160100	-1.07627900
H	-6.05456800	-2.72893900	0.58409500
H	-5.65158400	0.07038500	-2.66001500
H	-7.01472300	-1.58903700	-1.40561200
C	-0.97846700	-1.81181900	1.06237400
C	-0.20179000	-2.66659400	0.26259000
C	-1.19552800	-2.13236400	2.41411900
C	0.34637200	-3.82593800	0.81384600
H	-0.01497600	-2.42927200	-0.77905400
C	-0.64919500	-3.29718900	2.95313700
H	-1.77908300	-1.47105200	3.04756300
C	0.12283400	-4.14399500	2.15396700
H	0.96087300	-4.46714500	0.18946400
H	-0.82109500	-3.53783700	3.99888600
H	0.55619100	-5.04518100	2.57926800
5			
N	1.46759300	1.39163900	-0.03265900

C	2.80913600	1.32837100	0.35936300
C	3.51340200	0.21229300	-0.19132300
C	3.54499700	2.22109700	1.13976400
C	4.90984200	0.01738000	0.00629300
C	4.93114000	2.02195300	1.34253800
H	3.04772600	3.07595400	1.57154000
C	3.33359700	-1.72278100	-1.48466800
C	5.49202700	-1.11875900	-0.60782900
C	5.61717500	0.95714100	0.79802500
H	5.46528300	2.74374900	1.95528600
C	4.71254700	-1.98110000	-1.35012200
H	2.67434000	-2.39212200	-2.02486800
H	6.55645100	-1.30212000	-0.48239100
H	6.68118800	0.82152200	0.96981000
H	5.13694400	-2.85866600	-1.82658600
C	0.79956500	2.60252900	0.00270200
O	1.12496600	3.54543600	0.73147800
C	-0.34211700	2.79272000	-0.95758800
C	-1.31419400	3.75484800	-0.63854000
C	-0.40321800	2.14982900	-2.20118700
C	-2.34335800	4.04314200	-1.53019400
H	-1.24060200	4.26650900	0.31500900
C	-1.42981300	2.44931600	-3.10186100
H	0.34730600	1.42148400	-2.48768700
C	-2.40275300	3.39189800	-2.76750800
H	-3.09665700	4.78120300	-1.26669100
H	-1.45693200	1.94154200	-4.06190700
H	-3.20022700	3.62594800	-3.46852400
N	2.76578300	-0.66135900	-0.92870400
Ni	0.85276400	-0.30348300	-0.68438800
P	-1.08030800	-0.55079500	0.59248800
C	-0.65397000	-1.85201700	1.83920600
C	0.02552600	-3.00825100	1.41241800
C	-1.00232700	-1.72908800	3.19392100
C	0.34892200	-4.01047100	2.32757100
H	0.28899300	-3.12176900	0.36630200
C	-0.67237600	-2.73600100	4.10375100
H	-1.52986600	-0.84944300	3.54532400
C	0.00556800	-3.87729000	3.67467800
H	0.87272800	-4.89828200	1.98324000
H	-0.94840700	-2.62418300	5.14897000
H	0.26310800	-4.65863400	4.38484000
C	-1.72960500	0.83611600	1.61323800
C	-0.84721300	1.53669600	2.45340500

C	-3.08094600	1.21159200	1.58090200
C	-1.31003700	2.58606700	3.24624700
H	0.20500900	1.27285400	2.48178000
C	-3.53943900	2.26462000	2.37455100
H	-3.77689800	0.68626900	0.93617100
C	-2.65720200	2.95299400	3.20839300
H	-0.61234200	3.12472700	3.88062800
H	-4.58850600	2.54574600	2.33770100
H	-3.01554900	3.77480700	3.82257000
C	-2.54981300	-1.21888000	-0.28725900
C	-2.88379800	-0.69667100	-1.54638300
C	-3.36279500	-2.21075500	0.28390300
C	-4.01862600	-1.15674000	-2.21678100
H	-2.25430300	0.05478000	-2.00979400
C	-4.49310800	-2.66932000	-0.39344400
H	-3.11264000	-2.62842800	1.25388900
C	-4.82392200	-2.14238000	-1.64379800
H	-4.26549100	-0.74690500	-3.19228900
H	-5.11306300	-3.44043600	0.05606600
H	-5.70370000	-2.50254700	-2.17058700
O	0.41014300	-1.96737300	-1.46444100
C	0.04000600	-1.88766100	-2.70464600
O	-0.13886900	-0.87166900	-3.37470500
O	-0.12838900	-3.12892300	-3.25139600
H	-0.41004300	-2.96046800	-4.16663300

6

N	0.11091200	-0.89548300	-0.21157800
C	1.43450000	-1.33070700	-0.21946300
C	2.37008700	-0.30045800	0.09769300
C	1.95473400	-2.60959400	-0.42788100
C	3.76653400	-0.53450300	0.23723900
C	3.34260400	-2.84536700	-0.29194000
H	1.28778200	-3.41462900	-0.69798600
C	2.61017800	1.98460500	0.56199700
C	4.57041800	0.58521000	0.56555100
C	4.24518700	-1.85243900	0.03408800
H	3.70358800	-3.85703500	-0.45838400
C	4.00026300	1.83231500	0.73000700
H	2.11422300	2.94460400	0.65675100
H	5.64285000	0.45069100	0.68305800
H	5.30686500	-2.06086200	0.12722800
H	4.60229900	2.69963300	0.97885400
C	-0.93539300	-1.77839100	-0.42119400
O	-0.80443900	-2.87842500	-0.96166400

C	-2.28211400	-1.37718700	0.10989400
C	-3.42239700	-1.85490900	-0.55048600
C	-2.43527800	-0.65003500	1.29792000
C	-4.69409800	-1.57506800	-0.05540000
H	-3.29098800	-2.44918600	-1.44909100
C	-3.70832300	-0.38588700	1.80511600
H	-1.55484400	-0.31122500	1.83651500
C	-4.84016700	-0.83957200	1.12478700
H	-5.57249800	-1.93820100	-0.58263900
H	-3.81586500	0.16692900	2.73492200
H	-5.83205300	-0.63141500	1.51803800
N	1.83866300	0.94679100	0.26168500
Ni	0.00308500	1.00154800	-0.16690700
O	-0.25446300	2.91760500	-0.20834000
C	-1.42259700	2.68689000	-0.65630500
O	-1.77903600	1.47769600	-0.82044500
O	-2.23433800	3.70195500	-0.93684700
H	-3.07136900	3.31813600	-1.25597300
7-ts			
N	-0.23689800	-1.17888300	0.18133100
C	-1.61021500	-1.34058400	0.21869200
C	-2.31545800	-0.14410000	-0.11060300
C	-2.35644300	-2.47932000	0.51527400
C	-3.73523000	-0.08878900	-0.15151700
C	-3.76899400	-2.42079500	0.47861500
H	-1.84208000	-3.39555400	0.77046000
C	-2.10550200	2.10291200	-0.70999000
C	-4.31290900	1.15609800	-0.50602700
C	-4.46004100	-1.26888500	0.15560000
H	-4.32434100	-3.32489700	0.71438300
C	-3.50685400	2.24095200	-0.78563600
H	-1.43235500	2.93114900	-0.90312800
H	-5.39546300	1.24501000	-0.55479000
H	-5.54574800	-1.25295600	0.13052200
H	-3.93058000	3.20167700	-1.05855200
C	0.69278400	-2.16808200	0.39238000
O	0.45592300	-3.33112800	0.71646300
C	2.05860000	-1.64368100	0.07329700
C	3.08791100	-2.53617100	-0.21996400
C	2.21331800	-0.24556000	-0.09467900
C	4.29555900	-2.05535300	-0.72965900
H	2.91232600	-3.59858500	-0.07789700
C	3.42627900	0.20190400	-0.65474100
C	4.45818100	-0.68766800	-0.96467300

H	5.10169200	-2.74657700	-0.96183600
H	3.58561800	1.26611600	-0.81192500
H	5.38965300	-0.31402700	-1.38226700
N	-1.53664800	0.94832800	-0.38716500
Ni	0.34919200	0.54485800	-0.20490200
O	0.87734900	2.40497100	-0.29235000
C	1.58098300	2.70541300	0.70828500
O	2.12443700	1.86220200	1.50441200
O	1.77970800	4.00754100	0.94742500
H	2.35223600	4.06915400	1.73230700
H	2.01534700	0.75892600	0.88530600
8			
N	-0.21881600	0.68452700	-0.00009400
C	1.10573400	1.06597800	-0.00003300
C	2.02700500	-0.03209000	-0.00002000
C	1.62824100	2.35984000	0.00002000
C	3.43623800	0.17846100	0.00005400
C	3.02614600	2.55706900	0.00009100
H	0.94658400	3.19912600	0.00000300
C	2.28212900	-2.34934800	-0.00006100
C	4.25601000	-0.97767700	0.00007200
C	3.92551600	1.50842300	0.00011000
H	3.39831800	3.57829400	0.00013400
C	3.68605800	-2.23388800	0.00001400
H	1.80406500	-3.32567900	-0.00011700
H	5.33701900	-0.86114000	0.00013300
H	4.99714100	1.68485900	0.00016900
H	4.29599200	-3.13118400	0.00002600
C	-1.33813200	1.51019200	-0.00008600
O	-1.29866600	2.73644600	-0.00011400
C	-2.56395700	0.66577500	-0.00003200
C	-3.85564300	1.19096700	-0.00002100
C	-2.32325500	-0.71842700	0.00002700
C	-4.94097400	0.31181700	0.00005500
H	-3.99429600	2.26891100	-0.00006800
C	-3.41739400	-1.58867000	0.00010900
C	-4.72113700	-1.06910500	0.00012200
H	-5.95672300	0.69843000	0.00006600
H	-3.28238800	-2.67005600	0.00016500
H	-5.56998700	-1.74961800	0.00018500
N	1.48015900	-1.29050900	-0.00007400
Ni	-0.48897500	-1.12919700	-0.00004000
9			
N	-0.19246600	-0.66623000	-0.52038400

C	1.09729200	-1.33937300	-0.59276800
C	2.20907200	-0.62223500	-0.09279000
C	1.26631500	-2.61593500	-1.07824800
C	3.49832600	-1.21902600	-0.05748200
C	2.55190300	-3.21159600	-1.06886600
H	0.41408400	-3.17517200	-1.45379700
C	2.99860900	1.37994400	0.79395500
C	4.55676400	-0.43242200	0.46939100
C	3.64216000	-2.53835600	-0.56044400
H	2.66828700	-4.21834600	-1.45787600
C	4.30629400	0.85282000	0.89774500
H	2.75696100	2.39984600	1.07732800
H	5.55774500	-0.85229200	0.52296400
H	4.62216900	-3.00716700	-0.54454900
H	5.09728200	1.47631200	1.30030300
C	-1.06639600	-1.19839900	0.53704800
O	-0.55281900	-1.71132000	1.50701100
C	-2.53121300	-1.11914800	0.30516500
C	-3.32829200	-1.96519200	1.09707100
C	-3.13530500	-0.27793000	-0.64427700
C	-4.70790500	-1.98928900	0.92481600
H	-2.84505200	-2.59657300	1.83509900
C	-4.52103600	-0.30191400	-0.80204900
H	-2.55510200	0.45432400	-1.19513400
C	-5.30593000	-1.15912200	-0.02872000
H	-5.31802800	-2.64998700	1.53404100
H	-4.98655600	0.36608000	-1.52050200
H	-6.38458300	-1.17291000	-0.15978800
N	1.99235700	0.66304600	0.31868100
Ni	0.22779200	1.30317000	-0.09131100
O	-1.31417200	2.14952600	-0.57345400
C	-0.78456100	3.34504700	-0.24742900
O	0.45822000	3.08977100	0.19958400
O	-1.31741500	4.42598500	-0.34087500
H	-0.67172800	-0.64951900	-1.42030400

10-ts

N	0.27360100	0.53752900	0.72586500
C	-0.61705100	-0.52883000	1.07184900
C	-1.72840200	-0.74206200	0.21085100
C	-0.47321700	-1.32223300	2.19401700
C	-2.68514800	-1.75704500	0.49893700
C	-1.42026300	-2.33331700	2.48295800
H	0.36788100	-1.15867700	2.86067800
C	-2.85129500	-0.12177700	-1.73533600

C	-3.76035400	-1.91244800	-0.41218900
C	-2.50503400	-2.55117000	1.66103400
H	-1.28457900	-2.93957400	3.37337800
C	-3.84250600	-1.10192100	-1.52368900
H	-2.89596600	0.53862800	-2.59663400
H	-4.51245100	-2.67386100	-0.22324000
H	-3.22987200	-3.32709000	1.88964500
H	-4.65441600	-1.19880500	-2.23611700
C	1.70305700	0.28812700	0.82851200
O	2.36805400	0.99307800	1.55601000
C	2.29809400	-0.82133600	0.02408300
C	3.61198100	-1.20064000	0.34430900
C	1.63707800	-1.46635200	-1.03185600
C	4.24648700	-2.21427700	-0.36776400
H	4.11763800	-0.68181400	1.15169000
C	2.27742200	-2.47620000	-1.74890100
H	0.63161200	-1.17094300	-1.30994800
C	3.57966600	-2.85523100	-1.41575100
H	5.26188700	-2.50180000	-0.11038600
H	1.76144300	-2.96349600	-2.57154500
H	4.07573900	-3.64350400	-1.97547800
N	-1.83068900	0.05451100	-0.90462200
Ni	-0.47846600	1.45206200	-0.88851200
O	-0.34723100	2.94632100	1.22888800
C	0.29872700	3.60472000	0.31585600
O	0.55370400	2.85318000	-0.82392100
O	0.67522900	4.76268900	0.32551800
H	0.04425400	1.54870900	1.20412900
11-ts			
N	2.54411000	-0.70517600	0.80536700
C	3.20117000	0.49700800	0.99476600
C	2.93442400	1.44269100	-0.04124300
C	4.05038200	0.88304200	2.03058200
C	3.50304600	2.74573000	-0.04083900
C	4.61527700	2.17918800	2.02783100
H	4.26781500	0.18101300	2.82361600
C	1.79263800	1.82775300	-2.03952300
C	3.15544500	3.59197300	-1.12394000
C	4.36226800	3.10112600	1.03046700
H	5.27407200	2.45156500	2.84837500
C	2.30700100	3.13897400	-2.11275100
H	1.13334900	1.42501100	-2.80051900
H	3.56465700	4.59848800	-1.16474500
H	4.80839100	4.09119500	1.05368400

