

Electronic Supplementary Information

Mechanistic Insight into Ni(I)-Catalyzed Regioselective Alkene Hydroarylation: Is It Carbonickelation or Hydronickelation?

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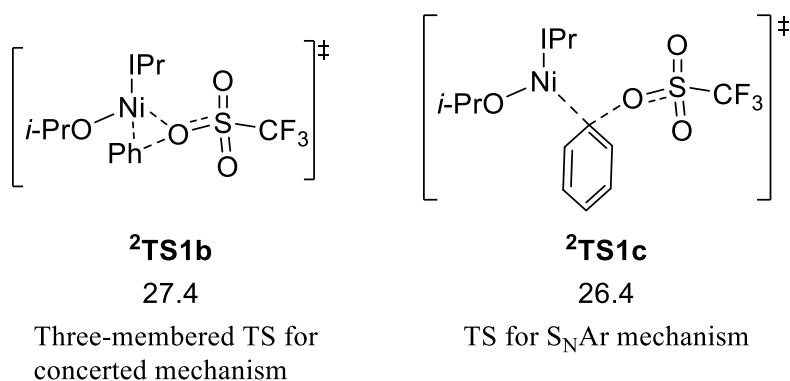


Figure S1. Higher-energy transition states of oxidative addition of **2a** to ²CAT1 that are isomers of ²TS1a in Figure 2.

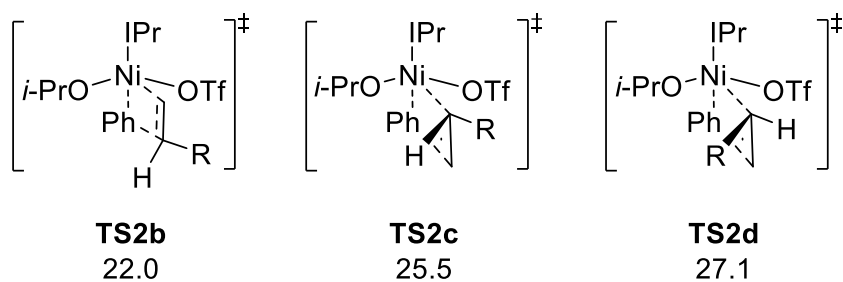


Figure S2. Higher-energy transition states of 3-butenylbenzene (**1a**) migratory insertion into ²IM1 that are isomers of ²TS2a in Figure 2.

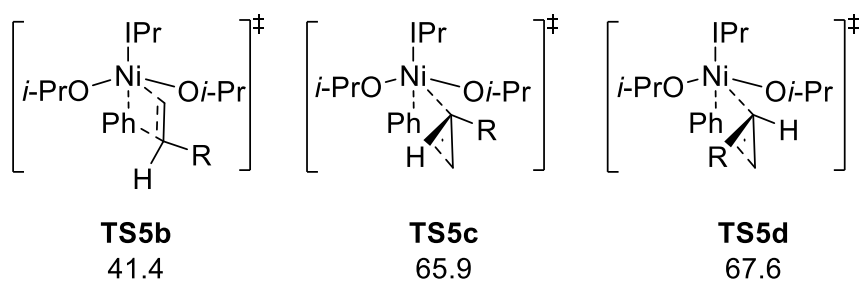


Figure S3. Higher-energy transition states of 3-butenylbenzene (**1a**) migratory insertion into ²IM5 that are isomers of ²TS5a in Figure 3.

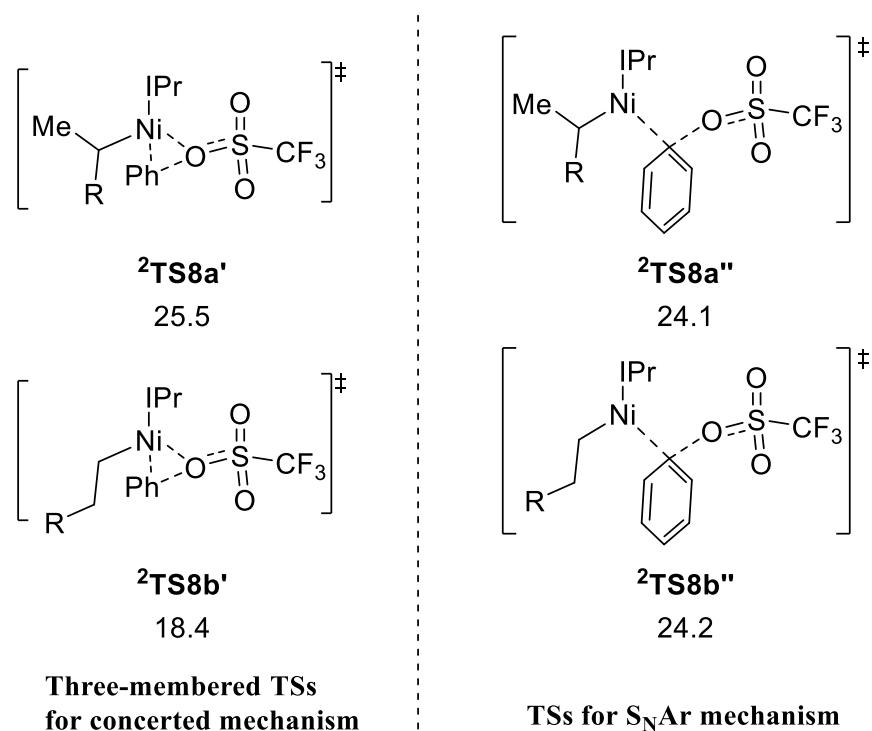


Figure S4. Higher-energy transition states of oxidative addition of **2a** to **²IM8a** that are isomers of **²TS8a** and **²TS8b** in Figure 4.

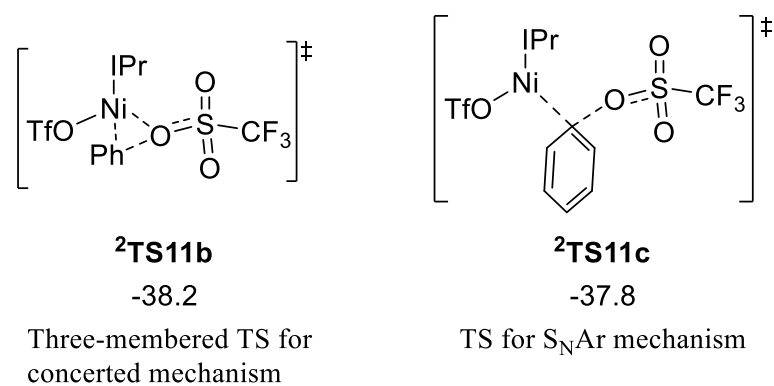


Figure S5. Higher-energy transition states of oxidative addition of **2a** to **²IM11** that are isomers of **²TS11a** in Figure 6.

Table S1. Relative energies of the doublet and quartet states of key structures selected from the most favored reaction pathway (see Figure 6).

	CAT1	TS6	TS7a
Doublet state	0.0	15.9	12.8
Quartet state	38.0	55.7	90.7
$\Delta\Delta G_{\text{sol}}^{\ddagger}$ (kcal/mol)	38.3	39.8	77.9

Cartesian Coordinates (Å) of Optimized Structures

1a

C	-4.014359	2.856831	0.913589
C	-2.622299	2.871019	0.997977
C	-1.837899	2.182772	0.064402
C	-2.483980	1.477517	-0.958062
C	-3.875730	1.459801	-1.047610
C	-4.646098	2.149971	-0.110663
H	-4.605684	3.401126	1.645007
H	-2.134612	3.426342	1.796243
H	-1.887469	0.940467	-1.692211
H	-4.358533	0.910286	-1.851241
H	-5.730198	2.140161	-0.180260
C	-0.333490	2.153468	0.190368
H	0.128325	2.057950	-0.799358
H	0.025490	3.099002	0.616687
C	0.153329	0.984183	1.078317
H	-0.192508	0.036077	0.648849
H	-0.327338	1.077681	2.062721
C	1.646872	0.967680	1.233938
H	2.084423	1.846833	1.710694
C	2.449238	-0.011629	0.816931
H	2.054216	-0.903101	0.333573
H	3.527258	0.034437	0.945325

2a

C	-1.846008	-0.610434	-0.163349
C	-0.712572	-0.804254	-0.944358
C	-2.208146	0.638108	0.329694
C	0.081389	0.302955	-1.243751
H	-0.470241	-1.794997	-1.309622
C	-1.399966	1.733745	0.027837
H	-3.103017	0.735383	0.934377
C	-0.258494	1.567546	-0.758986
H	0.969011	0.173369	-1.855223
H	-1.664984	2.715933	0.406977
H	0.366771	2.423533	-0.993746
O	-2.639016	-1.715617	0.218673
S	-3.625900	-2.424046	-0.882118
O	-3.027718	-2.409278	-2.206353
O	-4.114138	-3.626872	-0.239426

C	-5.031498	-1.186766	-0.900171
F	-4.648206	-0.080303	-1.535647
F	-6.065228	-1.734263	-1.532646
F	-5.376660	-0.882372	0.350966

²TM10a

C	0.863868	0.626692	4.494263
C	1.026238	-0.514348	5.204646
H	0.696485	1.646878	4.799922
H	1.044365	-0.704855	6.265389
C	1.162045	-1.077068	2.996295
N	1.199592	-1.537856	4.278831
N	0.946775	0.264168	3.154014
C	0.829596	1.214626	2.081291
C	1.921048	2.064819	1.826872
C	-0.378066	1.271441	1.360194
C	1.783225	2.983683	0.780840
C	-0.459202	2.206199	0.321851
C	0.611479	3.049313	0.032868
H	2.603733	3.650083	0.542605
H	-1.366821	2.278918	-0.265988
H	0.529327	3.765246	-0.780108
C	1.427668	-2.893899	4.711898
C	0.335304	-3.772553	4.779097
C	2.727734	-3.246584	5.095727
C	0.580354	-5.055063	5.275879
C	2.924147	-4.545606	5.577316
C	1.861161	-5.438604	5.670903
H	-0.233959	-5.767904	5.342530
H	3.919374	-4.862138	5.872685
H	2.030792	-6.443621	6.047520
Ni	1.222958	-2.171028	1.157577
C	-1.566115	0.389457	1.730428
H	-1.177341	-0.603135	1.980100
C	-2.579666	0.211475	0.593131
H	-3.323203	-0.538751	0.882180
H	-3.120265	1.141529	0.383011
H	-2.102314	-0.123710	-0.332317
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H	-3.123117	0.277369	3.248781

H	-1.616588	0.985324	3.845191	C	-1.949829	-4.191772	-0.508532
H	-2.681127	1.935400	2.791577	H	-1.365199	-5.067215	-0.814117
C	3.203642	1.981458	2.649784	H	-2.286737	-3.695685	-1.426057
H	2.914490	1.788977	3.689127	C	-1.033275	-3.227990	0.291077
C	4.095471	0.807191	2.205203	H	-0.812855	-3.703022	1.251232
H	4.974900	0.744390	2.857118	H	-1.608842	-2.321708	0.513194
H	3.566777	-0.145118	2.249479	C	0.264990	-2.868918	-0.438327
H	4.435741	0.942629	1.174912	H	0.821072	-3.770338	-0.705372
C	4.006914	3.289355	2.647979	C	0.037637	-1.998847	-1.662619
H	4.828373	3.215709	3.368452	H	-0.692069	-2.466128	-2.341148
H	4.455045	3.487245	1.667697	H	0.959050	-1.838027	-2.224564
H	3.388209	4.151362	2.921772	C	2.470643	-1.339574	-0.022022
C	-1.055912	-3.340018	4.336794	C	3.709324	-1.988673	-0.129962
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C	0.541583	0.469324	5.742830	H	7.187430	0.926603	1.140739
C	0.228405	-1.815419	5.021170	H	6.922549	2.399993	2.089680
C	-0.296069	-0.568910	5.349038	Ni	4.223509	-1.432402	2.314720
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H	-0.443400	-2.605907	4.711302	H	4.891422	0.418516	1.107561
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H	3.014397	-3.297506	4.040751	C	4.180398	-3.091722	-3.203143
C	1.183102	-4.375223	4.061310	C	4.069890	-2.847417	-4.577095
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H	3.525687	-3.534017	6.490544	H	4.314761	-1.859706	-4.961494
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H	1.435410	3.071525	6.505696	H	4.302841	0.537148	-1.220921
H	1.698237	2.054540	7.934271	C	4.597720	-0.522110	0.614506
H	2.938306	3.214063	7.417081	H	5.507006	-1.083837	0.362743
C	6.929940	-4.199603	5.032628	C	2.422454	-0.950682	1.972265
H	6.047019	-3.782074	5.521561	C	1.872388	0.306136	2.238036
C	7.916482	-4.622195	6.134801	C	1.584967	-1.971025	1.503838
H	8.819354	-5.073691	5.707764	C	0.501508	0.528780	2.084879
H	8.231896	-3.766043	6.743111	H	2.507199	1.120806	2.569059
H	7.454033	-5.361558	6.798638	C	0.215328	-1.745147	1.341031
C	6.438866	-5.400640	4.213150	H	1.998634	-2.946329	1.270378

C	-0.332581	-0.495714	1.635093
H	0.087213	1.506623	2.318698
H	-0.421467	-2.549110	0.978699
H	-1.397581	-0.320413	1.509575
O	4.776061	-3.217331	2.232423
C	4.754936	-3.927627	1.024370
H	4.227960	-3.340359	0.255275
C	3.981736	-5.243514	1.196008
H	2.968849	-5.041357	1.560462
H	3.905174	-5.795926	0.250565
H	4.478506	-5.892244	1.925603
C	6.184332	-4.172266	0.522821
H	6.720155	-3.220507	0.439028
H	6.735592	-4.796552	1.233953
H	6.191679	-4.668342	-0.456228

²M11

C	0.922588	1.784370	2.379314
C	2.188247	1.440061	2.025182
H	0.544456	2.382300	3.192553
H	3.144163	1.660711	2.472125
C	0.776754	0.516619	0.494483
N	2.075821	0.665508	0.875623
N	0.076824	1.209282	1.437524
C	-1.356385	1.351567	1.408617
C	-1.896143	2.459022	0.736569
C	-2.146745	0.358967	2.016408
C	-3.289409	2.585876	0.717746
C	-3.533260	0.531627	1.966636
C	-4.098510	1.635923	1.332333
H	-3.742962	3.425563	0.200598
H	-4.179742	-0.214261	2.414362
H	-5.178972	1.745131	1.302249
C	3.162511	0.024160	0.187612
C	3.575078	-1.241820	0.635370
C	3.721754	0.665166	-0.929377
C	4.607687	-1.865809	-0.072595
C	4.750266	-0.000791	-1.604347
C	5.190950	-1.251544	-1.178420
H	4.948534	-2.848767	0.236397
H	5.202530	0.458728	-2.477536
H	5.988006	-1.755361	-1.717777
Ni	0.056283	-0.412650	-0.976772