H	2.02597100	3.77191800	-2.94778800
C	2.59326600	-1.78442500	1.65271400
O	3.26020900	-1.87193200	2.68374800
C	1.63440300	-2.83372300	1.18202000
C	1.18927400	-3.81207600	2.07056000
C	1.08296600	-2.69735200	-0.11441600
C	0.14784800	-4.66302400	1.69577200
H	1.64664100	-3.86835400	3.05415000
C	0.00329800	-3.54074400	-0.44447200
C	-0.45770300	-4.51554800	0.44398400
H	-0.20305200	-5.42931900	2.38247900
H	-0.46335000	-3.45860000	-1.42331000
H	-1.28345800	-5.16266000	0.15925700
N	2.09752800	1.01427200	-1.03735100
Ni	1.52530800	-0.81966200	-0.75284800
O	0.81860700	-1.00372800	-2.56288000
C	1.36672700	-1.97514400	-3.14639800
O	2.05588400	-2.88653500	-2.56781000
O	1.20689100	-2.06330600	-4.47369500
H	1.67076400	-2.86860500	-4.76341800
H	1.80106800	-2.71496600	-1.34204600
P	-1.69941200	0.45743700	0.15206300
C	-3.07446200	-0.07059100	-0.97202800
C	-4.41859800	-0.18214200	-0.58138900
C	-2.72797400	-0.39279100	-2.29579000
C	-5.39257200	-0.59144200	-1.49426700
H	-4.70438400	0.04592200	0.44127300
C	-3.70476400	-0.79214500	-3.21036400
H	-1.68754200	-0.34337800	-2.60745400
C	-5.03906900	-0.89295200	-2.81152800
H	-6.42866300	-0.67481500	-1.17555400
H	-3.42038700	-1.03459700	-4.23123700
H	-5.79881600	-1.21157100	-3.52065800
C	-1.79949500	2.30707800	0.09177200
C	-2.79614100	3.03184000	-0.57904500
C	-0.76552500	3.01892200	0.72684600
C	-2.76471900	4.42899600	-0.60519800
H	-3.60068100	2.50530900	-1.08284800
C	-0.74148600	4.41295600	0.71131900
H	0.02487500	2.47442600	1.23861200
C	-1.74173300	5.12318500	0.04198000
H	-3.54553500	4.97398400	-1.13001200
H	0.06201200	4.94379500	1.21543800
H	-1.72098400	6.20974400	0.02247600

C	-2.37391600	0.08084800	1.83538200
C	-2.06920900	-1.18041700	2.37548300
C	-3.13740900	0.97491600	2.60311900
C	-2.53262100	-1.54488900	3.64019100
H	-1.46111400	-1.87888500	1.80635700
C	-3.59330500	0.61189900	3.87245800
H	-3.37109100	1.96065400	2.21173900
C	-3.29499800	-0.64903100	4.39280300
H	-2.28576600	-2.52439600	4.04126300
H	-4.18100800	1.31682100	4.45534000
H	-3.64781300	-0.92851000	5.38215200
12			
N	2.33840600	1.47143100	-0.06486000
C	3.45143800	0.66789400	0.00601700
C	3.17829700	-0.71599100	-0.24235000
C	4.77627900	1.03741400	0.26051600
C	4.22620900	-1.68481100	-0.27534000
C	5.79960300	0.06719700	0.25034800
H	4.99662200	2.07714800	0.45674500
C	1.57164700	-2.31073700	-0.76053600
C	3.86185800	-3.01714800	-0.58665300
C	5.55462700	-1.26640800	-0.01445000
H	6.81750000	0.39278200	0.45089700
C	2.54382500	-3.32705200	-0.84131200
H	0.52851800	-2.54572300	-0.93545100
H	4.63269400	-3.78319300	-0.62802700
H	6.35859000	-1.99681800	-0.03258800
H	2.23621900	-4.33740200	-1.09088600
C	2.34002000	2.84107200	0.11567000
O	3.31058900	3.53341200	0.42494000
C	0.97915300	3.36537100	-0.17774600
C	0.72550300	4.73546700	-0.25078100
C	0.00080700	2.39867300	-0.48314600
C	-0.52802600	5.17809300	-0.67359300
H	1.52429200	5.42855400	0.00050400
C	-1.23597300	2.86585600	-0.93994100
C	-1.49744200	4.24019900	-1.03607800
H	-0.74292200	6.24176600	-0.73997100
H	-2.02117900	2.17678600	-1.23463300
H	-2.46909900	4.57598600	-1.39323600
N	1.86424000	-1.04923900	-0.46308200
Ni	0.68057800	0.61076400	-0.33192300
P	-1.32993500	-0.44449200	0.03529800
C	-2.73772600	0.46643600	0.82491100

C	-2.63564300	0.84125300	2.17388100
C	-3.87699500	0.85517600	0.10419300
C	-3.64933600	1.57683400	2.78627700
H	-1.76620100	0.55671000	2.75743700
C	-4.89263900	1.58903400	0.72068600
H	-3.97881000	0.59143900	-0.94316100
C	-4.78282300	1.95208900	2.06266200
H	-3.55073700	1.85671800	3.83145200
H	-5.76781600	1.87880900	0.14529500
H	-5.57212000	2.52533100	2.54105200
C	-0.99567800	-1.77019200	1.29007600
C	-0.05768600	-1.47580100	2.29524900
C	-1.62685700	-3.02242400	1.30542300
C	0.22085600	-2.39941300	3.30337600
H	0.47102600	-0.52620500	2.27874000
C	-1.33689200	-3.95062600	2.30768000
H	-2.33693200	-3.28924100	0.53062500
C	-0.41846700	-3.64039000	3.31183200
H	0.94707300	-2.15181300	4.07262200
H	-1.83163000	-4.91830900	2.30117000
H	-0.19609900	-4.36418400	4.09115300
C	-2.07845300	-1.27825700	-1.42824400
C	-1.36893300	-1.21790400	-2.63888300
C	-3.31446500	-1.95127300	-1.40366500
C	-1.86805300	-1.83213400	-3.78991000
H	-0.42531700	-0.68005800	-2.67910200
C	-3.81040800	-2.56552300	-2.55343300
H	-3.90167800	-1.97755000	-0.49080800
C	-3.08639000	-2.51001000	-3.74772800
H	-1.30657200	-1.77244100	-4.71800000
H	-4.76599000	-3.08170100	-2.51844200
H	-3.47724800	-2.98581500	-4.64299200

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N	-1.66758400	1.15132400	0.19157000
C	-2.83861300	0.45712500	0.40428600
C	-2.74279300	-0.93986600	0.10798000
C	-4.06637600	0.94696200	0.85717900
C	-3.86194300	-1.81149400	0.25732200
C	-5.16641700	0.07571900	1.00419900
H	-4.15402800	1.99848400	1.09088400
C	-1.37456200	-2.67476300	-0.61574400
C	-3.66189300	-3.17493500	-0.06942500
C	-5.08957100	-1.27308400	0.71606300
H	-6.10628000	0.49267400	1.35735700

C	-2.42697300	-3.60503100	-0.50492900
H	-0.39052900	-2.99100600	-0.94470500
H	-4.49090400	-3.87183000	0.02801700
H	-5.94962600	-1.92598800	0.83390800
H	-2.24769400	-4.64408200	-0.76168800
C	-1.48295600	2.50152000	0.43102200
O	-2.32898300	3.27422600	0.87881200
C	-0.09713900	2.87983400	0.04472500
C	0.35907700	4.19513600	0.13441400
C	0.70220300	1.83270600	-0.45119500
C	1.65291200	4.49926800	-0.29058900
H	-0.30932900	4.95700700	0.52712600
C	1.99024700	2.16495800	-0.89327800
C	2.45995400	3.48444200	-0.81001800
H	2.02647800	5.51829000	-0.22978800
H	2.64328900	1.41161100	-1.32771200
H	3.46312100	3.71863400	-1.16133700
N	-1.51925500	-1.38674200	-0.32353400
Ni	-0.22357000	0.15160800	-0.42320900
Br	1.74254500	-1.21861700	-0.99920500
C	2.83446400	-0.95624900	0.67489700
C	4.22146000	-1.54690300	0.50543800
H	4.14635800	-2.61557900	0.26896000
H	4.72705700	-1.06508100	-0.34031800
H	2.82423800	0.12548900	0.80631500
H	2.24531200	-1.44041600	1.45376300
C	5.05690600	-1.35673900	1.78588700
H	5.11920000	-0.28675400	2.02470300
H	4.54332400	-1.83394500	2.63145600
C	6.46897200	-1.93682200	1.64811400
H	7.01801100	-1.45395700	0.83117100
H	7.04318200	-1.79067400	2.56918400
H	6.43769400	-3.01288100	1.43989300

14-ts

N	-0.78440100	1.43316900	0.04505200
C	-2.12728200	1.31511800	0.34848500
C	-2.66535600	0.01413900	0.09552800
C	-2.98955600	2.29234600	0.85074600
C	-4.03989400	-0.28309500	0.33104300
C	-4.34721700	1.98658600	1.08906900
H	-2.60069100	3.28134700	1.04661500
C	-2.23696600	-2.14110600	-0.67030300
C	-4.47356600	-1.59670400	0.02723300
C	-4.88056400	0.73750800	0.84152500

H	-4.98830300	2.77302000	1.47910500
C	-3.58045300	-2.51917500	-0.47421200
H	-1.50666400	-2.84163900	-1.06155100
H	-5.51520600	-1.86288700	0.19019900
H	-5.92950200	0.52438000	1.02631500
H	-3.88964600	-3.52962300	-0.72106600
C	-0.04509200	2.59650300	0.16405800
O	-0.45860900	3.67344100	0.59062500
C	1.33857500	2.34523400	-0.31752800
C	2.30166900	3.35573300	-0.35296300
C	1.61144100	1.04132700	-0.76130500
C	3.57268000	3.06951800	-0.84919200
H	2.03206500	4.34699400	0.00199300
C	2.88642800	0.76903500	-1.26820500
C	3.85754100	1.78057400	-1.30810500
H	4.33490000	3.84350500	-0.88616100
H	3.13946100	-0.21906300	-1.63821000
H	4.84426600	1.55482400	-1.70715000
N	-1.78994900	-0.92204500	-0.39249000
Ni	0.07537400	-0.11641000	-0.59651200
Br	1.10689500	-2.09397500	-1.31632500
C	1.01238500	-1.51612200	1.12747900
C	2.46436500	-1.62036600	1.46307800
H	3.01543000	-0.78917900	1.01339100
H	2.88691600	-2.55308300	1.07790700
H	0.51915100	-0.61699300	1.49171300
H	0.40005500	-2.40493600	1.23168900
C	2.63232300	-1.55934500	3.00533900
H	2.04352000	-2.35779900	3.47574300
H	2.23162900	-0.60862100	3.37942100
C	4.10470600	-1.69557600	3.41245800
H	4.70909800	-0.88994000	2.98044300
H	4.21043600	-1.64984700	4.50183000
H	4.52359700	-2.65004300	3.07319000

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N	-0.63201700	1.41538400	-0.07187500
C	-1.98608600	1.39736100	0.22838200
C	-2.60425700	0.12572600	0.02959700
C	-2.78329400	2.45562400	0.66308900
C	-3.99824000	-0.06620000	0.24411900
C	-4.16562700	2.25627900	0.88234500
H	-2.33416100	3.42742600	0.81111100
C	-2.29867700	-2.08840200	-0.61880600
C	-4.51077900	-1.36305900	-0.00470400

C	-4.77669700	1.03577200	0.68207000
H	-4.75865400	3.10351000	1.21624100
C	-3.66923600	-2.36592700	-0.43776200
H	-1.59915100	-2.84635400	-0.95724100
H	-5.57067300	-1.55319400	0.14583200
H	-5.84155300	0.90472300	0.85143600
H	-4.03956600	-3.36531500	-0.64091600
C	0.18686900	2.53030500	-0.01045600
O	-0.17058100	3.66428900	0.29603400
C	1.56624700	2.15066500	-0.40991600
C	2.58737800	3.09481700	-0.53943100
C	1.79039000	0.79845000	-0.69739700
C	3.84977900	2.68010300	-0.96165900
H	2.36712000	4.13485600	-0.31439700
C	3.05023400	0.38176800	-1.12309900
C	4.07318100	1.33165900	-1.25536600
H	4.65545100	3.40146300	-1.06771900
H	3.24421400	-0.65838800	-1.35495200
H	5.05473600	1.00688200	-1.59267000
N	-1.78404200	-0.88788200	-0.38756500
Ni	0.17459000	-0.22952300	-0.49857500
Br	0.99462700	-2.23516700	-1.40309200
C	0.63842400	-0.66280300	1.42756900
C	2.05453700	-0.98385800	1.81790400
H	2.68930000	-0.09596800	1.75101000
H	2.47245400	-1.74447600	1.15289700
H	0.21835000	0.21321000	1.91773000
H	-0.03692200	-1.51705800	1.46433700
C	2.07067600	-1.51273800	3.27535100
H	1.61936900	-0.76792200	3.94437900
H	1.44683600	-2.41376600	3.34390300
C	3.49389500	-1.83375000	3.74755300
H	4.13007000	-0.94129400	3.72418300
H	3.48739200	-2.21467100	4.77510700
H	3.95968300	-2.59373700	3.10955400