O	-0.839488	-1.240428	-2.583602
S	-1.739051	-2.142430	-1.756781
O	-2.064007	-3.445422	-2.319950
O	-1.233182	-2.079471	-0.343966
C	-3.342723	-1.199012	-1.673321
F	-3.971634	-1.247406	-2.849323
F	-4.127858	-1.737321	-0.731378
F	-3.113330	0.083239	-1.358149
C	-1.519679	-0.846746	2.702363
H	-0.603087	-1.091970	2.157288
C	-2.412639	-2.094107	2.658421
H	-1.843817	-2.962695	3.006989
H	-3.286158	-1.992395	3.313633
H	-2.750788	-2.297181	1.640607
C	-1.136633	-0.510667	4.156507
H	-0.671554	-1.378851	4.637770
H	-0.429386	0.322743	4.211166
H	-2.026532	-0.237791	4.736012
C	-1.019432	3.445530	-0.019471
H	0.021387	3.270735	0.269823
C	-1.124074	3.184089	-1.533305
H	-0.450313	3.848256	-2.087424
H	-0.861128	2.147124	-1.767449
H	-2.145529	3.357513	-1.890429
C	-1.347008	4.907287	0.321379
H	-0.649713	5.580012	-0.190528
H	-2.359230	5.180871	0.004103
H	-1.272246	5.090788	1.398880
C	2.887796	-1.946122	1.795931
H	2.267175	-1.213453	2.320739
C	1.949110	-3.049213	1.271827
H	2.514570	-3.816877	0.730656
H	1.430619	-3.535306	2.106585
H	1.192881	-2.643792	0.593345
C	3.892156	-2.504025	2.816537
H	4.565161	-1.721549	3.184578
H	3.358600	-2.929026	3.673820
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C	3.188228	1.995749	-1.437329
H	2.538471	2.417974	-0.664395
C	4.305948	3.015749	-1.703925
H	4.923139	3.170463	-0.812330
H	4.965023	2.692760	-2.517198
H	3.874772	3.980177	-1.994589

C	2.326202	1.775365	-2.693714
H	2.923203	1.354821	-3.510647
H	1.505081	1.076262	-2.493204
H	1.889079	2.720031	-3.035797

²IM12

C	0.605302	-3.202425	0.400714
C	-0.720064	-3.097687	0.673663
H	1.268932	-4.050887	0.396204
H	-1.448723	-3.832274	0.972294
C	0.044764	-1.023604	0.161984
N	-1.045866	-1.756339	0.520362
N	1.059656	-1.923351	0.101093
C	2.459587	-1.604624	-0.097087
C	3.028578	-1.812971	-1.362482
C	3.194672	-1.141613	1.013899
C	4.391049	-1.523719	-1.507536
C	4.547195	-0.859806	0.808456
C	5.139774	-1.046934	-0.438400
H	4.863290	-1.669089	-2.473323
H	5.142037	-0.479576	1.630352
H	6.192356	-0.815053	-0.574777
C	-2.296211	-1.147873	0.904730
C	-2.341083	-0.506331	2.156959
C	-3.397891	-1.202790	0.030795
C	-3.520324	0.169743	2.493477
C	-4.552656	-0.517300	0.420400
C	-4.609386	0.176708	1.627501
H	-3.586738	0.680409	3.449530
H	-5.417488	-0.523436	-0.233733
H	-5.517178	0.706494	1.903478
Ni	-0.008054	0.943753	-0.369429
C	-0.861825	2.895339	-0.409754
C	-1.880060	2.742548	0.518166
C	-0.949693	3.624488	-1.581005
C	-3.153612	3.172969	0.121259
H	-1.731074	2.265590	1.480071
C	-2.225913	4.058546	-1.945189
H	-0.081882	3.795979	-2.203651
C	-3.318970	3.822879	-1.102300
H	-3.998236	3.007540	0.782641
H	-2.363092	4.583350	-2.886238
H	-4.304525	4.173875	-1.393685

O	1.293018	4.005149	0.554193
S	2.241105	2.884753	0.652370
O	3.314936	2.950368	1.642303
O	1.538242	1.517581	0.696934
C	3.096944	2.829990	-1.000338
F	3.951791	3.851954	-1.090467
F	3.761764	1.683390	-1.147656
F	2.197666	2.935762	-1.994149
C	2.567548	-1.004904	2.395138
H	1.540394	-0.664963	2.250823
C	3.256216	0.031037	3.291701
H	2.668900	0.161719	4.207975
H	4.255099	-0.301219	3.599048
H	3.343647	1.000893	2.799576
C	2.531359	-2.367704	3.116020
H	2.050858	-2.264329	4.096457
H	1.979936	-3.124668	2.552216
H	3.549701	-2.740320	3.277009
C	2.235943	-2.385890	-2.524649
H	1.173975	-2.254257	-2.315579
C	2.521028	-1.666160	-3.851562
H	1.805227	-2.000973	-4.609040
H	2.414204	-0.585379	-3.736530
H	3.529107	-1.881875	-4.224754
C	2.506670	-3.896088	-2.663116
H	1.911393	-4.315466	-3.482095
H	3.565090	-4.085153	-2.878251
H	2.252839	-4.441379	-1.747115
C	-1.205953	-0.597861	3.170104
H	-0.416415	-1.220887	2.745298
C	-0.584023	0.768638	3.500878
H	-1.339035	1.475016	3.865563
H	0.172980	0.659082	4.284805
H	-0.083036	1.208845	2.634250
C	-1.688683	-1.307341	4.448700
H	-2.123033	-2.285926	4.217471
H	-0.847887	-1.457691	5.135027
H	-2.448682	-0.718499	4.974158
C	-3.374285	-2.033574	-1.241614
H	-2.335749	-2.130783	-1.563775
C	-3.925473	-3.444648	-0.951545
H	-3.366014	-3.953064	-0.159514
H	-4.973602	-3.393327	-0.633787
H	-3.872679	-4.064545	-1.853449

C	-4.154315	-1.401057	-2.403621
H	-5.236975	-1.430642	-2.231323
H	-3.850132	-0.365593	-2.563842
H	-3.953164	-1.962531	-3.321763
O	-1.708084	0.490850	-1.867937
S	-0.690196	0.062019	-2.880271
C	-1.048386	1.046873	-4.418291
F	-0.814881	2.348555	-4.226739
F	-0.269919	0.610116	-5.409486
F	-2.331946	0.878578	-4.750879
O	-0.751664	-1.332326	-3.323611
O	0.650352	0.570134	-2.400787

²IM13

C	0.827561	0.323166	0.650671
C	2.591690	1.392973	-0.280633
C	2.774889	1.387159	1.060448
N	1.679525	0.738353	1.621963
N	1.382342	0.748271	-0.518745
H	3.562483	1.779489	1.681312
H	3.186283	1.786716	-1.087332
C	1.487132	0.782898	3.062356
C	0.884375	1.940824	3.588798
C	2.034502	-0.235487	3.858033
C	0.876319	2.081002	4.979296
C	2.014505	-0.029920	5.240710
C	1.453442	1.114969	5.795083
H	0.410150	2.953463	5.424152
H	2.410886	-0.795946	5.895015
H	1.437212	1.238911	6.873727
C	0.750474	0.763486	-1.818888
C	0.064435	1.938050	-2.193420
C	0.912392	-0.338751	-2.674414
C	-0.503298	1.970522	-3.471053
C	0.336012	-0.243232	-3.946967
C	-0.368682	0.890393	-4.339469
H	-1.043761	2.854349	-3.793010
H	0.436337	-1.072496	-4.636874
H	-0.811015	0.935810	-5.330590
C	-3.202975	-3.332545	-1.005176
C	-2.773933	-3.044807	-2.298436
C	-2.464919	-1.729121	-2.652427
C	-2.584272	-0.705150	-1.716199

C	-3.041527	-0.981893	-0.412736
C	-3.340537	-2.308160	-0.068693
H	-3.400370	-4.355209	-0.704839
H	-2.659430	-3.844183	-3.024488
H	-2.122299	-1.498325	-3.654991
H	-2.335889	0.311440	-2.005041
H	-3.646483	-2.544719	0.941911
C	-1.847824	0.799939	0.841787
H	-1.689421	1.238825	1.819225
H	-1.514220	1.417867	0.013790
C	-3.190278	0.137572	0.619200
H	-3.515284	-0.301465	1.563695
C	-4.245774	1.188062	0.199184
H	-3.972645	1.623165	-0.770491
H	-5.198648	0.665337	0.047258
C	-4.424106	2.307867	1.238946
H	-3.476356	2.843338	1.366461
H	-4.655499	1.857999	2.211843
Ni	-0.710353	-0.847627	0.842541
O	0.016383	-2.627170	0.271467
C	1.732447	-1.555428	-2.272585
C	3.224781	-1.310582	-2.571621
C	1.256739	-2.844704	-2.951598
H	1.619149	-1.705580	-1.196075
H	3.615316	-0.443010	-2.030397
H	3.814407	-2.184036	-2.273063
H	3.383460	-1.141190	-3.643348
H	0.191904	-3.012101	-2.775534
H	1.442982	-2.831242	-4.032063
H	1.799152	-3.695092	-2.535665
C	-0.010156	3.168362	-1.297405
C	-1.397491	3.832509	-1.288528
C	1.057923	4.200826	-1.707060
H	0.211917	2.860146	-0.272988
H	-2.197793	3.115949	-1.085312
H	-1.430656	4.605964	-0.513360
H	-1.620401	4.318444	-2.244336
H	2.065905	3.778475	-1.667094
H	0.881442	4.553214	-2.729500
H	1.027038	5.066419	-1.035987
C	2.607702	-1.512286	3.260398
C	2.473785	-2.708490	4.212058
C	4.079337	-1.330962	2.841390
H	2.024706	-1.756329	2.366990

H	1.447150	-2.804557	4.573300
H	2.726319	-3.625798	3.677571
H	3.148915	-2.616350	5.071899
H	4.205181	-0.554820	2.079494
H	4.696850	-1.059447	3.706225
H	4.467155	-2.268738	2.428414
C	0.288520	3.031242	2.709264
C	1.270113	4.202512	2.522126
C	-1.062988	3.540184	3.238925
H	0.103360	2.600466	1.722072
H	2.210932	3.875635	2.068498
H	0.831095	4.970931	1.874013
H	1.503580	4.666436	3.486958
H	-1.731351	2.712237	3.488704
H	-0.934979	4.151640	4.138871
H	-1.543409	4.174440	2.484117
S	-1.665733	-0.868330	3.997213
O	-0.842233	-1.053662	5.187930
O	-2.359129	0.418817	3.807244
O	-0.972585	-1.364689	2.731203
C	-3.029367	-2.119651	4.175159
F	-3.898481	-2.023683	3.144566
F	-2.541968	-3.352814	4.212377
F	-3.702763	-1.871271	5.303826
C	-5.502452	3.280198	0.827597
C	-5.187288	4.422017	0.080510
C	-6.845795	3.034910	1.138214
C	-6.186144	5.297011	-0.347102
H	-4.146977	4.628593	-0.161347
C	-7.848571	3.906288	0.713185
H	-7.104298	2.154732	1.722437
C	-7.521626	5.040729	-0.032181
H	-5.921819	6.180846	-0.921570
H	-8.884903	3.702298	0.968122
H	-8.301282	5.722020	-0.360855
S	-0.142642	-3.920251	1.089850
O	0.919670	-4.092891	2.080615
O	-1.528318	-4.203607	1.471656
C	0.254092	-5.170085	-0.227662
F	1.532919	-5.048760	-0.621016
F	0.076592	-6.399248	0.265001
F	-0.538293	-5.023407	-1.301498

²TM14

Ni	-0.960856	-0.401250	0.756374
N	1.311030	1.237472	1.730797
N	-0.333223	1.091182	3.139473
C	2.973605	0.403681	0.115393
C	3.552068	0.524160	-1.151725
C	3.148241	1.520988	-2.037526
C	2.168970	2.436969	-1.668193
C	1.562563	2.371667	-0.408637
C	1.975246	1.333603	0.449418
C	1.701643	1.915622	2.878655
C	0.673277	1.818519	3.762177
C	0.070417	0.715720	1.904015
C	-1.657281	0.875998	3.698216
C	-1.853683	-0.221881	4.547870
C	-3.130159	-0.376643	5.098398
C	-4.152628	0.512963	4.794121
C	-3.926854	1.583331	3.932643
C	-2.671148	1.794648	3.359611
H	4.318980	-0.179078	-1.454768
H	3.605214	1.585341	-3.020683
H	1.871941	3.218248	-2.360607
H	2.655590	2.411636	2.941651
H	0.551661	2.192919	4.764803
H	-3.328798	-1.218278	5.751858
H	-5.142587	0.361006	5.213390
H	-4.745345	2.246025	3.679771
H	-0.471320	0.745851	0.022115
O	-1.269305	-2.392386	1.678592
C	0.542800	3.427652	-0.003678
C	-0.690923	3.431856	-0.922165
C	1.199418	4.818954	0.051042
H	0.194721	3.206625	1.007611
H	-1.226281	2.476560	-0.890606
H	-1.391713	4.211914	-0.606315
H	-0.414047	3.629973	-1.963247
H	2.063856	4.822685	0.724003
H	1.543761	5.138106	-0.938685
H	0.479661	5.561534	0.412699
C	3.441605	-0.652014	1.101442
C	4.594718	-0.101031	1.963447
C	3.863183	-1.962248	0.424258
H	2.603829	-0.881923	1.762996
H	4.302499	0.798095	2.515973

H	4.917552	-0.853352	2.691576	C	2.189289	2.476222	-0.092197
H	5.455765	0.157976	1.336512	C	2.583666	2.356505	1.198815
H	3.073249	-2.335470	-0.231432	N	1.856352	1.306765	1.745619
H	4.781868	-1.838940	-0.160335	N	1.228795	1.494666	-0.303531
H	4.062329	-2.720672	1.186284	H	3.305879	2.901553	1.784408
C	-0.733601	-1.190522	4.889485	H	2.503452	3.137909	-0.881803
C	-1.216332	-2.645942	4.967426	C	2.095874	0.844810	3.095122
C	-0.043965	-0.777791	6.203794	C	1.650625	1.651263	4.154828
H	0.010051	-1.143110	4.089824	C	2.783154	-0.367290	3.277426
H	-1.763409	-2.921879	4.063501	C	1.946613	1.217062	5.449360
H	-0.355566	-3.313525	5.069257	C	3.044676	-0.756313	4.593972
H	-1.862577	-2.810805	5.836660	C	2.637968	0.029900	5.666739
H	0.369815	0.235324	6.150129	H	1.604785	1.795153	6.299311
H	-0.756503	-0.801613	7.036311	H	3.547905	-1.696968	4.781535
H	0.776218	-1.465892	6.438240	H	2.834697	-0.300831	6.681904
C	-2.420825	2.974144	2.428902	C	0.708673	1.191231	-1.611661
C	-1.805376	4.163081	3.192906	C	-0.436923	1.869070	-2.060863
C	-3.673164	3.434280	1.670915	C	1.402110	0.244648	-2.382901
H	-1.704182	2.644647	1.672926	C	-0.893143	1.562353	-3.345664
H	-0.864799	3.902190	3.686726	C	0.897300	-0.032757	-3.659031
H	-1.603328	4.992634	2.504799	C	-0.236992	0.618867	-4.134357
H	-2.499949	4.523018	3.960480	H	-1.782149	2.051206	-3.727392
H	-4.169002	2.601778	1.168852	H	1.403246	-0.761295	-4.284904
H	-4.393302	3.920334	2.339456	H	-0.614391	0.390870	-5.127260
H	-3.386250	4.174741	0.915894	C	-3.768399	-0.052541	0.230778
S	-4.078145	-0.382794	0.771949	C	-3.971616	-0.498819	-1.075970
O	-3.991572	-1.247739	1.945842	C	-2.897859	-1.004751	-1.810484
O	-5.218651	0.521265	0.620383	C	-1.627679	-1.096128	-1.233700
O	-2.756981	0.368755	0.470899	C	-1.455369	-0.667756	0.077528
C	-4.125791	-1.513954	-0.708327	C	-2.499861	-0.123096	0.818651
F	-2.930539	-2.122619	-0.860899	H	-4.595288	0.352447	0.808006
F	-5.064192	-2.445594	-0.549303	H	-4.960255	-0.443643	-1.522823
F	-4.378719	-0.813889	-1.818124	H	-3.038973	-1.336655	-2.835560
S	-0.215058	-3.094144	0.855501	H	-0.798382	-1.488412	-1.807078
O	-0.601407	-4.299300	0.137883	H	-2.349178	0.198872	1.839891
O	0.504744	-2.015773	0.074011	Ni	0.173038	-1.011819	1.007091
C	1.017864	-3.675048	2.119902	O	0.307901	-2.711346	0.579649
F	1.480406	-2.639558	2.848660	C	-0.519031	-3.842134	0.382224
F	2.052023	-4.264463	1.515534	C	-0.251965	-4.850264	1.501227
F	0.437103	-4.547505	2.943877	H	0.782280	-5.209199	1.441084
				H	-0.392990	-4.384317	2.477199
				C	-0.246040	-4.443385	-0.998825
				H	-0.870638	-5.329276	-1.162912
				H	-0.459941	-3.721022	-1.792212
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C	1.020175	0.756246	0.821335				

H	0.805205	-4.743843	-1.078758
C	2.678847	-0.427636	-1.897200
C	3.889513	0.087807	-2.695723
C	2.587701	-1.960848	-1.939513
H	2.841068	-0.147521	-0.853685
H	3.974224	1.178319	-2.629341
H	4.815423	-0.351682	-2.308273
H	3.806278	-0.177851	-3.755745
H	1.774462	-2.325906	-1.307359
H	2.430621	-2.329071	-2.959865
H	3.523359	-2.397743	-1.571331
C	-1.139597	2.899379	-1.188303
C	-2.652183	2.970766	-1.436289
C	-0.515349	4.296064	-1.378438
H	-0.992409	2.598751	-0.145118
H	-3.112651	1.982614	-1.389785
H	-3.118708	3.603072	-0.673229
H	-2.880641	3.417973	-2.410996
H	0.546218	4.313715	-1.117419
H	-0.612855	4.619550	-2.421377
H	-1.027769	5.029517	-0.745757
C	3.233138	-1.229795	2.104418
C	3.289119	-2.726992	2.428938
C	4.570541	-0.726572	1.531002
H	2.492869	-1.127832	1.300148
H	2.355548	-3.059888	2.888375
H	3.439820	-3.291754	1.503012
H	4.122519	-2.963320	3.100891
H	4.509644	0.320326	1.215234
H	5.361977	-0.806214	2.285260
H	4.865086	-1.327811	0.662799
C	0.802991	2.894853	3.911862
C	0.918892	3.936815	5.032913
C	-0.671190	2.501775	3.689340
H	1.153465	3.378502	2.992567
H	1.963782	4.180771	5.255469
H	0.407623	4.858574	4.734915
H	0.445912	3.589266	5.957690
H	-0.782040	1.852636	2.818776
H	-1.051351	1.945187	4.551447
H	-1.282657	3.400831	3.544213
S	-0.579011	-1.495211	4.126252
O	0.263953	-2.697209	4.096635
O	-0.657446	-0.716985	5.365064

O	-0.405602	-0.596678	2.911250
C	-2.312024	-2.116490	3.868722
F	-3.178909	-1.090105	3.873863
F	-2.426472	-2.751050	2.687221
F	-2.650607	-2.968779	4.840182
H	-0.924502	-5.711959	1.409521
H	-1.568912	-3.522943	0.425750

²IM2

C	0.932907	0.461379	0.712825
C	2.656652	1.603627	-0.205580
C	2.876775	1.541651	1.128700
N	1.806615	0.844173	1.676371
N	1.454280	0.939531	-0.448978
H	3.674340	1.919550	1.746103
H	3.221721	2.046359	-1.008153
C	1.600805	0.725078	3.102268
C	0.956742	1.792263	3.753967
C	2.076827	-0.415576	3.763418
C	0.839841	1.710163	5.143082
C	1.932855	-0.444688	5.154171
C	1.329576	0.607040	5.835442
H	0.334460	2.501455	5.685344
H	2.278056	-1.310026	5.708513
H	1.208720	0.552303	6.912799
C	0.817590	0.996317	-1.745842
C	0.116874	2.177737	-2.064758
C	0.980952	-0.069461	-2.649206
C	-0.452953	2.267099	-3.339224
C	0.401097	0.083933	-3.915073
C	-0.309770	1.230963	-4.256501
H	-1.007504	3.157677	-3.615144
H	0.499771	-0.711090	-4.643577
H	-0.755438	1.316353	-5.243449
C	-3.661790	-3.297596	-1.461676
C	-3.039405	-3.061511	-2.688208
C	-2.409847	-1.835991	-2.914034
C	-2.402229	-0.855386	-1.922949
C	-3.024207	-1.081451	-0.687921
C	-3.653418	-2.313985	-0.472175
H	-4.149195	-4.249531	-1.270689
H	-3.042000	-3.826206	-3.459785
H	-1.924620	-1.636488	-3.864527

H	-1.916503	0.093395	-2.122028	C	2.734470	-1.559164	3.005692
H	-4.137554	-2.502179	0.480890	C	2.402903	-2.928801	3.614096
C	-1.770324	0.702862	0.623288	C	4.257982	-1.350828	2.923771
H	-1.782355	1.365437	1.484862	H	2.332080	-1.567772	1.988655
H	-1.387495	1.196620	-0.264083	H	1.321930	-3.054410	3.721271
C	-3.094497	0.004056	0.374961	H	2.778776	-3.723330	2.961002
H	-3.442741	-0.439529	1.308362	H	2.866457	-3.067534	4.597676
C	-4.163976	1.057966	-0.044564	H	4.511045	-0.411256	2.420350
H	-3.865026	1.514935	-0.997274	H	4.701809	-1.324545	3.926214
H	-5.096340	0.515077	-0.245623	H	4.727218	-2.168536	2.364454
C	-4.432354	2.152755	1.002873	C	0.418847	2.997081	2.993818
H	-3.527801	2.750240	1.159068	C	1.424253	4.163000	3.022867
H	-4.654746	1.681014	1.965120	C	-0.958247	3.457912	3.497080
Ni	-0.514975	-0.744905	1.112257	H	0.290384	2.699458	1.948867
O	0.428754	-2.233894	0.575694	H	2.392603	3.875701	2.600671
C	0.168457	-3.604015	0.812266	H	1.042120	5.014034	2.446442
C	-0.990743	-3.851783	1.777867	H	1.592561	4.498875	4.052456
H	-1.122486	-4.927136	1.950625	H	-1.672767	2.631895	3.541067
H	-0.815259	-3.366845	2.739212	H	-0.893945	3.902583	4.496416
H	-1.926779	-3.460985	1.363305	H	-1.355246	4.228892	2.825607
C	-0.070235	-4.314097	-0.522599	S	-2.153525	-0.454587	4.019655
H	-0.268395	-5.381820	-0.365968	O	-1.596865	-0.370640	5.367819
H	-0.929464	-3.870081	-1.034396	O	-2.974891	0.666401	3.531634
H	0.804773	-4.220063	-1.169586	O	-1.146312	-0.952821	2.995135
C	1.771063	-1.319873	-2.285819	C	-3.323852	-1.897596	4.092864
C	3.288883	-1.050127	-2.330666	F	-3.846922	-2.154528	2.875350
C	1.444095	-2.512404	-3.193453	F	-2.691383	-2.996943	4.515564
H	1.494201	-1.603222	-1.263156	F	-4.328505	-1.624552	4.929418
H	3.597117	-0.280859	-1.618614	H	1.078909	-4.033604	1.263643
H	3.835823	-1.966403	-2.081864	C	-5.564346	3.052865	0.569965
H	3.598744	-0.732503	-3.333985	C	-5.315716	4.221616	-0.160556
H	0.372825	-2.732527	-3.198923	C	-6.894460	2.712095	0.847705
H	1.776855	-2.346602	-4.225508	C	-6.364419	5.028470	-0.603188
H	1.968037	-3.400455	-2.828182	H	-4.288020	4.503732	-0.377741
C	0.002189	3.350345	-1.097535	C	-7.947030	3.514447	0.407765
C	-1.411370	3.953134	-1.047199	H	-7.102139	1.810527	1.419529
C	1.029111	4.444879	-1.444253	C	-7.685223	4.676458	-0.320853
H	0.233266	2.987707	-0.092922	H	-6.150314	5.934240	-1.164553
H	-2.171586	3.188582	-0.871586	H	-8.971772	3.235565	0.638150
H	-1.471698	4.684874	-0.234032	H	-8.503684	5.304484	-0.661531
H	-1.664914	4.474974	-1.976399				
H	2.052962	4.060316	-1.427163				
H	0.838768	4.850116	-2.444560	²TM3			
H	0.964905	5.268500	-0.724230	C	0.932907	0.461379	0.712825

C	2.656652	1.603627	-0.205580	H	-3.527801	2.750240	1.159068
C	2.876775	1.541651	1.128700	H	-4.654746	1.681014	1.965120
N	1.806615	0.844173	1.676371	Ni	-0.514975	-0.744905	1.112257
N	1.454280	0.939531	-0.448978	O	0.428754	-2.233894	0.575694
H	3.674340	1.919550	1.746103	C	0.168457	-3.604015	0.812266
H	3.221721	2.046359	-1.008153	C	-0.990743	-3.851783	1.777867
C	1.600805	0.725078	3.102268	H	-1.122486	-4.927136	1.950625
C	0.956742	1.792263	3.753967	H	-0.815259	-3.366845	2.739212
C	2.076827	-0.415576	3.763418	H	-1.926779	-3.460985	1.363305
C	0.839841	1.710163	5.143082	C	-0.070235	-4.314097	-0.522599
C	1.932855	-0.444688	5.154171	H	-0.268395	-5.381820	-0.365968
C	1.329576	0.607040	5.835442	H	-0.929464	-3.870081	-1.034396
H	0.334460	2.501455	5.685344	H	0.804773	-4.220063	-1.169586
H	2.278056	-1.310026	5.708513	C	1.771063	-1.319873	-2.285819
H	1.208720	0.552303	6.912799	C	3.288883	-1.050127	-2.330666
C	0.817590	0.996317	-1.745842	C	1.444095	-2.512404	-3.193453
C	0.116874	2.177737	-2.064758	H	1.494201	-1.603222	-1.263156
C	0.980952	-0.069461	-2.649206	H	3.597117	-0.280859	-1.618614
C	-0.452953	2.267099	-3.339224	H	3.835823	-1.966403	-2.081864
C	0.401097	0.083933	-3.915073	H	3.598744	-0.732503	-3.333985
C	-0.309770	1.230963	-4.256501	H	0.372825	-2.732527	-3.198923
H	-1.007504	3.157677	-3.615144	H	1.776855	-2.346602	-4.225508
H	0.499771	-0.711090	-4.643577	H	1.968037	-3.400455	-2.828182
H	-0.755438	1.316353	-5.243449	C	0.002189	3.350345	-1.097535
C	-3.661790	-3.297596	-1.461676	C	-1.411370	3.953134	-1.047199
C	-3.039405	-3.061511	-2.688208	C	1.029111	4.444879	-1.444253
C	-2.409847	-1.835991	-2.914034	H	0.233266	2.987707	-0.092922
C	-2.402229	-0.855386	-1.922949	H	-2.171586	3.188582	-0.871586
C	-3.024207	-1.081451	-0.687921	H	-1.471698	4.684874	-0.234032
C	-3.653418	-2.313985	-0.472175	H	-1.664914	4.474974	-1.976399
H	-4.149195	-4.249531	-1.270689	H	2.052962	4.060316	-1.427163
H	-3.042000	-3.826206	-3.459785	H	0.838768	4.850116	-2.444560
H	-1.924620	-1.636488	-3.864527	H	0.964905	5.268500	-0.724230
H	-1.916503	0.093395	-2.122028	C	2.734470	-1.559164	3.005692
H	-4.137554	-2.502179	0.480890	C	2.402903	-2.928801	3.614096
C	-1.770324	0.702862	0.623288	C	4.257982	-1.350828	2.923771
H	-1.782355	1.365437	1.484862	H	2.332080	-1.567772	1.988655
H	-1.387495	1.196620	-0.264083	H	1.321930	-3.054410	3.721271
C	-3.094497	0.004056	0.374961	H	2.778776	-3.723330	2.961002
H	-3.442741	-0.439529	1.308362	H	2.866457	-3.067534	4.597676
C	-4.163976	1.057966	-0.044564	H	4.511045	-0.411256	2.420350
H	-3.865026	1.514935	-0.997274	H	4.701809	-1.324545	3.926214
H	-5.096340	0.515077	-0.245623	H	4.727218	-2.168536	2.364454
C	-4.432354	2.152755	1.002873	C	0.418847	2.997081	2.993818

C	1.424253	4.163000	3.022867
C	-0.958247	3.457912	3.497080
H	0.290384	2.699458	1.948867
H	2.392603	3.875701	2.600671
H	1.042120	5.014034	2.446442
H	1.592561	4.498875	4.052456
H	-1.672767	2.631895	3.541067
H	-0.893945	3.902583	4.496416
H	-1.355246	4.228892	2.825607
S	-2.153525	-0.454587	4.019655
O	-1.596865	-0.370640	5.367819
O	-2.974891	0.666401	3.531634
O	-1.146312	-0.952821	2.995135
C	-3.323852	-1.897596	4.092864
F	-3.846922	-2.154528	2.875350
F	-2.691383	-2.996943	4.515564
F	-4.328505	-1.624552	4.929418
H	1.078909	-4.033604	1.263643
C	-5.564346	3.052865	0.569965
C	-5.315716	4.221616	-0.160556
C	-6.894460	2.712095	0.847705
C	-6.364419	5.028470	-0.603188
H	-4.288020	4.503732	-0.377741
C	-7.947030	3.514447	0.407765
H	-7.102139	1.810527	1.419529
C	-7.685223	4.676458	-0.320853
H	-6.150314	5.934240	-1.164553
H	-8.971772	3.235565	0.638150
H	-8.503684	5.304484	-0.661531

²IM4

C	-5.725495	-8.111796	-0.565136
C	-7.032825	-8.262834	-0.245187
H	-4.976671	-8.820204	-0.880686
H	-7.666197	-9.133015	-0.214660
C	-6.514198	-6.058720	0.028320
N	-7.501852	-6.997653	0.105084
N	-5.424859	-6.764285	-0.382356
C	-4.073566	-6.262019	-0.400152
C	-3.621305	-5.532747	-1.507698
C	-3.266620	-6.540448	0.714993
C	-2.300926	-5.071402	-1.481004
C	-1.956064	-6.054276	0.697112