16-ts

N	-0.75686000	1.35937300	0.15472600
C	-2.11413400	1.26298800	0.41631400
C	-2.66031400	-0.01491600	0.10198100
C	-2.96755700	2.24604100	0.91199000
C	-4.04345400	-0.29625700	0.28182300
C	-4.33958600	1.95912000	1.09568700
H	-2.56975000	3.22546900	1.13788700
C	-2.23337200	-2.14591100	-0.73358000

C	-4.48548900	-1.59275300	-0.07925100
C	-4.88179200	0.72616000	0.79611100
H	-4.98092900	2.74519800	1.48527300
C	-3.58815700	-2.50824200	-0.58528900
H	-1.49644600	-2.83605900	-1.12909200
H	-5.53473900	-1.85054200	0.04271100
H	-5.93912300	0.52558700	0.94321400
H	-3.90140600	-3.50589800	-0.87467600
C	-0.03683900	2.52798000	0.11406900
O	-0.44977100	3.65113500	0.39960100
C	1.33860500	2.24109800	-0.38620400
C	2.20332500	3.26132200	-0.78058100
C	1.70162900	0.89201200	-0.53939900
C	3.44344800	2.93509900	-1.33119900
H	1.87863800	4.29101800	-0.66129100
C	2.94211500	0.56579600	-1.09113400
C	3.80300900	1.59322300	-1.49315800
H	4.12674200	3.72169500	-1.63955200
H	3.23172000	-0.46984000	-1.22014500
H	4.76354100	1.33853800	-1.93381100
N	-1.78108600	-0.94432900	-0.39584800
Ni	0.11452800	-0.22491800	-0.40255800
Br	1.03813700	-2.18639200	-1.33994300
C	1.26207100	-0.20969000	1.36501100
C	2.58691700	-0.88847500	1.61842500
H	3.41712400	-0.19937600	1.43708300
H	2.70869400	-1.74532500	0.94991400
H	1.14883800	0.76044300	1.83971800
H	0.41932300	-0.85722500	1.63296000
C	2.63846800	-1.37591300	3.08546700
H	2.46963100	-0.52924300	3.76458900
H	1.82094500	-2.08732700	3.26372500
C	3.97923700	-2.04200700	3.41801800
H	4.81359300	-1.34387200	3.28172300
H	3.99763800	-2.38712500	4.45784000
H	4.15942700	-2.90913300	2.77202100

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N	-0.38885800	0.85563600	-0.75929700
C	-1.32431100	1.86080300	-0.56887700
C	-2.50417500	1.38763400	0.07201400
C	-1.24190500	3.20849400	-0.90300700
C	-3.59093100	2.25376400	0.36865300
C	-2.32697000	4.06808600	-0.61187200
H	-0.34568900	3.58200400	-1.37894600

C	-3.58327000	-0.45513200	1.01910400
C	-4.70665800	1.68005200	1.02670600
C	-3.47796500	3.62102900	0.00442000
H	-2.24076800	5.11601600	-0.88588200
C	-4.69912300	0.34018200	1.35135900
H	-3.53921100	-1.51418600	1.24433500
H	-5.56013100	2.30662900	1.27371500
H	-4.29731800	4.29953100	0.22332100
H	-5.53891300	-0.12297400	1.85834600
C	0.92134000	1.04123700	-1.09737300
O	1.45252300	2.10205300	-1.42479000
C	1.65231900	-0.26939400	-0.96399000
C	0.95128400	-1.43834000	-1.34641300
C	2.94276900	-0.36528800	-0.39347000
C	1.51586900	-2.71324300	-1.16398600
H	0.07843700	-1.34704200	-2.00436500
C	3.47390800	-1.65011600	-0.23220900
C	2.77818800	-2.81058100	-0.60222300
H	0.95898200	-3.59460600	-1.46053600
H	4.46011400	-1.76063400	0.20608800
H	3.23720900	-3.78276700	-0.44793500
N	-2.52315100	0.05307400	0.40045800
Ni	-0.92958100	-0.85844600	-0.20389600
Br	-1.53491400	-3.02700600	0.41145800
C	3.70111800	0.88008600	0.03937800
C	5.06733500	0.65356800	0.69737400
H	5.73276800	0.11287200	0.00880300
H	4.95987900	0.01806200	1.58827300
H	3.81532700	1.53468500	-0.83165800
H	3.06429500	1.45274600	0.72770800
C	5.73983100	1.97266400	1.10249300
H	5.84392700	2.61197400	0.21495300
H	5.08097600	2.51708000	1.79336300
C	7.11162900	1.77139200	1.75477000
H	7.80390100	1.26033800	1.07414700
H	7.56519400	2.72952700	2.03264800
H	7.03346900	1.16364800	2.66476400
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N	0.74005800	0.20057600	-0.11880300
C	1.81937000	-0.68458900	-0.16874300
C	3.10589900	-0.08715400	0.06743300
C	1.73533900	-2.04438500	-0.42309500
C	4.27757400	-0.90261900	0.03611800
C	2.90941500	-2.83310400	-0.45086100

H	0.76618700	-2.49020800	-0.59553900
C	4.32031800	1.81303700	0.53407000
C	5.51550200	-0.25384900	0.27775600
C	4.15577200	-2.29145900	-0.22881500
H	2.81098600	-3.89618000	-0.65337200
C	5.54229300	1.09969300	0.52658500
H	4.31670500	2.88461000	0.72879900
H	6.43241500	-0.83860400	0.26317500
H	5.04922800	-2.90986900	-0.25192400
H	6.47512000	1.62221100	0.71494100
C	-0.60096000	-0.06721500	-0.29094300
O	-1.03830500	-1.20013000	-0.48035300
C	-1.48154000	1.15149300	-0.22892700
C	-1.03733500	2.34926100	-0.81535100
C	-2.75518000	1.09863400	0.38362900
C	-1.82776700	3.49551600	-0.80603700
H	-0.07161100	2.37401800	-1.31297000
C	-3.52304600	2.27217600	0.39628800
C	-3.07825900	3.45612200	-0.18926400
H	-1.47038700	4.40725100	-1.27631700
H	-4.49572400	2.24949900	0.88277700
H	-3.70589300	4.34309200	-0.16342400
N	3.14689200	1.25142900	0.31422800
C	-3.33617700	-0.14818100	1.02039100
C	-4.21449700	-0.96344600	0.04879900
H	-5.02810600	-0.32626100	-0.32754900
H	-3.60207300	-1.24660400	-0.81410200
H	1.02639000	1.14586100	0.11862200
H	-2.54135200	-0.79620600	1.39879100
H	-3.94606400	0.15576200	1.88228600
C	-4.80506600	-2.22098600	0.69801900
H	-5.39063400	-1.93751400	1.58499900
H	-3.98443100	-2.85478800	1.06159400
C	-5.68763300	-3.02880100	-0.25973800
H	-5.11974500	-3.35166400	-1.14076100
H	-6.08977300	-3.92581900	0.22560900
H	-6.53757400	-2.43245600	-0.61467600

19-ts

N	1.34960600	0.92349800	-1.52335900
C	0.98662900	2.25396800	-1.58526300
C	0.78080900	2.85955400	-0.30380100
C	0.79498600	3.04611200	-2.72084600
C	0.38695400	4.22406700	-0.17936200
C	0.40713200	4.39729100	-2.58650100

H	0.94729300	2.60531600	-3.69587400
C	0.78913000	2.55809300	2.00302900
C	0.20049400	4.72169900	1.13360700
C	0.20260600	4.99144400	-1.35695300
H	0.26711000	4.98222700	-3.49209500
C	0.39834800	3.89529900	2.21836100
H	0.95792000	1.87973900	2.83285100
H	-0.10192900	5.75702300	1.27087500
H	-0.09716100	6.03227800	-1.27557700
H	0.25759500	4.25110600	3.23380200
C	1.57103000	0.11003100	-2.61777100
O	1.53399700	0.45772600	-3.79799300
C	1.85305000	-1.27239600	-2.14626300
C	2.07375300	-2.32443800	-3.03817500
C	1.84435100	-1.46529200	-0.75460100
C	2.28725500	-3.60912900	-2.53934600
H	2.06422200	-2.11511200	-4.10468700
C	2.05132700	-2.76092400	-0.26625600
C	2.27126400	-3.82225400	-1.15734200
H	2.46127200	-4.44011300	-3.21824800
H	2.04157000	-2.95987200	0.80039300
H	2.42805000	-4.82426000	-0.76318400
N	0.97637900	2.05488500	0.78917000
Ni	1.48036800	0.16571700	0.20450000
Br	1.91503700	-0.64843700	2.37042700
C	3.75981000	0.41167400	1.04173100
C	4.77244200	-0.68585200	1.09691100
H	4.44488600	-1.53103400	0.48397200
H	4.90232600	-1.04425700	2.12261000
H	3.58062700	0.82830700	0.05340300
H	3.78136100	1.16537300	1.82105500
C	6.12301400	-0.15687400	0.54463600
H	6.44037700	0.72375100	1.11872400
H	5.98807900	0.17393500	-0.49307500
C	7.21321200	-1.23382600	0.60663900
H	6.92956300	-2.11506400	0.01999700
H	8.15863800	-0.85179900	0.20616600
H	7.39137600	-1.55938700	1.63816800
P	-2.04444100	-0.52966200	0.14981300
C	-2.63939000	-1.62067000	-1.22227800
C	-3.90488100	-1.51393600	-1.82166400
C	-1.74750100	-2.59767500	-1.69642100
C	-4.27145600	-2.36942700	-2.86261000
H	-4.60421400	-0.75729200	-1.47836500

C	-2.11866200	-3.45660300	-2.73197600
H	-0.75569000	-2.68104200	-1.26066800
C	-3.38075600	-3.34380200	-3.31835400
H	-5.25366700	-2.27250400	-3.31864400
H	-1.41291000	-4.20233700	-3.08778300
H	-3.66626500	-4.00574300	-4.13194000
C	-3.20762600	0.91048900	0.05073400
C	-2.89208800	1.92327500	-0.87314500
C	-4.34610400	1.06958600	0.85636100
C	-3.69928800	3.05405000	-0.99757400
H	-2.00873400	1.82559500	-1.49963800
C	-5.14854600	2.20734900	0.73745400
H	-4.60782300	0.30360500	1.57989700
C	-4.82941300	3.20066000	-0.18949000
H	-3.43653500	3.82375200	-1.71842800
H	-6.02657900	2.31377300	1.36979300
H	-5.45502400	4.08489400	-0.27997700
C	-2.62781400	-1.41691500	1.66732000
C	-2.09577100	-0.99672900	2.89926700
C	-3.52695000	-2.49449200	1.65947100
C	-2.46835500	-1.62031500	4.09023600
H	-1.37995800	-0.17885900	2.92208500
C	-3.89104700	-3.12633700	2.85097400
H	-3.94284700	-2.84308100	0.71921400
C	-3.36689200	-2.68949100	4.06874700
H	-2.04860200	-1.27899000	5.03313300
H	-4.58739600	-3.96087000	2.82573500
H	-3.65112800	-3.18296600	4.99452000

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N	-1.18986100	0.87235600	1.40496200
C	-0.96757300	2.23688300	1.45377100
C	-0.69772600	2.83433200	0.18325400
C	-0.98178400	3.06394500	2.57849300
C	-0.45551200	4.23314000	0.05531400
C	-0.73092700	4.44671400	2.44369500
H	-1.18603700	2.62730900	3.54551200
C	-0.47657100	2.48726300	-2.10930500
C	-0.22157400	4.72445200	-1.25477900
C	-0.47282900	5.03676000	1.22233600
H	-0.74677700	5.06004300	3.34089600
C	-0.23386600	3.86096200	-2.32808600
H	-0.49243800	1.77011400	-2.92357400
H	-0.03830000	5.78689400	-1.39730300
H	-0.28755600	6.10400800	1.14014100