C	-1.476770	-5.324475	-0.387672
H	-1.916332	-4.505346	-2.323396
H	-1.308123	-6.240598	1.548242
H	-0.456632	-4.950928	-0.381078
C	-8.805062	-6.769462	0.672452
C	-8.893379	-6.436171	2.038855
C	-9.941634	-6.934391	-0.142685
C	-10.174117	-6.288219	2.583634
C	-11.196333	-6.795567	0.461203
C	-11.314667	-6.478950	1.811239
H	-10.273435	-6.028216	3.632556
H	-12.090995	-6.919055	-0.139426
H	-12.298744	-6.370465	2.258627
Ni	-6.678981	-4.062153	0.316379
C	-9.502903	-2.177694	-0.369985
C	-10.237264	-3.146148	0.327941
C	-9.652388	-0.837641	0.006409
C	-11.087700	-2.784979	1.372885
H	-10.137953	-4.194052	0.069912
C	-10.500512	-0.470228	1.051797
H	-9.084661	-0.074216	-0.521309
C	-11.223121	-1.445439	1.741026
H	-11.637132	-3.558195	1.902044
H	-10.591370	0.576171	1.331537
H	-11.881068	-1.164389	2.558967
C	-3.772839	-7.326851	1.916378
H	-4.792986	-7.658020	1.707981
C	-3.843650	-6.444764	3.171947
H	-4.258427	-7.016913	4.010803
H	-2.849826	-6.088382	3.466361
H	-4.471610	-5.573278	2.975510
C	-2.929162	-8.590641	2.152874
H	-3.339931	-9.171125	2.986890
H	-2.912393	-9.232310	1.264183
H	-1.891803	-8.339896	2.401534
C	-4.509007	-5.278405	-2.713335
H	-5.534021	-5.515671	-2.419294
C	-4.486412	-3.807387	-3.154134
H	-5.198943	-3.646324	-3.970983
H	-4.752934	-3.147019	-2.324191
H	-3.498169	-3.509863	-3.521594
C	-4.135950	-6.217679	-3.874133
H	-4.810374	-6.065607	-4.724959
H	-3.110659	-6.032549	-4.214957

H	-4.202188	-7.267826	-3.567539
C	-7.682030	-6.270506	2.946293
H	-6.777267	-6.313845	2.339956
C	-7.675988	-4.897720	3.639086
H	-8.503938	-4.799715	4.351036
H	-6.737560	-4.763159	4.186456
H	-7.754213	-4.087171	2.908380
C	-7.607258	-7.419630	3.966359
H	-7.559877	-8.392366	3.463553
H	-6.712731	-7.312742	4.589979
H	-8.481683	-7.425702	4.627579
C	-9.849629	-7.221692	-1.635162
H	-8.831216	-6.992868	-1.964722
C	-10.133851	-8.700328	-1.955303
H	-9.445084	-9.378024	-1.441049
H	-11.152267	-8.971880	-1.653815
H	-10.040161	-8.874066	-3.033151
C	-10.802174	-6.327226	-2.444080
H	-11.850151	-6.599420	-2.274672
H	-10.680428	-5.275472	-2.176675
H	-10.597737	-6.433727	-3.511007
C	-10.099955	-5.744119	-6.100053
C	-9.882804	-4.483573	-5.543122
C	-8.777251	-4.234084	-4.717634
C	-7.893847	-5.292087	-4.470403
C	-8.105663	-6.557738	-5.019375
C	-9.211538	-6.790216	-5.838703
H	-10.962186	-5.909580	-6.740450
H	-10.579121	-3.675254	-5.754467
H	-7.030335	-5.125083	-3.839662
H	-7.400699	-7.358132	-4.809737
H	-9.377155	-7.772057	-6.273296
C	-8.572299	-2.856235	-4.121724
H	-7.508922	-2.700776	-3.906471
H	-8.839206	-2.115230	-4.884380
C	-9.406455	-2.573909	-2.838798
H	-10.208009	-3.315528	-2.750487
H	-9.906231	-1.602851	-2.940183
C	-8.585382	-2.547883	-1.521665
H	-7.851280	-1.737141	-1.623625
C	-7.809645	-3.842827	-1.277339
H	-8.479613	-4.708857	-1.296088
H	-7.079248	-3.994524	-2.075598
O	-5.157157	-3.945042	1.323895

H	-6.955944	-2.634245	0.435497
C	-4.573295	-2.707657	1.677112
H	-5.335162	-2.037217	2.108732
C	-3.981333	-2.025204	0.439181
H	-3.501313	-1.072488	0.697662
H	-3.236490	-2.681683	-0.025125
H	-4.771729	-1.826540	-0.292871
C	-3.490230	-2.943100	2.733914
H	-2.716976	-3.611197	2.338193
H	-3.018572	-1.997247	3.028157
H	-3.917932	-3.405846	3.629310

²IM5

C	0.989081	0.654767	0.842690
C	2.074592	2.427291	-0.091684
C	2.296192	2.470915	1.242587
N	1.636239	1.378262	1.797908
N	1.265913	1.319762	-0.317776
H	2.873395	3.143790	1.855176
H	2.402292	3.063685	-0.896455
C	1.856179	1.028690	3.181242
C	0.888807	1.371373	4.134372
C	3.077671	0.419168	3.501686
C	1.170380	1.064296	5.469073
C	3.315506	0.138106	4.850280
C	2.370697	0.451144	5.823751
H	0.446468	1.307413	6.239456
H	4.243195	-0.347530	5.137436
H	2.569828	0.217429	6.865906
C	0.837448	0.903631	-1.625414
C	-0.069005	1.719770	-2.323017
C	1.354671	-0.298891	-2.146955
C	-0.484631	1.283279	-3.585585
C	0.884249	-0.699825	-3.401765
C	-0.028157	0.079202	-4.111916
H	-1.186847	1.886499	-4.152170
H	1.244031	-1.626945	-3.833021
H	-0.377183	-0.252939	-5.085634
C	-3.778849	0.639436	0.933635
C	-4.239205	0.488838	-0.374638
C	-3.387188	-0.043861	-1.345485
C	-2.088088	-0.431152	-1.010414
C	-1.627712	-0.299509	0.304524

C	-2.477489	0.247468	1.271432	H	5.899641	0.364027	3.665883
H	-4.431345	1.050904	1.700172	H	6.175498	0.488028	1.922976
H	-5.250645	0.786902	-0.637123	C	-0.385018	2.098013	3.733131
H	-3.730877	-0.158166	-2.370744	C	-0.167990	3.622592	3.777907
H	-1.447696	-0.862581	-1.770924	C	-1.602163	1.698908	4.578021
H	-2.146955	0.337775	2.300326	H	-0.608079	1.830642	2.696788
Ni	0.026390	-1.094955	0.924605	H	0.646275	3.929384	3.112813
O	-0.410514	-2.733942	0.284035	H	-1.076813	4.150474	3.466042
C	-1.611141	-3.409243	-0.012961	H	0.085623	3.948072	4.793662
C	-1.923505	-4.449737	1.066790	H	-1.730509	0.612408	4.602831
H	-1.102061	-5.171006	1.150921	H	-1.516900	2.054421	5.611182
H	-2.054117	-3.964866	2.038558	H	-2.509793	2.143994	4.155255
C	-1.465172	-4.054412	-1.395378	O	0.938466	-1.547330	2.500446
H	-2.380071	-4.586666	-1.683528	H	-2.844433	-4.996258	0.827255
H	-1.254162	-3.288462	-2.149122	H	-2.450698	-2.702664	-0.057586
H	-0.633502	-4.769250	-1.392863	C	0.489617	-2.659340	3.247408
C	2.459212	-1.078548	-1.439615	H	0.248907	-3.488473	2.566861
C	3.830311	-0.509422	-1.853329	C	-0.777603	-2.286949	4.028170
C	2.387879	-2.593910	-1.660007	H	-1.162691	-3.139940	4.601518
H	2.362568	-0.922632	-0.362634	H	-0.555104	-1.470213	4.725203
H	3.904059	0.560508	-1.628166	H	-1.563525	-1.951057	3.342159
H	4.632999	-1.026367	-1.315066	C	1.597780	-3.116016	4.201121
H	3.998329	-0.640861	-2.928836	H	1.885401	-2.297335	4.869033
H	1.417304	-2.981948	-1.339726	H	1.258854	-3.964108	4.809510
H	2.566519	-2.870403	-2.705738	H	2.484354	-3.430000	3.642270
H	3.162652	-3.081009	-1.057745				
C	-0.558972	3.054552	-1.776094				
C	-2.088130	3.192943	-1.791557				
C	0.097989	4.212350	-2.552122	²TM6			
H	-0.248912	3.131925	-0.730579	C	0.366201	0.553944	-2.627142
H	-2.560492	2.421964	-1.181936	C	-0.983965	0.526645	-2.486002
H	-2.372038	4.174192	-1.393745	H	0.994831	0.677329	-3.494409
H	-2.494115	3.119821	-2.806856	H	-1.782859	0.620359	-3.204044
H	1.191926	4.147609	-2.536381	C	-0.078202	0.248897	-0.406430
H	-0.213729	4.201509	-3.602874	N	-1.232321	0.342022	-1.130605
H	-0.194258	5.177462	-2.123067	N	0.896628	0.383567	-1.353201
C	4.108816	0.050483	2.443541	C	2.300122	0.347365	-1.045934
C	4.245502	-1.473436	2.297146	C	2.939489	1.547919	-0.697068
C	5.464770	0.718761	2.724738	C	2.959965	-0.892310	-1.077475
H	3.761457	0.425449	1.477476	C	4.300437	1.482929	-0.379273
H	3.272426	-1.910622	2.063027	C	4.320254	-0.904716	-0.752294
H	4.957889	-1.711721	1.497453	C	4.984581	0.270389	-0.408372
H	4.613091	-1.930373	3.223371	H	4.825741	2.389779	-0.095957
H	5.367483	1.808575	2.793101	H	4.861667	-1.845543	-0.756691
				H	6.040315	0.239248	-0.154126

C	-2.539202	0.248843	-0.540128
C	-3.119635	-1.021559	-0.397096
C	-3.161732	1.430491	-0.104866
C	-4.382319	-1.087684	0.201648
C	-4.422991	1.311716	0.487972
C	-5.028453	0.066116	0.637987
H	-4.858389	-2.054058	0.336899
H	-4.930774	2.201811	0.846020
H	-6.006493	-0.006314	1.105308
C	-2.476174	2.784213	-0.211477
H	-1.596483	2.668954	-0.852051
C	-1.979168	3.239934	1.172405
H	-2.820044	3.388721	1.859928
H	-1.311177	2.492792	1.614526
H	-1.433318	4.187265	1.090937
C	-3.378278	3.844981	-0.861556
H	-3.729872	3.520238	-1.847281
H	-4.258480	4.061290	-0.245978
H	-2.826581	4.783549	-0.986145
C	-2.398841	-2.290196	-0.825884
H	-1.487745	-2.000056	-1.357455
C	-1.968956	-3.107437	0.404979
H	-1.400664	-3.992600	0.096222
H	-1.339919	-2.508450	1.072066
H	-2.841191	-3.446061	0.976262
C	-3.246230	-3.131613	-1.793903
H	-4.163130	-3.494954	-1.316414
H	-3.536022	-2.551186	-2.677006
H	-2.679359	-4.007332	-2.129804
C	2.187472	2.867445	-0.615683
H	1.178864	2.708056	-1.008361
C	2.846920	3.958343	-1.474812
H	3.851456	4.204861	-1.113129
H	2.935609	3.642228	-2.520263
H	2.250209	4.877001	-1.443531
C	2.041281	3.314179	0.849728
H	1.542143	2.542427	1.445721
H	3.020941	3.508827	1.301534
H	1.449419	4.234956	0.911290
C	2.223084	-2.185754	-1.390463
H	1.229965	-1.926954	-1.770307
C	2.927808	-3.009183	-2.479875
H	3.066405	-2.423447	-3.395519
H	3.913683	-3.356751	-2.151456

H	2.332643	-3.895710	-2.726312
C	2.022313	-3.008252	-0.104726
H	2.986565	-3.313551	0.318151
H	1.490884	-2.425039	0.654880
H	1.440724	-3.913426	-0.315789
Ni	0.129924	-0.010687	1.499395
H	0.295171	-0.216790	3.012569

²IM7a

C	-1.422226	0.214922	1.279364
N	-1.609340	-0.229399	0.000027
C	-0.513531	-0.944414	-0.471952
C	-2.790343	0.066005	-0.759741
N	-0.179087	-0.259322	1.596175
C	0.393521	-0.959595	0.536766
C	0.451079	-0.073851	2.874981
C	-3.936871	-0.719452	-0.553216
C	-2.756336	1.147069	-1.656672
C	-5.077949	-0.405201	-1.299050
C	-3.967972	-1.851785	0.461585
C	-5.067983	0.646084	-2.212520
C	-3.918797	1.412992	-2.388041
C	-1.511427	2.000370	-1.843830
C	-4.892445	-1.497432	1.639130
C	-4.369867	-3.188076	-0.183261
C	-1.807861	3.494700	-1.643221
C	-0.869198	1.727958	-3.215548
C	0.382408	-1.123078	3.809628
C	1.089820	1.148031	3.141758
C	0.985668	-0.917689	5.054300
C	-0.403065	-2.393399	3.512470
C	1.623301	0.284739	5.350540
C	1.676788	1.301967	4.403163
C	1.175529	2.245172	2.091472
C	-1.871156	-2.218114	3.946484
C	0.210333	-3.648931	4.147435
C	2.504240	2.134909	1.321275
C	0.982893	3.649388	2.677692
H	-5.983291	-0.988659	-1.160653
H	-5.962702	0.873219	-2.785560
H	-3.926260	2.237997	-3.093610
H	0.934042	-1.690219	5.813444
H	2.052742	0.437530	6.334778

H	2.166980	2.236556	4.653601
H	-2.959537	-1.973259	0.866075
H	-0.789727	1.717298	-1.073124
H	-0.402477	-2.546338	2.428069
H	0.356514	2.098311	1.384071
H	-4.867799	-2.286951	2.398996
H	-5.929767	-1.377605	1.305695
H	-4.577736	-0.559406	2.108265
H	-4.328985	-3.994789	0.557614
H	-3.697874	-3.446586	-1.008960
H	-5.390639	-3.154038	-0.580413
H	-0.883334	4.074376	-1.750085
H	-2.207119	3.665392	-0.639114
H	-2.523127	3.872079	-2.383393
H	0.048812	2.315130	-3.332830
H	-1.549845	1.999812	-4.030975
H	-0.614187	0.668454	-3.334679
H	-2.457349	-3.110022	3.693806
H	-2.323185	-1.353269	3.453901
H	-1.935040	-2.062851	5.030238
H	-0.322550	-4.541119	3.800374
H	0.134741	-3.631212	5.240353
H	1.268165	-3.756696	3.884016
H	2.559977	2.902312	0.540333
H	2.605390	1.154643	0.841707
H	3.360321	2.269735	1.993431
H	0.960600	4.385551	1.866973
H	1.793558	3.932248	3.359562
H	0.030058	3.714689	3.210766
H	-0.490403	-1.363968	-1.464777
H	1.375332	-1.398787	0.612211
H	-2.024462	2.866254	1.551912
Ni	-2.522472	1.528505	2.190381
C	0.957686	2.351910	8.373001
C	-0.212196	2.485816	7.625796
C	-1.085285	1.403856	7.452017
C	-0.751482	0.180743	8.045906
C	0.416457	0.039444	8.796625
C	1.277047	1.126255	8.963008
H	1.618945	3.205156	8.499189
H	-0.454349	3.441665	7.166986
H	-1.416511	-0.670032	7.915333
H	0.652764	-0.917592	9.254566
H	2.184601	1.021581	9.551159