H	-0.05901000	4.21330800	-3.33936100
C	-1.57094800	0.08257200	2.46894700
O	-1.69438300	0.45798600	3.63545100
C	-1.78132800	-1.31054500	1.99983500
C	-2.10250000	-2.34969900	2.87888600
C	-1.62426300	-1.54709100	0.62847500
C	-2.27029200	-3.63962000	2.37884300
H	-2.21472700	-2.12118800	3.93550000
C	-1.79747900	-2.83464200	0.12539600
C	-2.11527200	-3.87543600	1.00907200
H	-2.52115000	-4.45823700	3.04810300
H	-1.70188200	-3.03327300	-0.93507900
H	-2.24578100	-4.88113200	0.61592800
N	-0.69919100	1.99621000	-0.89964100
Ni	-1.16148800	0.06974900	-0.31570400
Br	-1.09042700	-0.84681500	-2.53589400
C	-3.15468900	0.50499000	-0.57402800
C	-4.16781300	-0.60214400	-0.70587200
H	-4.28099000	-1.14612100	0.23706400
H	-3.84674700	-1.31987900	-1.46717100
H	-3.31575800	1.15681200	0.28282300
H	-3.01620200	1.06875400	-1.49459000
C	-5.54042900	-0.01364000	-1.11530100
H	-5.86155400	0.72749800	-0.37072300
H	-5.43655100	0.52475300	-2.06697700
C	-6.61205500	-1.10176500	-1.25336500
H	-6.75681700	-1.63637100	-0.30702200
H	-7.57636100	-0.67069500	-1.54633800
H	-6.32863900	-1.83952200	-2.01339400
P	1.59736200	-0.50878000	-0.06490500
C	2.35450700	0.04043600	1.53096900
C	3.50815500	0.83365000	1.62914000
C	1.71754800	-0.36801400	2.71623900
C	3.99830300	1.22203300	2.87836800
H	4.03123900	1.14831100	0.73286100
C	2.20965500	0.01837200	3.96193000
H	0.83984500	-1.00361800	2.66812700
C	3.34956800	0.82080700	4.04669600
H	4.89291600	1.83700300	2.93437100
H	1.69355400	-0.30104200	4.86279800
H	3.73029800	1.12900200	5.01682300
C	2.64408700	0.29469100	-1.36002400
C	2.68527200	1.69919900	-1.42954300
C	3.35087400	-0.44166500	-2.32278200

C	3.42760300	2.34465600	-2.41848200
H	2.14958800	2.29545300	-0.69699600
C	4.08238800	0.20655700	-3.32022900
H	3.33576900	-1.52558200	-2.29576500
C	4.12673400	1.59996200	-3.37087200
H	3.45349000	3.43087800	-2.44622700
H	4.62297500	-0.38374400	-4.05545700
H	4.70020900	2.10223200	-4.14538400
C	2.09340800	-2.29023600	-0.15200500
C	1.48817800	-3.11747300	-1.11411700
C	3.05758900	-2.84456800	0.70553400
C	1.84940000	-4.46168300	-1.21944400
H	0.73783400	-2.70526800	-1.78121500
C	3.40699100	-4.19214600	0.60356900
H	3.53781300	-2.22639500	1.45629100
C	2.80582400	-5.00420800	-0.35938100
H	1.37465300	-5.08593200	-1.97201300
H	4.15370200	-4.60475800	1.27710700
H	3.08009200	-6.05301800	-0.43793700

21-ts

N	-0.54635800	1.06207300	-0.06378000
C	0.46985100	1.98545200	-0.17598400
C	1.60204400	1.54281200	-0.92057500
C	0.47386900	3.31524400	0.25695200
C	2.64725900	2.42525200	-1.31720600
C	1.52681500	4.18074400	-0.10191500
H	-0.34478300	3.68842400	0.86099700
C	2.58559900	-0.27710100	-1.99911900
C	3.67392600	1.87084500	-2.12150800
C	2.59171900	3.77294300	-0.88536700
H	1.48515700	5.21003900	0.24505900
C	3.63323000	0.53796900	-2.47347300
H	2.54474700	-1.33619200	-2.21923400
H	4.48721600	2.50833300	-2.45978400
H	3.38298200	4.46150200	-1.16585700
H	4.40171700	0.09515800	-3.09830400
C	-1.50384500	1.22821800	0.96311300
O	-1.16760600	1.47712400	2.11937900
C	-2.93743700	1.12424200	0.57263800
C	-3.90873900	1.10952200	1.58616100
C	-3.33868100	1.11501000	-0.77139100
C	-5.26100300	1.07094500	1.26120600
H	-3.57987400	1.12898100	2.61983900
C	-4.69562600	1.07961600	-1.09379600

H	-2.58567200	1.12500300	-1.55092100
C	-5.65672600	1.05658100	-0.08068800
H	-6.00872500	1.05205600	2.04953900
H	-5.00188800	1.07269200	-2.13647000
H	-6.71349300	1.02933100	-0.33457100
N	1.61285700	0.21071200	-1.23597900
Ni	0.09801200	-0.73072000	-0.43960500
O	-1.44424200	-1.50836800	0.25011100
C	-2.13661000	-1.86619200	-0.78999400
O	-1.82573900	-1.64019000	-1.96144500
O	-3.26726200	-2.53008900	-0.45583500
H	-3.70617500	-2.72679500	-1.30119000
Br	1.18531600	-2.85487500	-0.40378400
C	0.98074500	-1.32059800	1.74290000
H	0.28737600	-0.48587000	1.82192500
H	0.56395100	-2.25960900	2.08405800
C	2.40986900	-1.01893400	2.00796300
H	2.77398500	-0.23523200	1.33601600
H	3.03778500	-1.90408500	1.87657900
C	2.51887800	-0.49327200	3.47201400
H	1.88527800	0.39393000	3.58604300
H	2.13322100	-1.25214200	4.16397000
C	3.97097800	-0.15373600	3.82989500
H	4.36768600	0.62806200	3.17203000
H	4.03610400	0.20919600	4.86141200
H	4.61961500	-1.03268200	3.73989700
22			
N	-0.59175700	0.98873000	0.04322100
C	0.33631000	1.99349800	-0.13061800
C	1.50088000	1.60425900	-0.85183800
C	0.21508300	3.34118300	0.21762400
C	2.46321200	2.54929500	-1.30230700
C	1.18149400	4.27722000	-0.20765200
H	-0.63522500	3.67529000	0.80034600
C	2.65865500	-0.18583100	-1.79780000
C	3.54799700	2.04117800	-2.05768900
C	2.27962200	3.91419900	-0.96368900
H	1.04378300	5.31919200	0.06839600
C	3.63380100	0.68927300	-2.31612700
H	2.71046000	-1.25794500	-1.94300600
H	4.30553600	2.72662200	-2.42949800
H	3.00696200	4.65059900	-1.29143900
H	4.44938300	0.27623300	-2.90000600
C	-1.61557000	1.18079100	1.01729800

O	-1.34715000	1.51799900	2.16495500
C	-3.01896800	1.00652600	0.55734100
C	-4.03961700	0.97706500	1.52264700
C	-3.34963000	0.95497800	-0.80538400
C	-5.37020700	0.87822700	1.13088200
H	-3.76564000	1.03098100	2.57102000
C	-4.68682000	0.86486300	-1.19380100
H	-2.55914200	0.97314200	-1.54585800
C	-5.69571400	0.82383200	-0.22936800
H	-6.15591700	0.84437800	1.88056900
H	-4.93959500	0.82770200	-2.24994100
H	-6.73643400	0.75121300	-0.53493600
N	1.63366600	0.26083600	-1.07920200
Ni	0.19424200	-0.76122800	-0.22210400
O	-1.30277500	-1.61654400	0.48520900
C	-1.98311300	-1.91242600	-0.58458600
O	-1.66521500	-1.56136500	-1.72428600
O	-3.08650000	-2.63868300	-0.32166900
H	-3.51601100	-2.78027000	-1.18311500
Br	1.21101100	-2.89537700	-0.64477800
C	0.95448000	-0.79099300	1.72607900
H	0.29788000	-0.02952500	2.14279000
H	0.62688800	-1.80822200	1.91999300
C	2.42033000	-0.53190300	1.83938700
H	2.67876300	0.46812400	1.47447000
H	2.99078500	-1.27225600	1.27109300
C	2.81941600	-0.61940200	3.34132300
H	2.22885000	0.10238300	3.91902000
H	2.56709700	-1.61535200	3.72540800
C	4.31528400	-0.34794200	3.54185500
H	4.58661600	0.65510600	3.19204100
H	4.58198700	-0.41703400	4.60245800
H	4.92701600	-1.07334900	2.99307200

23-ts

N	-0.15564800	-1.05946000	-0.96332700
C	-1.51505900	-1.33273600	-0.95773300
C	-2.25261800	-0.50227200	-0.07072500
C	-2.20772700	-2.29466200	-1.68792700
C	-3.65761800	-0.62974400	0.09618700
C	-3.60825400	-2.41285700	-1.53373600
H	-1.66341700	-2.95515000	-2.34788500
C	-2.11079900	1.19835000	1.52794500
C	-4.26846900	0.23782900	1.03678000
C	-4.33227400	-1.61111700	-0.67339700

H	-4.12378300	-3.17257900	-2.11494000
C	-3.50350600	1.13883600	1.74755900
H	-1.46023700	1.87192200	2.07380000
H	-5.34174600	0.17606000	1.19763900
H	-5.40710300	-1.72683100	-0.56924900
H	-3.94895600	1.80158800	2.48174600
C	0.82193000	-1.85446500	-1.49735200
O	0.62777800	-2.88321600	-2.14168600
C	2.16438100	-1.21870000	-1.32598200
C	3.16000700	-1.54913100	-2.24433200
C	2.32569700	-0.13828400	-0.41998500
C	4.31293400	-0.76973300	-2.33759000
H	2.98324800	-2.38857400	-2.90991200
C	3.46372900	0.68621700	-0.60593000
C	4.45103200	0.36672400	-1.53422100
H	5.08731600	-1.02738100	-3.05512900
H	3.62070200	1.52713700	0.06130100
H	5.33462400	0.99332200	-1.61908000
N	-1.52845400	0.41165000	0.63910900
Ni	0.37644200	0.26532100	0.25594800
O	0.80317500	1.62200300	1.55498600
C	1.79123900	1.36933400	2.31931400
O	2.68378800	0.50562900	2.11691300
O	1.86578300	2.13936000	3.41734500
H	2.63881400	1.82820200	3.92061200
H	2.33275200	-0.09520500	0.88866100
Br	0.32755000	-1.61190200	2.08104500
C	0.39061000	1.71852100	-1.22675600
H	1.19346700	2.33067900	-0.82057000
H	0.70171900	1.14960400	-2.09992500
C	-0.90514200	2.46151700	-1.41005500
H	-1.71124100	1.78211900	-1.71043300
H	-1.21119100	2.94941500	-0.47792800
C	-0.74493300	3.54746000	-2.50461500
H	-0.43256800	3.07240900	-3.44379100
H	0.06249400	4.23436700	-2.21882500
C	-2.04058000	4.33598700	-2.72889600
H	-1.90776800	5.09573700	-3.50742400
H	-2.85751300	3.67483000	-3.04179300
H	-2.35722500	4.84791100	-1.81224100
BuBr			
C	-1.12670100	-0.21346800	0.00011900
C	0.02667500	0.77878200	0.00013600
H	-1.04752100	-0.86364600	-0.87981300

H	-1.04774700	-0.86339900	0.88025500
Br	1.78817300	-0.13581100	-0.00002900
H	0.03106100	1.41050500	-0.88943400
H	0.03116400	1.41034500	0.88981700
C	-2.48834000	0.50231100	-0.00015300
H	-2.55674200	1.15803300	-0.87936500
H	-2.55687500	1.15848700	0.87871300
C	-3.66645700	-0.47787800	0.00001000
H	-3.64321100	-1.12484700	0.88514100
H	-4.62402300	0.05458000	-0.00008200
H	-3.64320600	-1.12514500	-0.88490300
Br-			
Br	0.00000000	0.00000000	0.00000000
CO₂			
C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16959300
O	0.00000000	0.00000000	-1.16959300
HCO₃⁻			
C	-0.15844600	0.07272900	-0.00002900
O	0.14147800	1.29165200	0.00002600
O	1.00488900	-0.79894600	0.00002000
H	1.71628100	-0.13784000	0.00005400
O	-1.24206800	-0.53002300	-0.00003000
PPh₃			
P	0.00264000	-0.00223500	-1.20480200
C	-1.17871900	-1.18227900	-0.39983400
C	-1.92266700	-0.90102200	0.75676700
C	-1.36048500	-2.42704000	-1.02772700
C	-2.81448600	-1.84271100	1.27563200
H	-1.80946600	0.05850800	1.25229400
C	-2.24289900	-3.37175100	-0.50354300
H	-0.81012400	-2.65320700	-1.93829900
C	-2.97478000	-3.08024000	0.65008600
H	-3.38477400	-1.60718100	2.17074100
H	-2.36758100	-4.32977700	-1.00179000
H	-3.67050400	-3.81077900	1.05455800
C	-0.43026800	1.61194800	-0.40396400
C	-1.42023200	2.38720100	-1.03193100
C	0.18040900	2.11675300	0.75476700
C	-1.80564600	3.62025600	-0.50592100
H	-1.88917500	2.02221600	-1.94283800
C	-0.19718100	3.35672400	1.27565600
H	0.95624600	1.54156600	1.25103100
C	-1.19245800	4.10973200	0.64997300

H	-2.57647300	4.20333300	-1.00338100
H	0.28776300	3.73367700	2.17281200
H	-1.48421700	5.07472600	1.05650000
C	1.61620200	-0.43278900	-0.40120000
C	1.74636300	-1.21081500	0.75962900
C	2.78289000	0.03315900	-1.03116000
C	3.00886300	-1.50637000	1.27983500
H	0.85876700	-1.59082400	1.25655300
C	4.04299200	-0.25159400	-0.50562800
H	2.70093800	0.61978100	-1.94319600
C	4.15914700	-1.02548900	0.65137800
H	3.09238600	-2.11326200	2.17816200
H	4.93384300	0.12054000	-1.00488000
H	5.14050600	-1.25781900	1.05687500

1a

Ni	1.72255300	-0.17544300	-1.20813100
O	3.13538500	0.31211500	0.07888000
C	4.03790000	-0.08402200	-0.83117500
O	3.43335400	-0.48524100	-1.96112600
O	5.25544300	-0.08190600	-0.65541900
P	-0.19777100	-0.01832500	-0.21223700
C	-0.73934200	1.70639800	0.21838200
C	-0.31090600	2.73896900	-0.63057600
C	-1.51498400	2.03699400	1.34043500
C	-0.67314500	4.06370300	-0.38216600
H	0.33177200	2.49285000	-1.47220600
C	-1.87383600	3.36331100	1.59224600
H	-1.82725000	1.25800600	2.03004100
C	-1.45854900	4.37904100	0.72858500
H	-0.32746900	4.85064200	-1.04804900
H	-2.47140400	3.60327300	2.46903200
H	-1.73325900	5.41221100	0.92887100
C	-0.15830700	-0.87468500	1.43274600
C	1.09552200	-0.97962700	2.06333000
C	-1.29147000	-1.42237800	2.05481400
C	1.19177900	-1.60515000	3.30891700
H	1.98586700	-0.58644900	1.56432400
C	-1.18300400	-2.05179600	3.29724100
H	-2.26011500	-1.37063600	1.56448600
C	0.05968600	-2.14048100	3.92829000
H	2.16398500	-1.68247600	3.78974100
H	-2.06759900	-2.47684000	3.76727700
H	0.14575000	-2.63352500	4.89448800
C	-1.71437700	-0.73794800	-1.01426600

C	-3.00398900	-0.19179700	-0.92751900
C	-1.53051000	-1.90083600	-1.78181900
C	-4.08126200	-0.79819200	-1.58006500
H	-3.16845700	0.71599400	-0.35478600
C	-2.60682000	-2.51286100	-2.42352000
H	-0.52875000	-2.31357200	-1.88107600
C	-3.88756700	-1.96190100	-2.32538400
H	-5.07298100	-0.35715200	-1.50578500
H	-2.44323800	-3.41351800	-3.01048700
H	-4.72612600	-2.43171900	-2.83430600

3a

N	-2.97980200	0.00585200	0.05651300
C	-3.34843500	-1.34074500	0.16902100
C	-2.45278100	-2.38748700	-0.26065600
C	-4.60543600	-1.69842500	0.64905100
C	-2.94092600	-3.74245600	-0.27307100
C	-5.04260200	-3.03485900	0.67468200
H	-5.25950300	-0.91447000	1.00382400
C	-0.38800200	-3.10790800	-1.05394100
C	-2.08429500	-4.76174900	-0.75762800
C	-4.23921400	-4.04665200	0.20271300
H	-6.03907700	-3.25477100	1.05019100
C	-0.81204500	-4.44713800	-1.16645600
H	0.62970500	-2.83444900	-1.32067200
H	-2.45243100	-5.78502800	-0.79060700
H	-4.57621000	-5.08051300	0.19054500
H	-0.12634800	-5.19848900	-1.54635900
C	-3.40395500	0.98717300	0.92866100
O	-4.00524900	0.74440400	1.97850000
C	-3.07160100	2.40698500	0.55742500
C	-2.76003000	2.82196200	-0.74475900
C	-3.11243400	3.35788900	1.59098200
C	-2.45817900	4.16167000	-1.00048100
H	-2.72760800	2.12333200	-1.57357500
C	-2.82039600	4.69452600	1.33146000
H	-3.37620300	3.02157800	2.58851000
C	-2.48653200	5.09899800	0.03253700
H	-2.17906100	4.43688300	-2.01286900
H	-2.84933700	5.42202900	2.14015000
H	-2.24861400	6.14173900	-0.16820800
N	-1.15444500	-2.11371900	-0.62083000
Ni	-0.10259000	-0.27749100	-1.02742400
O	-1.59006700	0.32848700	-2.25040000
C	-0.79889200	1.31038600	-2.74282200

O	0.42530600	1.24980300	-2.25298300
O	-1.21615700	2.16943300	-3.52893900
H	-2.42474700	0.26045300	-0.79972100
P	1.79327100	-0.12489600	0.19288400
C	2.10082300	-0.95020000	1.83322900
C	1.27624400	-2.03470200	2.17191400
C	3.07517700	-0.53993100	2.75851700
C	1.43409600	-2.70574500	3.38672800
H	0.49296600	-2.33695100	1.48381600
C	3.23178100	-1.20672900	3.97481100
H	3.70561600	0.31497300	2.53397600
C	2.41445000	-2.29479700	4.29096900
H	0.78110900	-3.54050900	3.62988700
H	3.98937500	-0.87129000	4.67969000
H	2.53397100	-2.81026600	5.24115900
C	2.21909000	1.63989900	0.55355800
C	1.16074600	2.53067100	0.78211100
C	3.53505100	2.12493700	0.59900600
C	1.41247800	3.86921300	1.08569000
H	0.13771100	2.17945000	0.69452500
C	3.78718300	3.46544800	0.89842900
H	4.36527000	1.45845100	0.38054400
C	2.72602000	4.33847200	1.14802900
H	0.57624000	4.54345500	1.24899100
H	4.81224400	3.82898300	0.92570100
H	2.92251900	5.38432400	1.37373000
C	3.22993900	-0.67425500	-0.84486100
C	4.26877600	-1.50386900	-0.39802400
C	3.21502900	-0.25835700	-2.19256500
C	5.28108900	-1.90866500	-1.27437600
H	4.29212200	-1.83892700	0.63480600
C	4.23512100	-0.65807000	-3.05588100
H	2.39299300	0.36503900	-2.54748800
C	5.26905700	-1.48428400	-2.60324300
H	6.07874000	-2.55491100	-0.91354400
H	4.21571700	-0.32749100	-4.09176400
H	6.05700800	-1.79863100	-3.28438200

4a-ts

N	-2.25506700	0.17014900	-1.39526800
C	-2.93742700	-0.91349200	-0.86299500
C	-2.21046800	-2.09474900	-0.45532300
C	-4.33009500	-0.94257900	-0.77457400
C	-2.94439500	-3.24743200	-0.01078800
C	-5.03104000	-2.06852000	-0.30794700

H	-4.88099400	-0.06665400	-1.10033600
C	-0.19494200	-3.19387200	-0.08067500
C	-2.21085000	-4.40071100	0.36553200
C	-4.35931200	-3.21375300	0.05961500
H	-6.11718600	-2.03359900	-0.26269900
C	-0.83811200	-4.38008900	0.32686600
H	0.88921200	-3.13514700	-0.09050700
H	-2.75282300	-5.28720500	0.68842600
H	-4.89227500	-4.09753600	0.40200000
H	-0.24350100	-5.24241300	0.61330800
C	-2.54707300	1.48495200	-1.16692000
O	-2.21276000	2.38133600	-1.94551100
C	-3.21832200	1.89488800	0.13429800
C	-4.01801500	3.04578300	0.11406600
C	-2.99492600	1.25067900	1.35900200
C	-4.61373900	3.52215100	1.28118300
H	-4.14691200	3.56131400	-0.83250900
C	-3.57235800	1.73903300	2.53256100
H	-2.35787700	0.37285200	1.39659700
C	-4.39219100	2.86911500	2.49677800
H	-5.24208600	4.40956000	1.24580600
H	-3.38079700	1.23495300	3.47718300
H	-4.84770400	3.24363400	3.41091000
N	-0.83617900	-2.09668900	-0.46177900
Ni	0.41454400	-0.66842400	-1.35156600
O	-0.71568800	-0.68487000	-3.14450500
C	0.25145400	0.11055200	-3.71908500
O	1.18588300	0.42786000	-2.84423600
O	0.22555700	0.42660700	-4.90089800
H	-1.52928100	-0.11080600	-2.35077500
P	1.88739700	0.02288300	0.24541300
C	1.81912100	-0.76160100	1.92078700
C	2.57160000	-1.91225900	2.21878600
C	0.85515500	-0.34581000	2.85761700
C	2.38872000	-2.60260600	3.41842000
H	3.31427000	-2.26698800	1.50951000
C	0.67182700	-1.03678600	4.05579000
H	0.24570300	0.52857100	2.64849500
C	1.44041700	-2.16642500	4.34577300
H	2.99173600	-3.48357800	3.62741400
H	-0.07546200	-0.68922700	4.76545900
H	1.29761300	-2.70363800	5.28023300
C	3.68347800	-0.05316100	-0.22019600
C	4.73866500	-0.01518000	0.70623300

C	3.98008600	-0.09301500	-1.59407100
C	6.06520000	-0.04087300	0.27357300
H	4.52729400	0.02710100	1.77108500
C	5.31145800	-0.10769400	-2.01990300
H	3.16389100	-0.07551200	-2.31688600
C	6.35452200	-0.08981100	-1.09259700
H	6.87197900	-0.01741300	1.00325300
H	5.52816300	-0.13206700	-3.08515300
H	7.38862000	-0.10767800	-1.43024500
C	1.66001700	1.83019000	0.59541400
C	0.98900700	2.59157300	-0.37508900
C	2.14768000	2.46697700	1.74868200
C	0.79039300	3.96094400	-0.17807500
H	0.64361500	2.11618200	-1.28972000
C	1.94855700	3.83427900	1.93943200
H	2.67490300	1.89327500	2.50627400
C	1.26419800	4.58310100	0.97710000
H	0.24978600	4.52760900	-0.93078600
H	2.32548200	4.31490300	2.83991100
H	1.10148900	5.64765400	1.13131300

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N	1.68934700	1.56156100	-0.35766700
C	2.98326300	1.25638800	0.02351500
C	3.44782200	-0.06637700	-0.34524600
C	3.90843300	2.07709500	0.69161800
C	4.78582500	-0.49244900	-0.07464400
C	5.22038200	1.63788500	0.96008400
H	3.58958400	3.06412200	0.99038900
C	2.93047100	-2.09670800	-1.36787500
C	5.15045500	-1.79565000	-0.50189100
C	5.67425100	0.38734100	0.59252000
H	5.89364400	2.32003300	1.47722000
C	4.23303700	-2.59232800	-1.15196700
H	2.16210700	-2.67575400	-1.87184800
H	6.16233700	-2.14875000	-0.31049000
H	6.69061400	0.06388700	0.80627200
H	4.49290600	-3.59007400	-1.49526200
C	1.17822900	2.81337900	-0.16759100
O	1.67242800	3.73367800	0.51104500
C	-0.12620400	3.09612900	-0.88185300
C	-0.90212600	4.17420700	-0.42853200
C	-0.56285600	2.37965800	-2.00505100
C	-2.09567200	4.51131400	-1.06367200
H	-0.54009800	4.73390200	0.42766300

C	-1.75629200	2.71959500	-2.64826700
H	0.02565500	1.55893500	-2.40664100
C	-2.52739100	3.78351900	-2.17803000
H	-2.69130500	5.34289300	-0.69159400
H	-2.06783100	2.13298200	-3.50768200
H	-3.45892500	4.04735400	-2.67536100
N	2.55679500	-0.88775900	-0.97058700
Ni	0.63307000	-0.16351600	-0.94399000
P	-1.05313800	-0.53724000	0.63200200
C	-0.65411900	-2.12697700	1.51030400
C	-0.31291400	-3.22914600	0.70427000
C	-0.66622700	-2.28521100	2.90357500
C	-0.00896300	-4.45956000	1.28650100
H	-0.27779000	-3.10762800	-0.37644700
C	-0.34893800	-3.51783800	3.48239000
H	-0.91804100	-1.44355300	3.54187600
C	-0.02352200	-4.60916600	2.67655500
H	0.24972200	-5.30321400	0.65060400
H	-0.35814700	-3.62176600	4.56545300
H	0.22304600	-5.56800300	3.12736800
C	-1.22379300	0.66848900	2.02618200
C	-0.03284000	1.16370200	2.58854200
C	-2.44518200	1.17274100	2.49817900
C	-0.06531400	2.11649600	3.60605300
H	0.92475500	0.82159400	2.20776900
C	-2.47586800	2.13139900	3.51398400
H	-3.37775400	0.82432400	2.06716600
C	-1.28820100	2.60292000	4.07422300
H	0.86831400	2.49446100	4.01377800
H	-3.43317200	2.51329700	3.86210500
H	-1.31353700	3.35515400	4.85931700
C	-2.80458700	-0.88154300	0.11763400
C	-3.19890300	-0.50952000	-1.17578700
C	-3.73373600	-1.52825000	0.95107900
C	-4.50303200	-0.75929100	-1.61419200
H	-2.48229200	-0.05563700	-1.85364200
C	-5.03539400	-1.77171900	0.51288400
H	-3.43407400	-1.85157800	1.94442400
C	-5.42391000	-1.38343000	-0.77292000
H	-4.78944400	-0.47115600	-2.62258200
H	-5.74352700	-2.27129400	1.17066700
H	-6.43709100	-1.57844700	-1.11809300
O	0.00912500	-1.70778000	-2.19196400
C	-0.58385000	-1.47708200	-3.28991300