C	-2.306131	1.532384	6.573877
H	-3.027350	0.742902	6.820507
H	-2.811169	2.490674	6.746620
C	-1.923460	1.421362	5.078392
H	-1.325436	0.516331	4.952255
H	-1.266564	2.259566	4.819741
C	-3.109458	1.394897	4.149032
H	-3.732160	0.499372	4.210609
C	-3.642105	2.536073	3.542748
H	-3.210589	3.515273	3.726752
H	-4.663470	2.543411	3.163124

²IM7b

C	0.255926	0.878817	-0.339565
N	-0.896320	0.798117	-1.078162
C	-0.862863	-0.268673	-1.971756
C	-2.019003	1.697282	-0.953005
N	1.004784	-0.170306	-0.810503
C	0.335182	-0.880143	-1.803720
C	2.322858	-0.511608	-0.331302
C	-3.065057	1.356823	-0.071427
C	-2.041941	2.864453	-1.743636
C	-4.151517	2.237164	0.010139
C	-3.072066	0.062773	0.737477
C	-4.196566	3.401121	-0.751833
C	-3.153548	3.707315	-1.621753
C	-0.937969	3.200028	-2.742552
C	-3.319936	0.305501	2.237003
C	-4.098534	-0.932381	0.157052
C	-0.401305	4.632766	-2.571600
C	-1.420033	2.962359	-4.188640
C	2.441470	-1.420925	0.739742
C	3.444202	0.060993	-0.966780
C	3.734165	-1.742803	1.173177
C	1.235260	-2.072530	1.409778
C	4.858146	-1.188991	0.567215
C	4.711962	-0.298601	-0.493149
C	3.320365	1.020119	-2.147160
C	1.182975	-1.773248	2.919907
C	1.208953	-3.590433	1.137221
C	3.835058	0.368307	-3.446603
C	4.033241	2.359541	-1.882016
H	-4.973942	2.005716	0.680436

H	-5.049183	4.070159	-0.670205
H	-3.204036	4.613484	-2.218438
H	3.859399	-2.438360	1.997964
H	5.851318	-1.453577	0.920622
H	5.595910	0.124120	-0.962209
H	-2.081498	-0.392717	0.654099
H	-0.099416	2.522070	-2.558988
H	0.329898	-1.643585	0.971376
H	2.259657	1.245014	-2.291254
H	-3.294069	-0.648949	2.776642
H	-4.298395	0.763103	2.425259
H	-2.538498	0.950288	2.649960
H	-4.069747	-1.878161	0.711144
H	-3.896830	-1.151754	-0.898121
H	-5.118649	-0.535518	0.224245
H	0.432639	4.806305	-3.262088
H	-0.039957	4.797645	-1.552038
H	-1.167122	5.386606	-2.787921
H	-0.612758	3.167090	-4.902124
H	-2.263109	3.617834	-4.437618
H	-1.748661	1.927341	-4.336554
H	0.302869	-2.252950	3.364770
H	1.104919	-0.696018	3.097014
H	2.068242	-2.155727	3.442085
H	0.311867	-4.040399	1.578479
H	2.081673	-4.091605	1.572631
H	1.203558	-3.806651	0.062376
H	3.703510	1.049544	-4.295682
H	3.295750	-0.559408	-3.669245
H	4.901594	0.124196	-3.375108
H	3.872884	3.045843	-2.721879
H	5.115240	2.229396	-1.764030
H	3.649925	2.836652	-0.974044
H	-1.687050	-0.486153	-2.632787
H	0.770942	-1.740784	-2.286454
Ni	0.637511	2.035174	1.206718
C	-2.858301	6.464763	5.860541
C	-2.087502	6.115758	4.749675
C	-1.956715	4.778708	4.349772
C	-2.624838	3.796973	5.096766
C	-3.396905	4.139541	6.207574
C	-3.516509	5.476464	6.594609
H	-2.947105	7.509115	6.150076
H	-1.580650	6.892561	4.180314

H	-2.538453	2.754335	4.798426
H	-3.908789	3.362156	6.769797
H	-4.119508	5.745246	7.458175
C	-1.094500	4.395148	3.165846
H	-1.551244	3.561675	2.618374
H	-1.036175	5.243762	2.472536
C	0.324589	3.969245	3.585729
H	0.248214	3.154292	4.313941
H	0.799913	4.813009	4.114035
C	1.244197	3.534588	2.459641
C	1.195996	4.014178	1.148228
H	0.390416	4.658984	0.805300
H	2.094098	4.029926	0.531920
H	-0.179358	1.403941	2.387221
H	2.204919	3.151197	2.814867

²IM8a

C	-1.382368	-0.045338	1.176000
N	-1.567036	-0.453908	-0.111987
C	-0.478613	-1.181798	-0.586125
C	-2.748460	-0.142456	-0.867381
N	-0.149296	-0.543626	1.493831
C	0.417946	-1.238756	0.432911
C	0.458586	-0.316932	2.779237
C	-3.800433	-1.074651	-0.876791
C	-2.815269	1.095481	-1.526430
C	-4.952795	-0.736670	-1.593137
C	-3.721957	-2.365513	-0.074985
C	-5.046655	0.481562	-2.263440
C	-3.990670	1.387870	-2.227876
C	-1.684056	2.109921	-1.457875
C	-4.438324	-2.188060	1.277208
C	-4.270457	-3.578880	-0.840280
C	-2.097834	3.323295	-0.606315
C	-1.213304	2.538660	-2.857057
C	0.193991	-1.223685	3.819292
C	1.231191	0.843116	2.958600
C	0.744557	-0.944073	5.074339
C	-0.711192	-2.430785	3.628478
C	1.516138	0.195287	5.283139
C	1.757140	1.076807	4.233402
C	1.445663	1.851718	1.840466
C	-2.024722	-2.246003	4.409071

C	-0.005893	-3.740176	4.016531
C	2.938589	2.113785	1.585542
C	0.686882	3.156800	2.138981
H	-5.789408	-1.427258	-1.618459
H	-5.951967	0.727748	-2.811251
H	-4.080950	2.338806	-2.743871
H	0.538912	-1.605827	5.909594
H	1.897916	0.413333	6.274539
H	2.338657	1.975631	4.414147
H	-2.667393	-2.566636	0.138939
H	-0.833867	1.637354	-0.957519
H	-0.970697	-2.499119	2.567653
H	1.025352	1.435407	0.920058
H	-4.340717	-3.094924	1.885721
H	-5.506094	-1.990430	1.125717
H	-4.015601	-1.348347	1.838813
H	-4.100342	-4.493798	-0.262055
H	-3.781837	-3.692726	-1.814265
H	-5.349636	-3.499171	-1.011784
H	-1.267033	4.033501	-0.524299
H	-2.382282	3.011195	0.404631
H	-2.950341	3.846940	-1.054467
H	-0.358455	3.219471	-2.775934
H	-2.002878	3.064155	-3.405806
H	-0.907408	1.673791	-3.456210
H	-2.695246	-3.096490	4.238586
H	-2.538753	-1.331913	4.093259
H	-1.835099	-2.171869	5.486133
H	-0.660167	-4.597555	3.821276
H	0.253113	-3.756060	5.081052
H	0.919219	-3.877087	3.445475
H	3.065284	2.801185	0.741323
H	3.471212	1.184439	1.354589
H	3.421530	2.567812	2.457969
H	0.798002	3.863605	1.308149
H	1.070326	3.636300	3.046884
H	-0.380212	2.959646	2.286488
H	-0.453141	-1.580998	-1.587478
H	1.390533	-1.698433	0.506763
H	-2.493974	4.050900	3.394547
Ni	-2.394863	1.010541	2.421770
C	1.220656	2.428629	8.248671
C	0.098785	2.792279	7.502855
C	-0.988134	1.919799	7.355650

C	-0.913294	0.664594	7.975914
C	0.204640	0.293365	8.723110
C	1.279020	1.175509	8.863586
H	2.048403	3.125406	8.354693
H	0.060125	3.768378	7.024490
H	-1.745542	-0.027378	7.866816
H	0.235926	-0.682399	9.201644
H	2.148216	0.892451	9.451099
C	-2.154728	2.274023	6.469698
H	-3.067863	1.782716	6.830450
H	-2.337611	3.354325	6.497084
C	-1.882169	1.817714	5.012002
H	-1.595489	0.759730	5.068822
H	-0.977310	2.340793	4.670326
C	-3.023568	2.011967	3.993485
H	-3.921237	1.514327	4.402615
C	-3.360200	3.496103	3.784423
H	-3.674500	4.012796	4.708183
H	-4.172691	3.622693	3.057981

²TM8b

C	0.084377	0.437387	-0.677379
N	-0.913105	0.089755	-1.551366
C	-0.482992	-0.858267	-2.474448
C	-2.251417	0.633350	-1.527222
N	1.145591	-0.326377	-1.089713
C	0.815285	-1.120684	-2.183263
C	2.452075	-0.318140	-0.473027
C	-3.235283	-0.022682	-0.760049
C	-2.527622	1.788083	-2.286961
C	-4.528809	0.513719	-0.771970
C	-2.940591	-1.266937	0.071978
C	-4.830189	1.652294	-1.513938
C	-3.838302	2.280590	-2.261681
C	-1.465441	2.507955	-3.112114
C	-3.167472	-1.003830	1.573590
C	-3.759832	-2.479168	-0.413044
C	-1.232589	3.942023	-2.597503
C	-1.815096	2.502551	-4.613309
C	2.711567	-1.222727	0.576310
C	3.423895	0.580954	-0.956706
C	3.992595	-1.206932	1.141752
C	1.661002	-2.190923	1.111218

C	2.765267	-3.167146	5.340020	C	5.145049	-2.950255	4.492196
C	0.598926	-4.942651	5.584054	H	5.612422	-3.658190	5.185469
C	2.950865	-4.458557	5.843273	H	4.844461	-3.504794	3.600044
C	1.878261	-5.334041	5.970300	H	5.911798	-2.219399	4.208977
H	-0.215805	-5.654331	5.640542	H	-0.241212	-0.038006	-0.042520
H	3.948730	-4.790781	6.109412	C	-4.994121	-4.231938	1.537445
H	2.043766	-6.340391	6.343694	C	-4.021762	-3.536658	0.816581
Ni	1.696307	-1.921805	1.524282	C	-2.807571	-4.146676	0.478665
C	-2.023669	0.645234	2.814034	C	-2.581738	-5.469143	0.881864
H	-1.572686	-0.247154	3.259140	C	-3.553759	-6.168253	1.596597
C	-3.174784	0.171994	1.910066	C	-4.762765	-5.552694	1.927230
H	-3.818788	-0.521648	2.460681	H	-5.933516	-3.745730	1.787810
H	-3.799055	1.008897	1.577316	H	-4.208267	-2.511182	0.505256
H	-2.803131	-0.345984	1.021610	H	-1.627719	-5.939270	0.658661
C	-2.576061	1.513786	3.959343	H	-3.361279	-7.192482	1.903335
H	-3.344500	0.965797	4.516030	H	-5.519129	-6.097411	2.485566
H	-1.791366	1.802406	4.664516	C	-1.728931	-3.386289	-0.250526
H	-3.028999	2.430422	3.563948	H	-1.132377	-4.077526	-0.855075
C	2.926622	1.554298	1.886891	H	-2.170592	-2.647567	-0.930038
H	3.019857	0.548874	2.308143	C	-0.771268	-2.675468	0.743509
C	3.833558	1.605630	0.650458	H	-0.469861	-3.418300	1.484103
H	4.843143	1.285028	0.922618	H	-1.312943	-1.893330	1.285599
H	3.478173	0.932127	-0.133927	C	0.432909	-2.102511	0.015242
H	3.906870	2.619725	0.240964	H	0.896077	-2.863012	-0.609457
C	3.404766	2.551671	2.959433	C	0.185862	-0.794032	-0.704087
H	4.455510	2.366628	3.209715	H	-0.535649	-0.956066	-1.520608
H	3.317291	3.581905	2.594978	H	1.095696	-0.386462	-1.150279
H	2.817555	2.466813	3.879508	C	3.157679	-1.907201	0.288673
C	-1.029728	-3.233480	4.628342	C	4.288558	-1.793627	1.110067
H	-0.892364	-2.547856	3.785822	C	3.332760	-1.921134	-1.094411
C	-1.870795	-4.405777	4.110618	C	5.568061	-1.666391	0.562719
H	-2.205768	-5.055069	4.928758	H	4.186464	-1.816796	2.194063
H	-2.765878	-4.030089	3.606147	C	4.609883	-1.791446	-1.648211
H	-1.304910	-5.012840	3.400894	H	2.484087	-2.045761	-1.760249
C	-1.785991	-2.472090	5.733588	C	5.728427	-1.658064	-0.823122
H	-1.248153	-1.576973	6.061589	H	6.431517	-1.585687	1.218552
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C	3.949227	-2.233150	5.142176	O	1.597557	-4.996574	0.143939
H	3.634890	-1.435633	4.459197	S	1.703632	-5.117158	1.605770
C	4.366661	-1.570772	6.467237	O	0.758125	-6.018770	2.278868
H	3.545393	-0.992695	6.904217	O	1.839856	-3.789423	2.331262
H	4.667570	-2.329530	7.198819	C	3.389415	-5.833334	1.914379
H	5.214270	-0.892844	6.312303	F	3.586345	-6.031637	3.225971

F 3.520552 -7.001764 1.277908
 F 4.339658 -4.993015 1.471284

²IM9b

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H	2.947483	-1.975868	-0.685537	C	1.340314	-2.869154	4.775563
H	2.542101	-0.543594	-1.627924	C	0.225558	-3.715766	4.867698
C	3.188051	-0.097934	0.368738	C	2.641094	-3.257956	5.122252
H	3.578066	0.907736	0.126793	C	0.444369	-4.999380	5.373747
C	3.992549	-0.588480	1.554458	C	2.804083	-4.548399	5.634515
H	5.007577	-0.895729	1.284828	C	1.717142	-5.406627	5.765166
C	2.038459	-2.414708	1.924967	H	-0.383290	-5.695384	5.440946
C	0.996245	-1.579372	2.351561	H	3.796985	-4.894705	5.902875
C	1.735332	-3.625044	1.288822	H	1.866296	-6.412024	6.148158
C	-0.334612	-1.972328	2.196240	Ni	1.179876	-1.966614	1.288094
H	1.208635	-0.626121	2.826438	C	-1.658287	0.456771	1.821180
C	0.399789	-4.008111	1.126362	H	-1.305575	-0.541709	2.099938
H	2.530127	-4.256024	0.911980	C	-2.703708	0.281240	0.711984
C	-0.635167	-3.189918	1.583205	H	-3.459548	-0.442222	1.035307
H	-1.131064	-1.325129	2.555032	H	-3.222747	1.221594	0.493145
H	0.172508	-4.949867	0.633130	H	-2.261832	-0.087389	-0.217805
H	-1.670132	-3.494285	1.451680	C	-2.327984	1.072299	3.066307
O	4.460679	-4.151145	-0.123857	H	-3.189045	0.465889	3.368789
S	5.466248	-3.969862	0.935351	H	-1.642641	1.124817	3.915552
O	6.607723	-3.095092	0.634495	H	-2.683180	2.086206	2.847919
O	4.865974	-3.719280	2.308479	C	3.178505	1.894989	2.631689
C	6.158865	-5.677847	1.179322	H	2.890162	1.743728	3.677629
F	6.594302	-6.149110	0.006715	C	4.026302	0.675052	2.219203
F	7.179983	-5.674964	2.045416	H	4.881951	0.575104	2.896973
F	5.204658	-6.493612	1.649102	H	3.454599	-0.254192	2.251872
²TS10				H	4.403872	0.788813	1.199759
C	0.831004	0.664150	4.552463	C	4.030144	3.170990	2.585767
C	1.001222	-0.475075	5.266288	H	4.857764	3.085329	3.297582
H	0.686739	1.688687	4.855046	H	4.472285	3.327261	1.595275
H	1.044999	-0.659926	6.327108	H	3.447243	4.061809	2.844856
C	1.059377	-1.055867	3.065391	C	-1.157903	-3.255658	4.429415
N	1.134188	-1.508379	4.346138	H	-1.019036	-2.545984	3.606095
N	0.866981	0.290005	3.214276	C	-2.018786	-4.403356	3.890951
C	0.768558	1.210859	2.116301	H	-2.360653	-5.064090	4.696775
C	1.891934	2.004210	1.817054	H	-2.910700	-4.008564	3.394742
C	-0.442271	1.277311	1.399846	H	-1.461708	-5.004327	3.170547
C	1.777718	2.886693	0.737109	C	-1.887024	-2.511840	5.564057
C	-0.495351	2.167966	0.321139	H	-1.330307	-1.632404	5.903194
C	0.602613	2.961565	-0.006391	H	-2.874837	-2.176740	5.225815
H	2.618013	3.516069	0.468384	H	-2.030873	-3.175063	6.425190
H	-1.403886	2.248419	-0.264373	C	3.844566	-2.358384	4.883312
H	0.539499	3.646304	-0.847320	H	3.482223	-1.352923	4.648009
				C	4.740760	-2.237209	6.125314
				H	4.174047	-1.883780	6.994371

H	5.195670	-3.197808	6.390907	C	3.271430	-6.009894	1.873837
H	5.555895	-1.529402	5.936023	F	3.446237	-6.068538	3.199970
C	4.639797	-2.850596	3.659966	F	3.310285	-7.253434	1.383403
H	5.027234	-3.861361	3.826802	F	4.289587	-5.308109	1.345251
H	4.006758	-2.885465	2.770827				
H	5.488865	-2.184508	3.465084				
H	-0.409643	-0.591390	-1.285257				
C	-4.961219	-4.396317	1.123925	²TS11a			
C	-3.868385	-3.931906	0.392363	C	0.534029	-3.158246	0.410345
C	-2.703266	-4.702153	0.272726	C	-0.788136	-3.038316	0.686817
C	-2.656028	-5.950761	0.902726	H	1.189150	-4.013081	0.412412
C	-3.750837	-6.422258	1.628833	H	-1.524802	-3.762278	0.992751
C	-4.905475	-5.647309	1.743794	C	-0.007419	-0.968063	0.160829
H	-5.858319	-3.787718	1.203877	N	-1.100345	-1.693450	0.527818
H	-3.920783	-2.963049	-0.100958	N	0.997990	-1.885435	0.096848
H	-1.743670	-6.537156	0.847446	C	2.399235	-1.586458	-0.117616
H	-3.696050	-7.393203	2.113454	C	2.972459	-1.869354	-1.368015
H	-5.756459	-6.013345	2.311630	C	3.137799	-1.065023	0.965502
C	-1.512670	-4.183244	-0.494813	C	4.333111	-1.580078	-1.530249
H	-0.779276	-4.979980	-0.640558	C	4.489669	-0.791491	0.744742
H	-1.830619	-3.841811	-1.487569	C	5.081259	-1.039800	-0.491548
C	-0.809299	-3.014360	0.243359	H	4.805598	-1.779432	-2.486031
H	-0.534942	-3.401882	1.233190	H	5.086474	-0.372986	1.546625
H	-1.526688	-2.206052	0.415785	H	6.133072	-0.812588	-0.641865
C	0.386412	-2.503339	-0.600188	C	-2.343844	-1.096153	0.946352
H	0.913420	-3.362425	-1.003963	C	-2.397632	-0.574405	2.252261
C	-0.104621	-1.561632	-1.690956	C	-3.439560	-1.076588	0.065848
H	-0.984099	-1.997061	-2.182644	C	-3.589135	0.041279	2.652402
H	0.655284	-1.381689	-2.453519	C	-4.609362	-0.456880	0.519686
C	2.241027	-1.564997	-0.270985	C	-4.682538	0.104594	1.792460
C	3.345989	-2.397478	-0.505011	H	-3.664372	0.458195	3.652329
C	2.289137	-0.225985	-0.681501	H	-5.473717	-0.415475	-0.134036
C	4.503463	-1.869937	-1.080410	H	-5.601904	0.582282	2.120511
H	3.301815	-3.445378	-0.238366	Ni	0.014937	0.981483	-0.433004
C	3.446617	0.291438	-1.264450	C	-0.572549	2.984681	-0.474037
H	1.430355	0.420433	-0.552794	C	-1.440171	2.674543	0.586058
C	4.560513	-0.526598	-1.461840	C	-0.997282	3.617008	-1.647528
H	5.359148	-2.519861	-1.243555	C	-2.822022	2.774946	0.338080
H	3.470593	1.336875	-1.561550	H	-1.064501	2.390515	1.562021
H	5.459570	-0.126559	-1.922420	C	-2.363927	3.711152	-1.857719
O	1.648463	-5.282386	-0.050435	H	-0.275810	3.926992	-2.392205
S	1.656665	-5.207564	1.423414	C	-3.275626	3.275653	-0.875710
O	0.609863	-5.957597	2.132796	H	-3.519584	2.477912	1.112868
O	1.871737	-3.812285	1.960792	H	-2.731629	4.108846	-2.799448
				H	-4.342181	3.360721	-1.059124

O	1.001139	3.915792	0.174395
S	2.164609	2.991169	0.501706
O	3.041249	3.454784	1.569404
O	1.690927	1.570167	0.629768
C	3.170648	2.996007	-1.066813
F	3.843050	4.144595	-1.155606
F	4.026644	1.975963	-1.050919
F	2.359705	2.880280	-2.122304
C	2.515677	-0.859130	2.340696
H	1.490449	-0.519054	2.185859
C	3.217224	0.209006	3.188926
H	2.634000	0.389657	4.098771
H	4.214351	-0.116496	3.507995
H	3.311927	1.156587	2.655902
C	2.467466	-2.188554	3.120598
H	1.990831	-2.038772	4.097011
H	1.904548	-2.960262	2.588741
H	3.481443	-2.567390	3.294204
C	2.192997	-2.526767	-2.494507
H	1.128694	-2.372192	-2.313887
C	2.505508	-1.922812	-3.872412
H	1.792705	-2.308027	-4.607946
H	2.415596	-0.835142	-3.849972
H	3.513786	-2.186287	-4.213570
C	2.461233	-4.044437	-2.511952
H	1.876419	-4.523695	-3.305217
H	3.522043	-4.249848	-2.698596
H	2.195470	-4.521141	-1.562220
C	-1.253150	-0.733581	3.246417
H	-0.466691	-1.325338	2.773753
C	-0.627400	0.609532	3.655995
H	-1.383923	1.306919	4.033957
H	0.112993	0.457138	4.448853
H	-0.109419	1.078501	2.815245
C	-1.718924	-1.524129	4.482693
H	-2.159924	-2.484149	4.193622
H	-0.868668	-1.722154	5.144954
H	-2.469040	-0.970450	5.058139
C	-3.395433	-1.768355	-1.286369
H	-2.354301	-1.819344	-1.607256
C	-3.926957	-3.209505	-1.155108
H	-3.350603	-3.794521	-0.430665
H	-4.973515	-3.211322	-0.827562
H	-3.870486	-3.721676	-2.122017

C	-4.170399	-1.016072	-2.377842
H	-5.255072	-1.080487	-2.227486
H	-3.875145	0.034120	-2.411404
H	-3.945415	-1.461966	-3.352194
O	-1.545395	0.595327	-2.048441
S	-0.506519	0.075995	-2.994802
C	-0.706524	1.080855	-4.545692
F	-0.421238	2.370311	-4.324577
F	0.118671	0.614264	-5.486062
F	-1.968959	0.986612	-4.975601
O	-0.675552	-1.311126	-3.438221
O	0.845282	0.468182	-2.462886

²TS11c

C	3.268485	-0.640490	0.724630
C	2.724430	-1.882805	0.693182
H	4.242597	-0.294251	1.027220
H	3.120676	-2.846297	0.969219
C	1.140669	-0.434752	-0.040675
N	1.418187	-1.738659	0.228401
N	2.284325	0.232703	0.274602
C	2.362305	1.675919	0.334914
C	2.959121	2.381249	-0.724111
C	1.818084	2.309205	1.472747
C	3.034696	3.774049	-0.597694
C	1.916017	3.700981	1.539968
C	2.524253	4.425835	0.519083
H	3.485530	4.355820	-1.392716
H	1.501965	4.225031	2.393563
H	2.588937	5.508060	0.589587
C	0.440098	-2.798670	0.339686
C	-0.060320	-3.064000	1.627539
C	0.062398	-3.539219	-0.795586
C	-0.955209	-4.130095	1.770776
C	-0.829770	-4.597799	-0.591930
C	-1.329137	-4.895915	0.673339
H	-1.357866	-4.359048	2.752903
H	-1.145701	-5.193686	-1.439536
H	-2.020222	-5.724813	0.799594
Ni	-0.276269	0.430462	-1.065007
C	-2.217169	-0.198668	-0.964790
C	-2.671658	-0.226667	0.353930
C	-2.560793	-1.131639	-1.937658

C	-3.370316	-1.370796	0.747457
H	-2.445755	0.567464	1.053385
C	-3.266258	-2.252788	-1.503026
H	-2.248909	-0.997232	-2.968509
C	-3.664223	-2.380622	-0.168894
H	-3.688382	-1.458741	1.781753
H	-3.512892	-3.027435	-2.222644
H	-4.213740	-3.259275	0.151738
O	-1.948214	1.361634	-1.743645
S	-2.051132	2.703453	-0.875414
O	-3.418738	3.179188	-0.763884
O	-1.213655	2.521239	0.321613
C	-1.109073	3.845910	-2.025842
F	-1.659497	3.832605	-3.226593
F	-1.175067	5.071538	-1.501416
F	0.160775	3.455651	-2.081434
C	1.166877	1.520419	2.602209
H	0.689625	0.643510	2.156369
C	0.063809	2.295318	3.336703
H	-0.457269	1.620702	4.024943
H	0.472307	3.115343	3.938338
H	-0.665444	2.706250	2.635174
C	2.225191	1.027142	3.608014
H	1.752819	0.434285	4.400251
H	2.985896	0.403655	3.130094
H	2.730783	1.878783	4.077851
C	3.521199	1.680441	-1.953230
H	2.954453	0.756727	-2.102889
C	3.367264	2.518238	-3.231812
H	3.712561	1.940327	-4.091189
H	2.323751	2.786424	-3.412285
H	3.969572	3.433027	-3.193198
C	5.002207	1.313693	-1.737104
H	5.394961	0.793012	-2.617545
H	5.604457	2.216142	-1.577918
H	5.143250	0.660361	-0.870259
C	0.342401	-2.253579	2.852409
H	1.037348	-1.472616	2.540980
C	-0.866074	-1.547503	3.487314
H	-1.618193	-2.266352	3.831330
H	-0.547787	-0.955405	4.352802
H	-1.343452	-0.876294	2.768646
C	1.081773	-3.126984	3.880046
H	1.962299	-3.602374	3.434124

H	1.415080	-2.518020	4.728072
H	0.435821	-3.921590	4.269776
C	0.601976	-3.215361	-2.180900
H	0.619894	-2.128231	-2.284391
C	2.049238	-3.716339	-2.353032
H	2.723007	-3.285752	-1.606311
H	2.096993	-4.808761	-2.267707
H	2.420311	-3.430006	-3.342289
C	-0.280392	-3.762702	-3.310991
H	-0.227625	-4.856372	-3.376723
H	-1.326199	-3.474982	-3.176404
H	0.051882	-3.353860	-4.265460
O	0.621576	0.025137	-2.825380
S	0.144179	0.364034	-4.231689
O	-1.066230	-0.375871	-4.620534
O	0.214062	1.795145	-4.541887
C	1.512585	-0.426854	-5.219259
F	2.718425	-0.074661	-4.747623
F	1.422192	-0.050626	-6.496354
F	1.430591	-1.767492	-5.161291

²TS11b

Ni	8.233996	-3.452376	-0.712820
C	8.524577	-1.697272	0.031733
C	8.925607	0.504759	0.218086
C	8.834812	0.001451	1.474543
N	8.595236	-1.362827	1.344760
N	8.750871	-0.557457	-0.661853
H	8.918311	0.474332	2.436800
H	9.114226	1.502775	-0.140741
C	8.603248	-2.341963	2.407718
C	9.617115	-3.332153	2.373351
C	7.621807	-2.296437	3.417096
C	9.545434	-4.359139	3.320602
C	7.627145	-3.335948	4.358194
C	8.551604	-4.371185	4.295310
H	10.291513	-5.144463	3.310747
H	6.873986	-3.338672	5.136881
H	8.514142	-5.178353	5.021283
C	9.114130	-0.489608	-2.066218
C	8.119480	-0.293185	-3.035726
C	10.480873	-0.615359	-2.380164
C	8.535321	-0.229654	-4.369730

C	10.838669	-0.545103	-3.729935	H	12.725590	-2.112044	1.488041
C	9.876217	-0.358683	-4.715702	C	6.663220	-0.107441	-2.659635
H	7.794656	-0.086661	-5.147990	C	5.703179	-0.693871	-3.704483
H	11.881416	-0.648773	-4.009966	C	6.374673	1.387531	-2.421828
H	10.172729	-0.318271	-5.759758	H	6.475498	-0.619527	-1.714106
C	5.263154	-5.364195	1.080433	H	5.976005	-1.725991	-3.952583
C	4.369372	-5.510050	0.020080	H	4.684674	-0.686756	-3.313172
C	4.489167	-4.726251	-1.132075	H	5.702049	-0.114280	-4.635149
C	5.510467	-3.783566	-1.237877	H	7.020373	1.795958	-1.636725
C	6.421586	-3.725225	-0.188459	H	6.544758	1.968910	-3.336406
C	6.288734	-4.414659	1.012148	H	5.338916	1.523631	-2.103949
H	5.150524	-5.954032	1.985062	C	11.565015	-0.770156	-1.323153
H	3.547384	-6.214221	0.105131	C	12.345006	0.547015	-1.159119
H	3.766309	-4.814884	-1.937017	C	12.515617	-1.939710	-1.624378
H	5.599336	-3.137919	-2.100411	H	11.087743	-0.979627	-0.363782
H	6.947159	-4.252044	1.854571	H	13.097149	0.451555	-0.367519
O	5.661673	-1.195235	0.176621	H	12.860920	0.813795	-2.088239
S	4.286990	-1.136820	0.771934	H	11.677790	1.375719	-0.898465
O	3.795041	-2.436626	1.266265	H	11.967012	-2.878229	-1.728180
O	4.068122	0.042957	1.626597	H	13.079498	-1.774363	-2.548179
C	3.182497	-0.818168	-0.687868	H	13.243890	-2.047319	-0.812459
F	3.474032	0.354822	-1.281695	S	9.404565	-4.192758	-2.971394
F	1.901234	-0.783851	-0.307880	O	8.117276	-3.411310	-2.839889
F	3.312700	-1.788327	-1.621459	O	10.341504	-3.830562	-4.019062
O	9.945258	-4.297445	-1.551332	C	8.825170	-5.927442	-3.319926
C	6.607271	-1.172784	3.554693	F	8.179648	-5.960443	-4.483145
C	7.134354	-0.107342	4.539341	F	7.992563	-6.314421	-2.340488
C	5.232539	-1.661179	4.040456	F	9.869656	-6.752490	-3.357073
H	6.463707	-0.709383	2.575939				
H	8.129840	0.268224	4.277913				
H	6.444416	0.742197	4.568677	²TS12			
H	7.206656	-0.524588	5.550789	C	0.640306	0.496368	0.942906
H	4.856860	-2.482317	3.427261	C	2.289058	1.605607	-0.161468
H	5.265147	-1.974527	5.090954	C	2.699047	1.416117	1.114805
H	4.514429	-0.844094	3.948580	N	1.672112	0.753549	1.784492
C	10.849262	-3.223667	1.476709	N	1.016601	1.049823	-0.252858
C	11.544094	-4.561483	1.195618	H	3.606658	1.691163	1.625571
C	11.832723	-2.220548	2.112786	H	2.763165	2.084295	-1.001327
H	10.560337	-2.821375	0.506073	C	1.707401	0.663801	3.237086
H	10.842266	-5.308140	0.812121	C	1.197857	1.757427	3.966481
H	12.315375	-4.413522	0.434617	C	2.365131	-0.416624	3.840934
H	12.033125	-4.966182	2.088722	C	1.399883	1.756202	5.347941
H	11.377408	-1.231827	2.229894	C	2.550826	-0.358064	5.226294
H	12.146885	-2.568352	3.103431	C	2.082679	0.716281	5.971028