O	-1.04561200	-0.41341700	-3.73780700
O	-0.72298100	-2.61749900	-4.07935000
H	-1.18924400	-2.28558300	-4.86429900
6a			
N	-0.10619300	-1.02010800	0.10649200
C	-1.43549700	-1.39382300	0.13091800
C	-2.39331800	-0.33070200	-0.09511600
C	-1.97069200	-2.68429800	0.29136100
C	-3.79762800	-0.58672500	-0.17909000
C	-3.35498100	-2.92247800	0.20073400
H	-1.29106500	-3.49799500	0.49589900
C	-2.72036900	1.95923300	-0.42371700
C	-4.64925400	0.52673700	-0.40468800
C	-4.27017200	-1.91339800	-0.03048200
H	-3.70847800	-3.94510800	0.32586500
C	-4.11576300	1.79238200	-0.52656200
H	-2.24701000	2.93422800	-0.49585100
H	-5.72313400	0.36287000	-0.47494700
H	-5.33778700	-2.11364500	-0.08868500
H	-4.74915700	2.65898300	-0.69690900
C	0.87538800	-1.93162600	0.36891200
O	0.73903800	-3.04932100	0.90076500
C	2.27511800	-1.54385000	-0.06617000
C	3.35239000	-2.24094400	0.50035900
C	2.53830600	-0.60395500	-1.07077700
C	4.66149200	-1.98787400	0.09527800
H	3.12996000	-2.98919100	1.25431900
C	3.84726900	-0.35902900	-1.48965000
H	1.71013300	-0.06287300	-1.51759400
C	4.91392900	-1.04500200	-0.90583300
H	5.48651100	-2.52957700	0.55442000
H	4.03301400	0.37533600	-2.27053700
H	5.93453800	-0.84870100	-1.22924800
N	-1.89683300	0.93582300	-0.21919600
Ni	0.04983200	1.06663500	0.09782600
O	0.28344000	3.29924400	0.05085900
C	1.42312400	3.04859800	0.50407100
O	1.87864900	1.88773200	0.73348900
O	2.25469900	4.11095100	0.77580000
H	3.06569600	3.69154600	1.10847400
7a			
N	-0.22895100	-0.65375300	-0.37402100
C	1.03601100	-1.38514500	-0.47573800
C	2.18718900	-0.69744700	-0.06952700

C	1.09071400	-2.70336600	-0.95543500
C	3.46553300	-1.35338800	-0.13548600
C	2.32852100	-3.34152300	-1.02730600
H	0.17814900	-3.21284400	-1.25510500
C	3.16545900	1.29650100	0.72884700
C	4.59605400	-0.60577400	0.28047400
C	3.49608000	-2.68388200	-0.62510400
H	2.38659900	-4.36186600	-1.40030500
C	4.42402700	0.72895400	0.70616000
H	2.98592700	2.32203400	1.03258400
H	5.58240600	-1.06207400	0.25070100
H	4.45674200	-3.19083500	-0.69280600
H	5.27904600	1.32186800	1.02088800
C	-1.14747200	-1.14765000	0.62593300
O	-0.73502000	-1.68015200	1.63604500
C	-2.61106500	-1.03778400	0.31969100
C	-3.44493200	-1.98285700	0.94066100
C	-3.16966400	-0.07991800	-0.54153800
C	-4.81230000	-1.99505500	0.68213300
H	-2.99563300	-2.69977900	1.62027400
C	-4.54558300	-0.09096400	-0.78351600
H	-2.56042400	0.72273200	-0.94811100
C	-5.36612000	-1.04858700	-0.18609400
H	-5.44753000	-2.73727700	1.15958500
H	-4.97520000	0.66756500	-1.43260300
H	-6.43544800	-1.05165300	-0.38486700
N	2.04984100	0.59903000	0.36427500
Ni	0.32657600	1.32342400	-0.01410000
O	-1.23529500	2.21861900	-0.46400800
C	-0.63466100	3.40240800	-0.25021700
O	0.61701100	3.15072300	0.14098900
O	-1.14594400	4.50036400	-0.39257900
H	-0.69775100	-0.55425600	-1.27440800
8a-ts			
N	-0.19484300	-0.70707800	0.67584500
C	-0.29151300	0.65668400	0.89804000
C	0.61246200	1.60318600	0.27644500
C	-1.25946500	1.17221300	1.77094100
C	0.45595900	3.00670600	0.55329700
C	-1.39442600	2.54317300	2.03370400
H	-1.91708400	0.46715400	2.26827600
C	2.34007200	2.09033700	-1.23461600
C	1.31295300	3.92768100	-0.10228000
C	-0.55107000	3.45791700	1.44075700

H	-2.16716700	2.87714000	2.72265300
C	2.24592600	3.47109800	-1.00462000
H	3.07030300	1.70070700	-1.93733900
H	1.20613300	4.98870900	0.11157500
H	-0.64221800	4.52369900	1.63547100
H	2.90859200	4.14811100	-1.53577200
C	-1.28912900	-1.52717200	0.56475500
O	-1.27555000	-2.70827400	0.91101300
C	-2.54422500	-1.00613200	-0.12113000
C	-3.76894000	-1.59271700	0.22572300
C	-2.51890500	-0.05704100	-1.15186700
C	-4.94855500	-1.21263000	-0.41285600
H	-3.76739000	-2.36012500	0.99357400
C	-3.69573800	0.31011400	-1.80713200
H	-1.57201800	0.38037200	-1.45193700
C	-4.91578300	-0.25771500	-1.43312200
H	-5.89311700	-1.66862700	-0.12371200
H	-3.65852000	1.03942300	-2.61336700
H	-5.83323100	0.03430500	-1.93968700
N	1.58255900	1.17644500	-0.61306600
Ni	2.19505800	-0.64148000	-0.77252600
O	2.09576600	-1.57144100	1.05789200
C	2.60169500	-2.69386100	0.40443400
O	2.84398200	-2.41290600	-0.86014100
O	2.81507700	-3.74643000	0.98066500
H	0.90797800	-1.29362400	0.94329100
9a-ts			
N	-0.30086000	-1.25648900	0.11932200
C	-1.64807000	-1.37773100	0.20138700
C	-2.36454800	-0.15175000	-0.10566100
C	-2.41571700	-2.50996400	0.52700500
C	-3.79298900	-0.10681900	-0.07760800
C	-3.81982800	-2.44302700	0.54641400
H	-1.89031700	-3.42670700	0.76134600
C	-2.22296400	2.09771000	-0.69723900
C	-4.40543800	1.13537500	-0.38938400
C	-4.51544200	-1.28059000	0.25519200
H	-4.37720100	-3.34316100	0.80349400
C	-3.62656800	2.23125200	-0.69523200
H	-1.57134700	2.93780500	-0.91870000
H	-5.49182700	1.20686600	-0.38011500
H	-5.60259800	-1.25075000	0.27833900
H	-4.07403300	3.19276900	-0.93362100
C	0.62691900	-2.22634700	0.33840800

O	0.42180400	-3.39884000	0.70127700
C	2.02035600	-1.71612200	0.02550300
C	3.03373700	-2.67394300	-0.09395800
C	2.25226100	-0.32686500	-0.21935500
C	4.31815100	-2.30450400	-0.49615000
H	2.78380200	-3.71083200	0.11690200
C	3.56517900	-0.00916400	-0.63294500
C	4.57958500	-0.96285900	-0.78060100
H	5.10209700	-3.05427000	-0.59531500
H	3.81656200	1.03358000	-0.83630900
H	5.57382400	-0.65848200	-1.10939200
N	-1.61114900	0.95031700	-0.41851900
Ni	0.39434300	0.56489400	-0.34492200
O	0.87830600	2.84587300	-0.31857600
C	1.64836600	2.99639300	0.62004600
O	2.29698600	2.05571100	1.26654500
O	1.90987400	4.23918900	1.10155900
H	2.54102900	4.11827100	1.83208500
H	2.07878900	1.11934700	0.77209900

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N	-0.17705700	0.70826600	-0.00016000
C	1.11511900	1.09589200	-0.00006300
C	2.04733400	-0.01858400	-0.00000900
C	1.65511000	2.39579000	-0.00002200
C	3.45938100	0.20548900	0.00008400
C	3.04541200	2.59036900	0.00007400
H	0.96437800	3.22951700	-0.00006900
C	2.33478400	-2.33177300	0.00000500
C	4.29680900	-0.94140500	0.00013200
C	3.94727500	1.53612000	0.00012700
H	3.42607200	3.61123000	0.00010500
C	3.73719400	-2.20158600	0.00009100
H	1.86656200	-3.31204000	-0.00002500
H	5.37736300	-0.80928300	0.00020300
H	5.02090700	1.71059700	0.00019900
H	4.35684700	-3.09468500	0.00012900
C	-1.30484200	1.47798000	-0.00020000
O	-1.35843000	2.71956100	0.00009300
C	-2.53840600	0.60009300	-0.00000900
C	-3.79254800	1.22293700	0.00010300
C	-2.38968300	-0.82165700	-0.00004600
C	-4.95752400	0.45561500	0.00017600
H	-3.83048600	2.31018400	0.00010600
C	-3.59493700	-1.55349000	0.00002100

C	-4.85344200	-0.93936500	0.00013300
H	-5.93540500	0.93603300	0.00025600
H	-3.55724000	-2.64400900	0.00000800
H	-5.75861200	-1.54883000	0.00019300
N	1.50810600	-1.28559400	-0.00004400
Ni	-0.48651800	-1.24065900	-0.00014300

11a-ts

N	-1.62075000	1.22086400	0.18211000
C	-2.79390300	0.58957900	0.44419900
C	-2.76984100	-0.82952700	0.15819700
C	-3.99302200	1.12823200	0.94329700
C	-3.92515000	-1.64492000	0.36861400
C	-5.11641400	0.30753100	1.14669900
H	-4.02042600	2.18657100	1.16480400
C	-1.52563700	-2.63901600	-0.60685300
C	-3.80630500	-3.02268600	0.05247300
C	-5.10909000	-1.04998400	0.87207900
H	-6.02553000	0.76468800	1.53536800
C	-2.61560300	-3.51704600	-0.43400300
H	-0.56942400	-2.98915000	-0.98538800
H	-4.66537500	-3.67544800	0.19840500
H	-5.99043700	-1.66621200	1.03463200
H	-2.50041900	-4.56828400	-0.68483200
C	-1.35401300	2.55109300	0.38449700
O	-2.13820700	3.40079600	0.83716300
C	0.05488500	2.87073500	-0.02774000
C	0.51395200	4.19030700	0.05579300
C	0.86419000	1.80833000	-0.50696000
C	1.81319500	4.49989500	-0.34763300
H	-0.16114900	4.95466600	0.43472400
C	2.16346700	2.16331900	-0.91541300
C	2.63607600	3.48004000	-0.83847400
H	2.18103100	5.52337100	-0.28720100
H	2.82704400	1.39361400	-1.31102500
H	3.65066400	3.71485200	-1.16380800
N	-1.59364500	-1.34393800	-0.32130900
Ni	-0.14183100	0.11681700	-0.50597300
Br	1.73905200	-1.49305300	-1.28862600
C	2.63664900	-1.06944700	0.75662300
H	2.48167200	0.00570600	0.79153800
H	1.93951500	-1.61847500	1.38746900
C	4.05957100	-1.55857100	0.76741000
H	4.63227400	-1.03499300	-0.01033700
H	4.08683300	-2.62695900	0.50878600

C	4.75508900	-1.35292900	2.12993500
H	4.72622200	-0.28733000	2.39343600
H	4.18649000	-1.87693400	2.91075100
C	6.20822100	-1.84487000	2.13536300
H	6.68288400	-1.68847900	3.11207300
H	6.26434500	-2.91632700	1.90391300
H	6.80678500	-1.31412700	1.38432400
12a			
N	-0.79414300	1.52024000	0.02577000
C	-2.12914400	1.34594800	0.24418600
C	-2.57731600	-0.01727800	0.06947800
C	-3.08861200	2.30177000	0.60573200
C	-3.95079800	-0.37041200	0.23475500
C	-4.43791200	1.93295100	0.77713700
H	-2.76332000	3.32433800	0.74424900
C	-1.98626300	-2.20258200	-0.47619200
C	-4.29300500	-1.72922400	0.01674700
C	-4.88271600	0.63607800	0.59727700
H	-5.15236400	2.70581700	1.05580400
C	-3.32222700	-2.63890300	-0.34287400
H	-1.18526700	-2.86948400	-0.78292000
H	-5.33089900	-2.03759300	0.13027800
H	-5.93036800	0.37427200	0.72512700
H	-3.56514700	-3.68180700	-0.52536900
C	-0.08354500	2.67178800	0.21643800
O	-0.52387200	3.78666800	0.53410000
C	1.37626100	2.40729900	-0.02457900
C	2.30048700	3.45807000	-0.02850500
C	1.79475800	1.08416300	-0.27178000
C	3.64677400	3.20127400	-0.28546400
H	1.93563600	4.46362200	0.16699600
C	3.14148100	0.83555000	-0.54337200
C	4.06185200	1.89116900	-0.55044500
H	4.36936800	4.01526000	-0.28999000
H	3.46615700	-0.17453700	-0.77487400
H	5.10996800	1.68872400	-0.76745800
N	-1.62989300	-0.94542100	-0.26453200
Ni	0.31229700	-0.12559100	-0.34085400
Br	1.11255000	-1.77848600	-2.09204200
C	0.87064400	-0.59454100	1.52708700
C	1.96791000	-1.64069800	1.62898700
H	2.92542400	-1.20585300	1.31439100
H	1.76549700	-2.46391500	0.93160800
H	-0.09812400	-0.98683800	1.86158400

H	1.09858100	0.31269300	2.09249700
C	2.12983900	-2.21137300	3.05296900
H	1.17835500	-2.65908200	3.37578500
H	2.33183500	-1.38885600	3.75447300
C	3.24623500	-3.25816400	3.15584800
H	4.21617800	-2.82793200	2.87551900
H	3.33936700	-3.65709400	4.17462300
H	3.05654900	-4.10254400	2.48103900

13a-ts

N	-0.85771300	1.44199800	0.01639500
C	-2.19391500	1.29306700	0.25310600
C	-2.68116200	-0.06068700	0.08924900
C	-3.12534100	2.27375100	0.62376000
C	-4.05974800	-0.37677200	0.29324200
C	-4.47956700	1.94087200	0.82567400
H	-2.77307800	3.28912100	0.74718200
C	-2.16419000	-2.26186400	-0.45627500
C	-4.44233000	-1.72883600	0.09981100
C	-4.95902100	0.65365600	0.66978100
H	-5.16814600	2.73379700	1.11361700
C	-3.50519800	-2.66681000	-0.27487200
H	-1.38585800	-2.95196400	-0.77335100
H	-5.48426900	-2.00871900	0.24670900
H	-6.00863400	0.41693500	0.82845500
H	-3.77902000	-3.70602800	-0.43517400
C	-0.15443300	2.60449700	0.12996900
O	-0.58145900	3.73327400	0.42428600
C	1.29225800	2.35241300	-0.19644700
C	2.13604200	3.42167900	-0.50592800
C	1.76401900	1.01721200	-0.26996700
C	3.44789100	3.18971500	-0.92162200
H	1.72824300	4.42682400	-0.43217300
C	3.07667600	0.79655300	-0.71168800
C	3.90540900	1.87302600	-1.04161300
H	4.10224500	4.02335700	-1.16855800
H	3.43584800	-0.22106900	-0.82473300
H	4.91689700	1.67945900	-1.39585200
N	-1.77026900	-1.01192400	-0.27218300
Ni	0.25663200	-0.20304000	-0.42745700
Br	1.15731000	-2.15631700	-1.72593500
C	1.27359300	-0.14924200	1.40089800
C	2.48339000	-1.02591100	1.68467900
H	3.40708200	-0.44212700	1.58246200
H	2.52992700	-1.83028700	0.94005800

H	1.26281100	0.76798400	1.99186600
H	0.35093800	-0.69785900	1.64852000
C	2.43940800	-1.64117700	3.09603000
H	1.53377700	-2.25619800	3.19649700
H	2.34918100	-0.83996700	3.84440600
C	3.67237500	-2.49687700	3.41144100
H	4.59184200	-1.89988700	3.35659100
H	3.61699600	-2.93298300	4.41729000
H	3.77230200	-3.32048100	2.69356300

14a

N	0.41174700	-0.75981500	-0.60653500
C	1.38049800	-1.74616700	-0.52032200
C	2.65968800	-1.31212800	-0.00188600
C	1.27764000	-3.09873600	-0.88003900
C	3.76076600	-2.21317700	0.12968300
C	2.37283700	-3.97634800	-0.74612100
H	0.33219100	-3.45606200	-1.25939900
C	3.91368800	0.46273900	0.84392200
C	4.97131700	-1.68567500	0.64991300
C	3.59675600	-3.56700200	-0.25566700
H	2.23674600	-5.01520300	-1.04282500
C	5.05032400	-0.35631500	1.00560800
H	3.91661000	1.51657200	1.11015900
H	5.82899400	-2.34652500	0.76237200
H	4.43081000	-4.25833500	-0.15741700
H	5.96661800	0.06843300	1.40653400
C	-0.85312600	-1.04155100	-1.02390900
O	-1.32276400	-2.15605200	-1.32250700
C	-1.75963200	0.16894700	-1.15024200
C	-1.31066000	1.28278200	-1.87076000
C	-3.07762600	0.15551300	-0.63161000
C	-2.13854200	2.38431900	-2.09568700
H	-0.29464000	1.28056000	-2.25522600
C	-3.88708400	1.27527800	-0.85580900
C	-3.43225500	2.37879600	-1.58395500
H	-1.76378000	3.24084700	-2.64985300
H	-4.89475100	1.29708300	-0.45146500
H	-4.08975700	3.23190700	-1.73792200
N	2.76936200	-0.00072800	0.35993900
Ni	1.06279500	1.03201700	0.08609700
Br	1.23451500	3.29402200	0.77841900
C	-3.57853600	-1.04311000	0.16167900
C	-4.94601500	-0.89633300	0.83928700
H	-5.72521100	-0.71269700	0.08461000

H	-4.94778100	-0.01869300	1.50222300
H	-3.58464700	-1.91556400	-0.50135500
H	-2.83091100	-1.28807900	0.92901100
C	-5.33061900	-2.14004100	1.65223200
H	-5.32340300	-3.01955400	0.99286900
H	-4.56000800	-2.32691900	2.41330100
C	-6.69956900	-2.02070500	2.33122700
H	-7.49659200	-1.86605900	1.59239600
H	-6.94678200	-2.92345600	2.90361200
H	-6.72473500	-1.16981900	3.02395600

15a

N	1.53172100	1.22030900	-0.01634900
C	2.82777200	0.79948600	0.23609800
C	3.04451600	-0.62482300	0.14282600
C	3.93440600	1.59313600	0.55217200
C	4.34070200	-1.19030400	0.35044900
C	5.20873200	1.02146000	0.75219100
H	3.79183800	2.65983000	0.64736600
C	2.11658200	-2.73220000	-0.23025400
C	4.46270900	-2.59793600	0.24189500
C	5.42929500	-0.33652100	0.65605200
H	6.03767500	1.68353900	0.99064200
C	3.35896300	-3.37077200	-0.04670600
H	1.22063500	-3.30725400	-0.45025100
H	5.43764700	-3.05567100	0.39278600
H	6.41588700	-0.76353400	0.81401200
H	3.42776900	-4.45061000	-0.13199500
C	1.11763200	2.50288300	0.19301900
O	1.77087200	3.44258200	0.66449900
C	-0.33493800	2.73835800	-0.16877500
C	-1.05780800	3.68437300	0.57127300
C	-0.97704600	2.07683200	-1.22783700
C	-2.40230000	3.92699700	0.29482600
H	-0.54001300	4.22101800	1.35987800
C	-2.32307900	2.32908000	-1.51615900
H	-0.40477500	1.40797600	-1.87139100
C	-3.04227600	3.24660800	-0.74702000
H	-2.95288200	4.65444700	0.88605700
H	-2.79893800	1.82403400	-2.35337700
H	-4.08707100	3.44728200	-0.97047100
N	1.96426800	-1.41781600	-0.14273500
Ni	0.31868500	-0.26644600	-0.40193200
Br	-1.63190200	-1.71309400	-0.76189600
C	-2.94562800	-0.93752600	0.55950100

H	-2.44074300	-1.03681000	1.52029100
H	-3.00932100	0.11176500	0.27068800
C	-4.27109500	-1.67283200	0.48973200
H	-4.11668000	-2.73903300	0.69648300
H	-4.68076100	-1.59872100	-0.52523700
C	-5.27749500	-1.08931200	1.49933100
H	-4.85990900	-1.15946700	2.51279700
H	-5.41938400	-0.01944600	1.29624100
C	-6.63079200	-1.80733600	1.45049300
H	-6.52251000	-2.87390800	1.68071500
H	-7.32892100	-1.37758200	2.17682500
H	-7.08815500	-1.72509400	0.45734900

16a-ts

N	-0.19003700	-1.56404400	-0.00687400
C	-1.55108400	-1.80436200	0.12371000
C	-2.41198500	-0.73209300	-0.31042900
C	-2.17311900	-2.96164200	0.60210300
C	-3.83516100	-0.85995600	-0.27871900
C	-3.57980600	-3.07435400	0.63309300
H	-1.55289300	-3.77296600	0.95368100
C	-2.56020200	1.42926500	-1.18321500
C	-4.59641100	0.24261200	-0.73973000
C	-4.41084900	-2.06065700	0.20474700
H	-4.01198100	-3.99847000	1.00900200
C	-3.96809000	1.38257900	-1.19416400
H	-2.02068600	2.30748700	-1.52744800
H	-5.68173700	0.17373400	-0.73061800
H	-5.49206800	-2.16328700	0.23252700
H	-4.53241000	2.23631100	-1.55525500
C	0.75407400	-2.42006300	0.49159900
O	0.55973000	-3.43216100	1.17532800
C	2.17755400	-2.01205800	0.18285500
C	3.16887900	-2.29208600	1.13484400
C	2.55256700	-1.40308100	-1.02540200
C	4.49474600	-1.92974600	0.90482700
H	2.87608400	-2.80200800	2.04722700
C	3.88485900	-1.04998700	-1.26181200
H	1.81217400	-1.25798400	-1.81053800
C	4.85628800	-1.30288400	-0.29269600
H	5.25126700	-2.14196300	1.65608800
H	4.16028500	-0.58855500	-2.20626800
H	5.89195000	-1.02740800	-0.47367100
N	-1.81768700	0.41680100	-0.75599300
Ni	0.21172600	0.23916300	-0.70664200

Br	1.21234100	2.26102000	-1.40895100
C	1.23925400	1.80017500	0.91289700
H	1.27398600	0.73996200	1.17117300
H	2.23337400	2.23351800	0.94333000
C	0.14922900	2.60633400	1.55947100
H	-0.83099900	2.16962800	1.34350500
H	0.14989100	3.62658600	1.15993700
C	0.36160100	2.65191900	3.09264600
H	0.36174100	1.62983800	3.49264300
H	1.35059900	3.07526300	3.31220900
C	-0.72248900	3.48000000	3.79293900
H	-1.71855100	3.05740200	3.61646600
H	-0.55567000	3.50454800	4.87531000
H	-0.72751900	4.51460300	3.42999500

17a

N	0.00119700	1.49363500	-0.03008000
C	1.34033500	1.86477300	0.08181100
C	2.28155200	0.87666600	-0.36740400
C	1.86073100	3.08127700	0.52760800
C	3.68371900	1.13239600	-0.39545400
C	3.25321000	3.32566700	0.50435600
H	1.18148000	3.84045900	0.88550500
C	2.57676600	-1.27673800	-1.22679100
C	4.51785400	0.09462400	-0.87928800
C	4.15961000	2.39016600	0.05414500
H	3.60847600	4.29127500	0.85439400
C	3.97235600	-1.10139000	-1.30030700
H	2.09145500	-2.19731600	-1.53734100
H	5.59264700	0.25566800	-0.91584600
H	5.22595900	2.59677600	0.03919500
H	4.59467400	-1.90465100	-1.68045600
C	-1.02661600	2.27661800	0.45935000
O	-0.89091400	3.31083500	1.11559700
C	-2.40673800	1.76121000	0.15233100
C	-3.41947800	1.98196800	1.09808200
C	-2.72554800	1.10964700	-1.04932500
C	-4.71280600	1.52035100	0.86636500
H	-3.17136500	2.52024900	2.00738100
C	-4.02576600	0.65387400	-1.28425900
H	-1.97517100	1.00395300	-1.82906600
C	-5.01759100	0.84957500	-0.32339800
H	-5.48729700	1.68556000	1.61068800
H	-4.25758300	0.15147000	-2.21870300
H	-6.02762900	0.49139600	-0.50323700

N	1.77518100	-0.32373100	-0.77168500
Ni	-0.25126600	-0.37735100	-0.50468800
Br	-0.97250700	-2.35411100	-1.53439700
C	-0.54969800	-0.97390800	1.40677600
H	-0.40303200	-0.04953300	1.96368600
H	-1.60473500	-1.23726700	1.31057000
C	0.36756900	-2.09882500	1.80676700
H	1.41593600	-1.79119100	1.70761600
H	0.21313900	-2.96450100	1.15600600
C	0.11272500	-2.50598200	3.28115800
H	0.26210000	-1.63526600	3.93315900
H	-0.93641500	-2.80742600	3.39654400
C	1.03132800	-3.65050900	3.72477700
H	2.08712300	-3.36408500	3.64761700
H	0.83481400	-3.92862700	4.76638900
H	0.88018200	-4.54199800	3.10484600
18a			
N	-0.03930400	0.59427700	-0.98981000
C	1.30045000	0.87922500	-1.23773300
C	2.25121300	0.01604300	-0.58683400
C	1.81710700	1.87965900	-2.06408200
C	3.65671900	0.15818800	-0.79201600
C	3.20913400	2.00953800	-2.26558500
H	1.13270000	2.55659100	-2.55298100
C	2.57270600	-1.77287000	0.88412100
C	4.50385000	-0.74558300	-0.10326100
C	4.12488600	1.17853200	-1.65595800
H	3.55820300	2.79736800	-2.92802100
C	3.97194100	-1.70859900	0.72865400
H	2.10013800	-2.50640200	1.53153200
H	5.57964300	-0.66640000	-0.24023100
H	5.19214300	1.29235000	-1.82321100
H	4.60540400	-2.40897200	1.26281100
C	-1.05568900	1.45395800	-1.33999200
O	-0.90977300	2.57068600	-1.84448600
C	-2.44379200	0.95781400	-1.02556700
C	-3.40833200	1.90449500	-0.65071400
C	-2.81183200	-0.39401500	-1.12092900
C	-4.70415500	1.50380100	-0.33157800
H	-3.12181700	2.95088400	-0.61810700
C	-4.11652800	-0.79103100	-0.80987500
H	-2.10218500	-1.13427600	-1.48244500
C	-5.06069400	0.15312700	-0.40515000
H	-5.44012500	2.24444800	-0.02974800