H	1.008683	2.573768	5.943279	H	0.153998	-1.722974	-4.367702
H	3.043955	-1.182821	5.726905	H	1.069766	-2.804648	-3.320563
H	2.226430	0.732578	7.047462	C	-0.302097	3.630758	-0.342459
C	0.097719	1.299323	-1.345469	C	-1.521855	4.396817	0.189578
C	-0.634963	2.509258	-1.318526	C	0.673503	4.617064	-1.016447
C	-0.026146	0.366038	-2.390709	H	0.216038	3.199922	0.515165
C	-1.611416	2.702555	-2.300761	H	-2.256677	3.734582	0.654755
C	-1.016478	0.613933	-3.353498	H	-1.197421	5.120003	0.945244
C	-1.819818	1.748357	-3.293474	H	-2.031754	4.952763	-0.603077
H	-2.219801	3.599682	-2.290079	H	1.574594	4.111196	-1.375096
H	-1.156962	-0.094843	-4.160880	H	0.197126	5.101466	-1.876240
H	-2.600524	1.906375	-4.030930	H	0.978486	5.394835	-0.307606
C	-3.729643	-3.940949	0.412046	C	2.858604	-1.606507	3.041523
C	-3.971734	-3.849420	-0.959021	C	2.585306	-2.936755	3.759501
C	-3.446827	-2.781969	-1.689436	C	4.352092	-1.467708	2.697656
C	-2.702930	-1.793279	-1.041555	H	2.311050	-1.629901	2.098269
C	-2.491156	-1.892940	0.330970	H	1.531079	-3.021118	4.032659
C	-2.988797	-2.955489	1.073335	H	2.837755	-3.762806	3.092090
H	-4.108396	-4.785599	0.980513	H	3.189393	-3.035158	4.669344
H	-4.556746	-4.615301	-1.460023	H	4.559245	-0.548709	2.136527
H	-3.606627	-2.714120	-2.762356	H	4.963683	-1.449817	3.608085
H	-2.303853	-0.963775	-1.615964	H	4.669312	-2.316944	2.083595
H	-2.768623	-3.054909	2.124473	C	0.478333	2.921879	3.301996
C	-2.057264	0.949624	1.504146	C	1.452727	4.072340	2.985986
H	-1.741141	0.983440	2.541688	C	-0.713048	3.443312	4.120916
H	-1.719003	1.735031	0.842593	H	0.073353	2.557178	2.355532
C	-3.201901	0.252840	1.143159	H	2.266354	3.750640	2.329275
H	-3.698232	-0.346530	1.897753	H	0.926530	4.899123	2.492873
C	-3.962230	0.668818	-0.083975	H	1.896650	4.458954	3.910353
H	-3.248045	0.932372	-0.867870	H	-1.358825	2.622196	4.437697
H	-4.581809	-0.146112	-0.459377	H	-0.381526	3.985225	5.013767
C	-4.838736	1.920995	0.201375	H	-1.296001	4.147407	3.515058
H	-4.354328	2.554325	0.952150	S	-1.232442	-1.080820	4.322362
H	-5.793526	1.603246	0.639676	O	-0.294558	-1.628684	5.297358
Ni	-0.944222	-0.778418	0.999361	O	-1.629484	0.335824	4.445407
O	0.238315	-2.151842	0.198453	O	-0.922743	-1.495343	2.900564
C	0.940936	-0.797568	-2.544197	C	-2.819794	-1.986999	4.659513
C	2.225198	-0.302712	-3.241299	F	-3.805898	-1.536754	3.846938
C	0.354213	-1.981193	-3.321156	F	-2.683564	-3.301786	4.449752
H	1.206801	-1.155906	-1.547869	F	-3.201547	-1.785927	5.921760
H	2.714877	0.497964	-2.679078	C	-5.061711	2.739643	-1.053694
H	2.938786	-1.127881	-3.338588	C	-4.905961	4.130338	-1.025515
H	2.001253	0.077862	-4.245095	C	-5.373850	2.129476	-2.276040
H	-0.568792	-2.346696	-2.864868	C	-5.039509	4.893243	-2.187013

H	-4.666625	4.619246	-0.084978
C	-5.508245	2.886775	-3.439599
H	-5.499793	1.051447	-2.324473
C	-5.333908	4.272035	-3.401493
H	-4.909543	5.971018	-2.142322
H	-5.749303	2.394135	-4.377645
H	-5.433341	4.861308	-4.308384
S	0.664058	-3.549263	0.689207
O	2.125723	-3.644713	0.745776
O	-0.146756	-4.066807	1.787387
C	0.238579	-4.639425	-0.765409
F	1.164468	-4.522948	-1.728713
F	0.215375	-5.910040	-0.353167
F	-0.957446	-4.336245	-1.285797

²TS13

Ni	-1.032247	-0.481203	0.341643
N	1.196482	1.149172	1.525502
N	-0.448936	0.990756	2.913355
C	3.069056	0.475625	0.070573
C	3.845741	0.745493	-1.061893
C	3.539212	1.801360	-1.912512
C	2.459207	2.632437	-1.636166
C	1.661860	2.423616	-0.507307
C	1.966567	1.314529	0.310924
C	1.612395	1.743958	2.711930
C	0.580797	1.644648	3.580825
C	-0.075067	0.658135	1.650270
C	-1.739546	0.860059	3.561465
C	-1.872842	-0.101289	4.570115
C	-3.051200	-0.081439	5.323883
C	-4.054813	0.838593	5.053468
C	-3.908395	1.755423	4.014377
C	-2.742969	1.796694	3.247004
H	4.702540	0.116874	-1.278042
H	4.147288	1.981867	-2.793805
H	2.238627	3.460969	-2.299137
H	2.586561	2.192431	2.803774
H	0.460875	1.973140	4.599626
H	-3.190562	-0.816632	6.109751
H	-4.972198	0.826942	5.634568
H	-4.718807	2.436891	3.785720
C	-1.734444	-1.117319	-1.572866

H	-2.739098	-1.377817	-1.285733
H	-1.095834	-1.932882	-1.891480
C	-2.585070	1.223013	-1.922324
H	-2.198866	2.237882	-2.036573
H	-3.048298	1.167452	-0.938477
C	-0.286098	0.445609	-2.889490
C	-0.362690	1.445027	-3.871013
C	0.853875	-0.373495	-2.848347
C	0.660729	1.603851	-4.805916
H	-1.232998	2.087300	-3.932108
C	1.872047	-0.210107	-3.780900
H	0.957216	-1.120769	-2.070960
C	1.778751	0.773176	-4.768432
H	0.574659	2.373802	-5.567096
H	2.748617	-0.848063	-3.726471
H	2.574532	0.893911	-5.497878
C	-3.692104	0.968303	-2.970536
H	-4.074798	-0.048188	-2.834679
H	-3.289916	1.029889	-3.987905
C	-1.447309	0.207786	-1.969815
H	-0.772195	0.701723	-0.584171
O	-1.180327	-2.336754	1.252531
C	0.603304	3.450261	-0.125470
C	-0.097882	4.091852	-1.331161
C	1.240488	4.555532	0.741663
H	-0.162890	2.953297	0.473176
H	-0.402789	3.344552	-2.065091
H	-0.987162	4.636313	-0.996285
H	0.552591	4.811761	-1.840742
H	1.666906	4.155360	1.664919
H	2.040887	5.056795	0.185401
H	0.490932	5.305217	1.015443
C	3.483018	-0.626404	1.031848
C	4.583041	-0.119675	1.985861
C	3.967354	-1.894103	0.311966
H	2.610659	-0.896078	1.627890
H	4.256753	0.745061	2.571712
H	4.869449	-0.911092	2.687670
H	5.476791	0.176323	1.424292
H	3.229978	-2.238210	-0.415824
H	4.921217	-1.728229	-0.201466
H	4.126243	-2.693485	1.041105
C	-0.808253	-1.150640	4.838514
C	-1.394802	-2.569089	4.746867

C	-0.119646	-0.917936	6.194225
H	-0.047088	-1.068971	4.059441
H	-1.898050	-2.714263	3.788943
H	-0.595626	-3.310469	4.848622
H	-2.122643	-2.750283	5.545627
H	0.349162	0.071845	6.246948
H	-0.839611	-0.987932	7.017740
H	0.658563	-1.671243	6.362856
C	-2.567981	2.830501	2.142756
C	-1.847990	4.081611	2.679890
C	-3.883028	3.225420	1.456271
H	-1.940313	2.377572	1.371262
H	-0.858492	3.847196	3.084539
H	-1.720151	4.821848	1.881314
H	-2.438682	4.546119	3.477944
H	-4.457853	2.345185	1.165351
H	-4.508845	3.846961	2.107790
H	-3.666408	3.815167	0.558239
S	-4.168957	-0.728025	1.472607
O	-3.810622	-1.508385	2.654536
O	-5.321493	0.181714	1.531078
O	-2.995978	-0.046494	0.777848
C	-4.730175	-2.011730	0.245156
F	-3.799022	-2.953580	0.040893
F	-5.843994	-2.596051	0.683949
F	-4.996651	-1.434091	-0.952296
C	-4.798473	1.978443	-2.773223
C	-5.648298	1.878086	-1.661831
C	-4.945054	3.066314	-3.639910
C	-6.620046	2.848892	-1.426173
H	-5.548405	1.044914	-0.973033
C	-5.921217	4.037517	-3.407785
H	-4.291332	3.151895	-4.505602
C	-6.759753	3.931990	-2.297741
H	-7.266406	2.756028	-0.558172
H	-6.025343	4.874198	-4.093444
H	-7.518585	4.687397	-2.113375
S	0.022992	-2.958687	0.588080
O	-0.206263	-4.121963	-0.261722
O	0.811488	-1.825075	-0.009721
C	1.036809	-3.581219	2.015922
F	1.388430	-2.564455	2.821123
F	2.146983	-4.167792	1.559379
F	0.328343	-4.464793	2.715707

²TS14

Ni	-1.158424	-0.294231	0.770970
N	1.235969	1.283681	1.629487
N	-0.302742	1.065608	3.131751
C	2.629086	0.382754	-0.189017
C	3.131925	0.544399	-1.483788
C	2.844716	1.685125	-2.229965
C	2.055252	2.698251	-1.695603
C	1.520541	2.588063	-0.408031
C	1.821584	1.416907	0.312691
C	1.683243	1.948351	2.766346
C	0.713122	1.819102	3.708894
C	0.022554	0.724856	1.860017
C	-1.605336	0.810439	3.704343
C	-1.722041	-0.150722	4.720329
C	-2.995228	-0.358980	5.260779
C	-4.099400	0.339553	4.784546
C	-3.955485	1.269396	3.758129
C	-2.704037	1.534429	3.193200
H	3.748849	-0.234408	-1.916241
H	3.240615	1.783877	-3.236601
H	1.841220	3.582121	-2.286758
H	2.633584	2.455013	2.784241
H	0.643622	2.183504	4.720095
H	-3.124429	-1.094618	6.047075
H	-5.081879	0.151578	5.207556
H	-4.827239	1.797488	3.389662
H	-0.818126	0.799210	-0.227781
O	-1.596688	-2.168983	1.991344
C	0.705310	3.728736	0.187195
C	-0.344634	4.296452	-0.780355
C	1.644165	4.845383	0.682824
H	0.165138	3.347712	1.057757
H	-0.998921	3.511000	-1.163814
H	-0.956021	5.042743	-0.259946
H	0.122825	4.800873	-1.633284
H	2.370878	4.471829	1.412124
H	2.205327	5.276716	-0.153793
H	1.067400	5.648206	1.155891
C	2.984740	-0.824638	0.661971
C	4.177597	-0.493023	1.580010
C	3.272749	-2.085918	-0.160131

H	2.126448	-1.046062	1.297339
H	3.966885	0.363033	2.229971
H	4.412535	-1.351063	2.219775
H	5.068574	-0.254049	0.987616
H	2.439166	-2.315501	-0.828571
H	4.190416	-1.987306	-0.751479
H	3.407693	-2.936210	0.513181
C	-0.529169	-0.943405	5.227802
C	-0.861446	-2.433150	5.404274
C	0.003542	-0.349441	6.545064
H	0.262382	-0.876762	4.476529
H	-1.341900	-2.832738	4.509585
H	0.056781	-3.000055	5.587574
H	-1.526092	-2.598575	6.259630
H	0.298875	0.699801	6.435238
H	-0.763583	-0.395419	7.326638
H	0.876610	-0.912499	6.893530
C	-2.555022	2.611559	2.123356
C	-2.218590	3.964874	2.777640
C	-3.774388	2.730266	1.198652
H	-1.711311	2.348847	1.481282
H	-1.299815	3.907239	3.371338
H	-2.080591	4.735256	2.010733
H	-3.030667	4.283967	3.440885
H	-4.069729	1.758309	0.794045
H	-4.638103	3.166051	1.713107
H	-3.531229	3.382605	0.354344
S	-2.720342	0.416947	-1.662826
O	-3.977382	1.044128	-2.047779
O	-1.511405	1.321508	-1.566505
O	-2.789066	-0.469046	-0.424850
C	-2.258612	-0.792217	-2.998769
F	-3.200252	-1.727180	-3.100297
F	-2.145808	-0.141953	-4.159416
F	-1.091587	-1.361480	-2.694933
S	-0.726599	-3.019077	1.103872
O	-1.297105	-4.239616	0.551432
O	-0.017232	-2.090536	0.143897
C	0.629712	-3.601893	2.234733
F	1.204224	-2.557018	2.866570
F	1.571062	-4.241993	1.535765
F	0.134175	-4.431174	3.156132