H	-4.39377600	-1.83816100	-0.89718200
H	-6.07277400	-0.15767200	-0.16004100
N	1.76086100	-0.94194600	0.24986700
Ni	-0.27859500	-0.87699700	0.25670900
O	-0.73723300	-2.50122500	1.29305100
C	-0.75089900	-3.24773300	0.25510000
O	-0.53208300	-2.79811100	-0.89850100
O	-1.00649800	-4.55432400	0.45377700
H	-0.97831100	-4.97044400	-0.42566400
C	-0.54759800	0.31340800	1.85202200
H	-1.63158700	0.42041600	1.74319500
H	-0.29010200	-0.43979200	2.59970100
C	0.21099300	1.60797700	1.97030400
H	-0.06869400	2.30061700	1.16975100
H	1.28997700	1.43000300	1.87944600
C	-0.06083800	2.28264000	3.33753000
H	-1.13933300	2.45750200	3.44707900
H	0.22600500	1.59707000	4.14615200
C	0.69470600	3.60801400	3.48809200
H	0.40270600	4.32044200	2.70755400
H	0.48775000	4.07082500	4.45973500
H	1.77842300	3.45747100	3.41239700

19a-ts

N	-0.63103000	-1.32151500	-0.40124300
C	-1.99331200	-1.17388500	-0.55250000
C	-2.44966900	0.17421500	-0.37317500
C	-2.93531400	-2.14965300	-0.87573200
C	-3.83002400	0.50780300	-0.50876000
C	-4.30038900	-1.81036500	-1.00164000
H	-2.59787100	-3.16501100	-1.03394500
C	-1.87945100	2.39100300	0.06587600
C	-4.18877800	1.86574900	-0.33129800
C	-4.75557300	-0.52019100	-0.82281700
H	-5.00782700	-2.59807800	-1.24745300
C	-3.22096000	2.80518900	-0.04883700
H	-1.09914100	3.10922900	0.29439600
H	-5.23280300	2.15504400	-0.42375200
H	-5.80906000	-0.27517700	-0.92299700
H	-3.46909700	3.85217200	0.08986200
C	0.10076000	-2.38815900	-0.83861600
O	-0.32084400	-3.44493600	-1.31317700
C	1.57177400	-2.06525900	-0.76565600
C	2.46586200	-2.78642000	-1.55601100
C	2.01137100	-0.98115500	0.04104600

C	3.81182200	-2.41885600	-1.59162300
H	2.08510000	-3.61570700	-2.14469100
C	3.37583200	-0.63032500	-0.02596700
C	4.26881100	-1.33674900	-0.83078300
H	4.50829400	-2.97459100	-2.21450800
H	3.75394200	0.17698300	0.59690200
H	5.31858000	-1.05640000	-0.85894000
N	-1.50430000	1.13019000	-0.08985700
Ni	0.31511900	0.25477600	0.27119700
O	-0.17775600	0.21090900	2.26295600
C	0.50209200	-0.55680300	2.98317100
O	1.49708800	-1.26310000	2.60632300
O	0.15260800	-0.63795700	4.28264600
H	0.76078600	-1.27776800	4.69243100
H	1.66058400	-1.04783500	1.31554400
C	1.36862200	1.90064600	0.57842100
H	2.22563500	1.61912000	1.19351500
H	0.67844100	2.49650000	1.18182700
C	1.75147300	2.53675500	-0.74545600
H	2.41559000	1.86644000	-1.30661200
H	0.86063900	2.68820100	-1.37281400
C	2.45757400	3.90117300	-0.56633800
H	3.35293300	3.76210700	0.05426800
H	1.79825900	4.57815100	-0.00567700
C	2.84632900	4.54529200	-1.90169200
H	3.34320200	5.50989900	-1.74697500
H	3.53215700	3.90254100	-2.46674800
H	1.96377000	4.72036500	-2.52909500
20a			
N	0.67017700	-1.33316600	-0.02639700
C	2.02899000	-1.09353500	-0.02316600
C	2.35907600	0.30239900	-0.03520100
C	3.07398200	-2.01607300	-0.01563000
C	3.71451900	0.74125300	-0.04059500
C	4.41548800	-1.57145800	-0.02333500
H	2.83779300	-3.07139900	-0.00709200
C	1.56233300	2.48806800	-0.03667600
C	3.93956600	2.13902000	-0.05128800
C	4.74742200	-0.23232200	-0.03566900
H	5.20544800	-2.31784000	-0.01892600
C	2.87057600	3.01058000	-0.05018200
H	0.70209700	3.15001000	-0.02334700
H	4.96050100	2.51296400	-0.05846700
H	5.78449600	0.09070700	-0.04180300

H	3.01626600	4.08569600	-0.05648700
C	0.06369800	-2.58056100	-0.01389300
O	0.64009500	-3.66500600	-0.01675500
C	-1.42065200	-2.41084600	-0.01975100
C	-2.26924200	-3.51959700	-0.06680300
C	-1.93380500	-1.09883700	0.00398500
C	-3.65011500	-3.32956700	-0.10086900
H	-1.82704700	-4.51208200	-0.08368800
C	-3.31649500	-0.92148900	-0.02599200
C	-4.16930300	-2.03269600	-0.08578200
H	-4.31948900	-4.18487700	-0.13980100
H	-3.75523300	0.07204900	-0.00061000
H	-5.24595500	-1.88025000	-0.11372500
N	1.30917200	1.18595200	-0.03275300
Ni	-0.48338400	0.17064900	0.02328900
C	-1.57289100	1.54565600	0.88223900
H	-0.85011500	2.05828000	1.52982200
H	-2.34988300	1.10251400	1.50638200
C	-2.15592900	2.48744900	-0.17465500
H	-1.36894100	2.86841700	-0.84405500
H	-2.85959300	1.94600600	-0.82136300
C	-2.89075500	3.69642200	0.44366900
H	-2.19243600	4.25318800	1.08416200
H	-3.68476100	3.32745800	1.10694000
C	-3.48975900	4.63558700	-0.60915600
H	-4.00543800	5.48178000	-0.14066600
H	-2.71261500	5.04259900	-1.26810600
H	-4.21676900	4.11043200	-1.24067500

21a-ts

N	-0.19645600	1.21034600	-0.46920700
C	1.05641800	1.67129400	-0.80314600
C	2.00934900	0.68090200	-1.26056600
C	1.49226300	3.00895600	-0.84042600
C	3.28073000	1.05673300	-1.80234600
C	2.74711400	3.36212000	-1.36748200
H	0.83640500	3.77679700	-0.45510200
C	2.46764200	-1.58307400	-1.56473200
C	4.12282200	0.01003600	-2.25710000
C	3.63886700	2.42488800	-1.85503700
H	3.01718500	4.41681800	-1.38687800
C	3.71952100	-1.30245000	-2.15012700
H	2.12370900	-2.60196700	-1.41639000
H	5.09120700	0.26302900	-2.68512800
H	4.60547700	2.71362500	-2.26065300

H	4.34911400	-2.11927900	-2.49113400
C	-1.09084200	2.05420900	0.13684000
O	-0.80342300	3.03806600	0.84427000
C	-2.55231000	1.76366600	-0.10785400
C	-3.49882000	2.39925700	0.70876100
C	-2.99876700	0.97125200	-1.17324500
C	-4.86308400	2.23197400	0.48016800
H	-3.13489500	3.02952500	1.51386500
C	-4.36471100	0.81233200	-1.41038100
H	-2.27044600	0.47791100	-1.80714800
C	-5.30030400	1.43725500	-0.58361500
H	-5.58694800	2.72220200	1.12827100
H	-4.69745500	0.18542000	-2.23399900
H	-6.36498500	1.30437200	-0.76524500
N	1.65323700	-0.62837500	-1.14226400
Ni	-0.17961100	-0.95544900	-0.26736000
O	-2.10527100	-1.57470100	0.19889700
C	-2.22424900	-2.23328300	-0.86892200
O	-1.36829200	-2.29404800	-1.79126600
O	-3.39838500	-2.93286600	-1.03023200
H	-3.28801200	-3.37124100	-1.89027400
Br	0.79961400	-2.76906800	1.37729900
C	0.26836500	-0.71504800	2.42235300
H	-0.54203500	-0.22055800	1.89406100
H	-0.09254000	-1.24807700	3.29676300
C	1.53640000	0.07254200	2.60206600
H	1.97075500	0.31750500	1.62767100
H	2.27769400	-0.53450600	3.13842000
C	1.28343600	1.39283100	3.36672600
H	0.57371400	2.00397600	2.79668600
H	0.81608000	1.17227400	4.33756800
C	2.57627400	2.18867300	3.58414500
H	3.03034000	2.45763000	2.62289800
H	2.38214300	3.11903100	4.13215200
H	3.31494500	1.60967800	4.15465800
22a			
N	-0.56988600	1.23260600	-0.04048200
C	0.47970900	2.07369400	-0.31875300
C	1.61109800	1.49601100	-1.00556400
C	0.52438100	3.46283400	-0.10790600
C	2.66301700	2.31089600	-1.53093600
C	1.57229000	4.25086300	-0.61501200
H	-0.27468000	3.93388400	0.44927500
C	2.62082700	-0.45542100	-1.77820700

C	3.69840000	1.64447100	-2.23460100
C	2.62677200	3.71156500	-1.32840100
H	1.54056400	5.32446700	-0.43722200
C	3.67368400	0.27475600	-2.37119800
H	2.57764700	-1.54045000	-1.80130900
H	4.50903900	2.23371100	-2.65991200
H	3.42591000	4.33411900	-1.72291900
H	4.45484200	-0.25542400	-2.90828200
C	-1.55328100	1.65629300	0.83356400
O	-1.35540000	2.36307800	1.83144300
C	-2.96539600	1.24838400	0.50704800
C	-3.94807600	1.38737800	1.49717200
C	-3.34460800	0.85504300	-0.78234600
C	-5.28384800	1.11384900	1.21222400
H	-3.63840200	1.71795900	2.48338400
C	-4.68423200	0.58884700	-1.06976600
H	-2.57873900	0.73678100	-1.54081700
C	-5.65611800	0.71511400	-0.07529800
H	-6.03689300	1.21177400	1.99138700
H	-4.96858200	0.27631600	-2.07189000
H	-6.69909700	0.50194700	-0.30039300
N	1.63668100	0.14026200	-1.12291500
Ni	0.03877800	-0.82596400	-0.14087800
O	-1.77413000	-1.75498100	0.35320100
C	-1.97982900	-1.93335300	-0.87626600
O	-1.24464800	-1.45242800	-1.78783800
O	-3.05912800	-2.68361200	-1.23789300
H	-3.01048100	-2.72107500	-2.20803200
Br	1.22419700	-3.11570900	-0.15213800
C	0.66581600	-0.65137900	1.87686400
H	0.00014600	0.14841300	2.19784800
H	0.32373100	-1.64674300	2.15223200
C	2.13266400	-0.38509800	2.07035200
H	2.41328400	0.57102900	1.61055400
H	2.71561800	-1.17555100	1.58539600
C	2.49919800	-0.32830000	3.57301100
H	1.90058900	0.44954200	4.06615600
H	2.22512200	-1.28046300	4.04706700
C	3.99047900	-0.05156200	3.79870800
H	4.28351300	0.90942800	3.35752700
H	4.23611500	-0.01838000	4.86791100
H	4.60927400	-0.83033300	3.33577100
23a-ts			
N	-0.36559500	0.90009500	-0.89593300

C	-1.72284900	1.02378100	-0.97973100
C	-2.46969300	0.17700000	-0.07499000
C	-2.46136500	1.87741100	-1.81184200
C	-3.89736000	0.21019000	-0.03255600
C	-3.86801000	1.90537100	-1.74872900
H	-1.92012500	2.50221900	-2.50853900
C	-2.37474200	-1.49335100	1.54706500
C	-4.53230700	-0.67696400	0.87422000
C	-4.59186900	1.10261400	-0.88621700
H	-4.39845500	2.58516600	-2.41348700
C	-3.78161300	-1.52718300	1.65681000
H	-1.73461900	-2.15347000	2.12535900
H	-5.61918800	-0.68042400	0.93354300
H	-5.67852500	1.13400500	-0.85984700
H	-4.25026900	-2.22165500	2.34816200
C	0.53821800	1.50543500	-1.70899700
O	0.28162800	2.26922800	-2.65430700
C	1.96672700	1.25399600	-1.27515500
C	2.89309500	2.20465300	-1.73055500
C	2.34733100	0.23295200	-0.36082600
C	4.20277900	2.22279200	-1.25798900
H	2.53985200	2.94387700	-2.44335400
C	3.67064000	0.31755900	0.12443300
C	4.58678100	1.28257800	-0.30276000
H	4.90698400	2.97171800	-1.61597500
H	4.01611500	-0.43128400	0.83502900
H	5.59831800	1.28826900	0.10147000
N	-1.75787300	-0.66747600	0.72086100
Ni	0.29425800	-0.53054800	0.30437700
O	0.80160900	-2.10391500	1.60350100
C	1.78292500	-2.73092200	1.17168100
O	2.62520400	-2.32170700	0.29103800
O	2.03165400	-3.96082300	1.68017800
H	2.79623000	-4.29838600	1.18240000
H	2.26860900	-1.24666300	-0.09978000
C	0.55779600	0.66534300	1.95350900
H	1.59721500	0.44724800	2.19760100
H	-0.12292300	0.12897200	2.61750300
C	0.25475300	2.13666100	1.81846800
H	0.91181500	2.58940500	1.06721400
H	-0.77401500	2.28601100	1.46874500
C	0.43738000	2.88496100	3.15828800
H	1.46851600	2.74825200	3.51353500
H	-0.21302900	2.43337700	3.92128400

C	0.12905700	4.38278700	3.04357700
H	0.26430500	4.89771700	4.00348200
H	0.78598000	4.86399800	2.30866800
H	-0.90533500	4.54813200	2.71709600
Br	-0.08112000	-2.25479200	-1.57504800