²TS15

C	0.955210	0.496747	0.750466
C	2.591082	1.850251	-0.068545
C	2.652212	1.902252	1.283291
N	1.639988	1.078409	1.765288
N	1.544755	0.988629	-0.379155
H	3.305984	2.433635	1.954334
H	3.180084	2.330178	-0.831133
C	1.420752	0.937950	3.186846
C	0.695516	1.945464	3.841923
C	2.024228	-0.140492	3.850274
C	0.640140	1.881424	5.238042
C	1.945872	-0.151059	5.244329
C	1.272642	0.854876	5.931203
H	0.082808	2.634360	5.784809
H	2.392037	-0.970455	5.797303
H	1.209371	0.817913	7.014571
C	1.113515	0.676174	-1.718496
C	0.190219	1.539684	-2.340360
C	1.642311	-0.467213	-2.346667
C	-0.264081	1.181785	-3.614433
C	1.146999	-0.781681	-3.617863
C	0.193612	0.022878	-4.236958
H	-0.984048	1.813615	-4.122971
H	1.514739	-1.663821	-4.129565
H	-0.181479	-0.244793	-5.220757
C	-4.631653	-3.063093	-1.650496
C	-4.170818	-2.793448	-2.940384
C	-3.430590	-1.632137	-3.173300
C	-3.159505	-0.751233	-2.127781
C	-3.615457	-1.008413	-0.826405
C	-4.354823	-2.177535	-0.606109
H	-5.207623	-3.963732	-1.454618
H	-4.384106	-3.481023	-3.754091
H	-3.058122	-1.412406	-4.170587
H	-2.574271	0.139985	-2.329782
H	-4.711177	-2.394905	0.396382
C	-1.901811	0.412440	0.398761
H	-1.756086	1.110168	1.221389
H	-1.562830	0.862995	-0.535734
C	-3.357185	-0.036561	0.308359
H	-3.614779	-0.526884	1.248624
C	-4.314532	1.178142	0.162317
H	-4.161103	1.660509	-0.812069

H	-5.344916	0.800216	0.149872	H	4.762054	-1.801405	2.504741
C	-4.179536	2.227339	1.279734	C	0.007112	3.072739	3.083397
H	-3.187533	2.687724	1.231555	C	0.853839	4.358582	3.110274
H	-4.238904	1.725501	2.251480	C	-1.410613	3.348154	3.610127
Ni	-0.472276	-0.876871	0.735612	H	-0.091978	2.759467	2.037550
O	0.697283	-2.472224	0.299124	H	1.842865	4.206688	2.665616
C	-0.402075	-3.101335	0.077603	H	0.352321	5.160269	2.555380
C	-0.839297	-3.338138	-1.356560	H	0.998745	4.700587	4.141538
H	-1.911860	-3.523523	-1.427766	H	-1.995268	2.427010	3.655436
H	-0.573240	-2.490951	-1.989961	H	-1.386019	3.792375	4.611728
H	-0.308747	-4.229482	-1.720471	H	-1.920683	4.061789	2.952512
C	-0.885272	-4.099667	1.106781	S	-1.655881	-0.970553	3.791672
H	-1.957460	-4.286510	1.019509	O	-1.114049	-1.045577	5.148209
H	-0.352113	-5.041590	0.916148	O	-2.487518	0.190384	3.432842
H	-0.645420	-3.754462	2.110280	O	-0.634982	-1.342525	2.736175
C	2.776129	-1.265529	-1.717190	C	-2.836234	-2.406617	3.717241
C	4.127560	-0.606064	-2.061804	F	-3.340716	-2.563385	2.471751
C	2.803904	-2.740620	-2.134091	F	-2.216332	-3.547763	4.052397
H	2.642951	-1.239901	-0.633601	F	-3.858301	-2.210527	4.554645
H	4.182182	0.428162	-1.711203	H	-1.567737	-1.890220	0.364015
H	4.948817	-1.161797	-1.595427	C	-5.231784	3.302408	1.165616
H	4.290105	-0.603587	-3.146066	C	-5.008503	4.441168	0.381158
H	1.842209	-3.221619	-1.953233	C	-6.471772	3.166989	1.802551
H	3.069285	-2.863043	-3.190914	C	-5.993819	5.417564	0.233838
H	3.561047	-3.269209	-1.545713	H	-4.048331	4.561248	-0.116456
C	-0.236196	2.854921	-1.697681	C	-7.461242	4.139936	1.659773
C	-1.681395	3.264153	-2.017193	H	-6.657096	2.290720	2.419464
C	0.721676	3.984795	-2.127147	C	-7.225725	5.269456	0.873611
H	-0.157098	2.742140	-0.611444	H	-5.799141	6.295672	-0.376510
H	-2.394279	2.468821	-1.789410	H	-8.415032	4.018701	2.166416
H	-1.954561	4.140020	-1.419177	H	-7.994181	6.029639	0.763846
H	-1.802510	3.540939	-3.070293				
H	1.758964	3.765642	-1.860626				
H	0.677622	4.131137	-3.212442	²TS1a			
H	0.440033	4.926843	-1.643514	C	-1.806616	2.054320	2.232773
C	2.734675	-1.248978	3.089665	C	-2.848580	1.254610	1.895128
C	2.385511	-2.640944	3.635209	H	-1.730362	2.877801	2.923532
C	4.255373	-1.012678	3.073480	H	-3.874454	1.241596	2.224409
H	2.381201	-1.230389	2.056037	C	-1.057091	0.566083	0.675229
H	1.301392	-2.764670	3.682514	N	-2.377867	0.360113	0.934206
H	2.797804	-3.410328	2.972776	N	-0.726644	1.621334	1.472213
H	2.801335	-2.806675	4.635800	C	0.551028	2.281500	1.367406
H	4.505943	-0.049197	2.614471	C	1.545341	2.010489	2.320921
H	4.661358	-1.014137	4.092057	C	0.750332	3.151282	0.273374

C	2.760292	2.694439	2.190423	H	2.361342	-0.605868	4.450908
C	1.985863	3.798163	0.186585	C	-0.338573	3.393117	-0.765214
C	2.976718	3.581218	1.141999	H	-0.901719	2.461900	-0.873516
H	3.552616	2.512807	2.907606	C	-1.314138	4.488642	-0.294414
H	2.180007	4.474440	-0.638453	H	-1.784505	4.228443	0.658095
H	3.929991	4.095363	1.056840	H	-0.787748	5.441544	-0.164679
C	-3.265325	-0.438970	0.121257	H	-2.109617	4.636968	-1.034073
C	-4.012565	0.236468	-0.861782	C	0.210829	3.735083	-2.156560
C	-3.369752	-1.823311	0.346447	H	0.668817	4.730222	-2.186427
C	-4.887104	-0.522583	-1.647641	H	0.960002	3.006640	-2.481539
C	-4.256737	-2.533353	-0.471700	H	-0.608008	3.732227	-2.884144
C	-5.005120	-1.894860	-1.458180	Ni	0.595166	-0.493745	0.065060
H	-5.481073	-0.030825	-2.411866	O	0.454329	-1.720042	1.473117
H	-4.364599	-3.602866	-0.334847	C	1.379510	-2.693959	1.875109
H	-5.687250	-2.471286	-2.077300	H	2.402096	-2.277922	1.894890
C	-2.585582	-2.506934	1.453968	C	1.392514	-3.904910	0.931116
H	-1.568278	-2.098970	1.466177	H	0.400451	-4.369820	0.902045
C	-2.444297	-4.018990	1.247369	H	1.665205	-3.610965	-0.085115
H	-3.399661	-4.548661	1.351192	H	2.118660	-4.657063	1.263398
H	-2.027801	-4.251569	0.261278	C	1.023557	-3.137152	3.300346
H	-1.762795	-4.425636	2.000519	H	1.758895	-3.848004	3.697242
C	-3.224447	-2.223439	2.827441	H	0.977366	-2.271569	3.967796
H	-3.266446	-1.151756	3.043395	H	0.037929	-3.618529	3.308373
H	-4.245352	-2.622742	2.879011	C	0.562180	-1.196106	-1.804275
H	-2.631042	-2.696303	3.618074	C	0.470384	-0.018270	-2.582358
C	-3.947963	1.747522	-1.050743	C	-0.386148	-2.234585	-1.942892
H	-3.104740	2.132523	-0.474576	C	-0.684688	0.193110	-3.333548
C	-3.712792	2.161444	-2.510670	H	1.274608	0.706349	-2.573622
H	-3.633863	3.252602	-2.580634	C	-1.526443	-1.987855	-2.691504
H	-2.789556	1.722732	-2.892921	H	-0.249292	-3.160629	-1.398484
H	-4.536013	1.849940	-3.163155	C	-1.689039	-0.776541	-3.383832
C	-5.223956	2.411039	-0.500378	H	-0.781914	1.114536	-3.901488
H	-6.107386	2.082206	-1.059511	H	-2.308773	-2.738780	-2.730249
H	-5.386119	2.158680	0.552649	H	-2.585064	-0.606806	-3.970885
H	-5.155913	3.501911	-0.583370	O	2.178187	-1.865873	-1.910379
C	1.326494	1.008174	3.443793	S	3.277547	-1.302190	-0.975813
H	0.564220	0.296748	3.111714	O	2.687451	-0.277367	-0.066153
C	0.826904	1.712534	4.718376	O	4.148710	-2.323491	-0.416857
H	1.566148	2.438903	5.077220	C	4.331863	-0.294886	-2.135236
H	-0.112362	2.248603	4.546402	F	3.613239	0.704357	-2.663700
H	0.655011	0.980408	5.515558	F	5.350827	0.220703	-1.448363
C	2.592607	0.190190	3.737014	F	4.794346	-1.067701	-3.114979
H	2.976502	-0.271323	2.823557				
H	3.386128	0.803198	4.180058				

²TS1c

Ni	0.628533	0.110167	1.190795
C	0.719564	0.689577	-0.678245
C	1.333653	0.769124	-2.860011
C	0.556350	1.852611	-2.622455
N	0.184192	1.790226	-1.282467
N	1.433287	0.073935	-1.658680
H	0.239032	2.653904	-3.265877
H	1.834673	0.427461	-3.750909
C	-0.522850	2.829533	-0.574873
C	0.158728	3.520155	0.450761
C	-1.861398	3.118281	-0.917902
C	-0.559476	4.477209	1.176591
C	-2.522097	4.095309	-0.163637
C	-1.888694	4.757546	0.882849
H	-0.061501	5.017057	1.975355
H	-3.555390	4.327100	-0.394505
H	-2.428968	5.501473	1.461361
C	2.423086	-0.968394	-1.484736
C	2.057085	-2.315755	-1.608871
C	3.754192	-0.559186	-1.275545
C	3.086431	-3.266237	-1.591504
C	4.741206	-1.548071	-1.249564
C	4.414976	-2.889782	-1.428035
H	2.834511	-4.316768	-1.696097
H	5.775270	-1.263126	-1.082718
H	5.196170	-3.644571	-1.416128
C	-2.355300	0.983763	3.203021
C	-2.378173	-0.053842	4.135682
C	-1.883086	-1.320172	3.790621
C	-1.338372	-1.548810	2.531055
C	-1.229379	-0.463444	1.651565
C	-1.828660	0.776000	1.923953
H	-2.779674	1.953892	3.445379
H	-2.813032	0.107330	5.117249
H	-1.931307	-2.137591	4.504843
H	-0.968542	-2.525520	2.244193
H	-1.880745	1.550953	1.171233
O	-1.608699	-1.052814	-0.166789
S	-3.073452	-1.129579	-0.637127
O	-4.008989	-0.464659	0.273421
O	-3.156243	-0.874145	-2.079063
C	-3.476502	-2.939015	-0.462601
F	-2.858356	-3.656980	-1.414436

F	-4.793416	-3.117949	-0.585397
F	-3.086752	-3.400197	0.735733
C	-2.593078	2.448250	-2.072460
C	-2.527187	3.336013	-3.333068
C	-4.067336	2.147526	-1.753174
H	-2.107964	1.491875	-2.286798
H	-1.504535	3.599789	-3.621273
H	-2.997634	2.823399	-4.179037
H	-3.065634	4.275816	-3.163201
H	-4.180346	1.625173	-0.802053
H	-4.667220	3.065134	-1.728605
H	-4.478045	1.498650	-2.530976
C	1.640436	3.340644	0.758368
C	1.903578	3.053940	2.245662
C	2.433121	4.570150	0.279329
H	2.015112	2.484593	0.198287
H	1.353531	2.171642	2.592269
H	2.968329	2.861100	2.407964
H	1.613296	3.898693	2.879782
H	2.278624	4.745337	-0.790965
H	2.126285	5.475158	0.815843
H	3.505242	4.421160	0.451656
C	0.612533	-2.770041	-1.683918
C	0.300438	-3.636435	-0.450036
C	0.295952	-3.510569	-2.992130
H	-0.034017	-1.893507	-1.632851
H	0.516231	-3.081345	0.467462
H	-0.750250	-3.926373	-0.439765
H	0.906779	-4.549645	-0.440467
H	0.516403	-2.884308	-3.864021
H	0.876979	-4.435876	-3.086659
H	-0.766668	-3.770739	-3.020963
C	4.134692	0.890862	-1.021480
C	5.202325	1.396575	-2.003996
C	4.579807	1.064748	0.442508
H	3.248648	1.512058	-1.171911
H	5.415470	2.455504	-1.818709
H	6.143147	0.845555	-1.897301
H	4.867884	1.291373	-3.042094
H	3.821833	0.680135	1.131939
H	5.510824	0.517747	0.632115
H	4.763682	2.123526	0.661679
O	1.925973	-0.677428	2.140736
C	2.103297	-1.911338	2.781849

H	1.244154	-2.569962	2.560598
C	2.138937	-1.690448	4.296276
H	1.207859	-1.217383	4.625976
H	2.262406	-2.638470	4.834373
H	2.973334	-1.029154	4.558240
C	3.369793	-2.590590	2.258296
H	4.245896	-1.967482	2.473648
H	3.516718	-3.572005	2.726280
H	3.305934	-2.724925	1.175552

²TS1b

C	-1.906235	3.106729	-0.486834
C	-2.911793	2.213680	-0.309369
H	-1.917258	4.163088	-0.697521
H	-3.983465	2.324243	-0.339876
C	-0.954831	1.077717	-0.092708
N	-2.311338	0.977610	-0.077747
N	-0.720968	2.393444	-0.353392
C	0.599032	2.904529	-0.626928
C	1.311966	3.539231	0.403211
C	1.117957	2.709190	-1.923158
C	2.588460	4.020715	0.089050
C	2.400296	3.203338	-2.178338
C	3.125234	3.856416	-1.184249
H	3.175585	4.513790	0.855480
H	2.841729	3.066138	-3.158946
H	4.122640	4.228250	-1.401311
C	-3.047679	-0.261298	-0.088806
C	-3.506062	-0.721093	-1.335764
C	-3.301275	-0.933249	1.120501
C	-4.272690	-1.891679	-1.352397
C	-4.064881	-2.103006	1.043836
C	-4.552598	-2.573149	-0.173729
H	-4.646587	-2.271494	-2.298731
H	-4.280607	-2.656554	1.950017
H	-5.147343	-3.482182	-0.201426
Ni	0.475487	-0.078072	0.600242
O	0.359224	0.487906	2.389193
C	0.785445	-0.177761	3.538327
C	2.308072	-0.372322	3.591406
H	2.659496	-0.944134	2.728595
H	2.810912	0.601638	3.573137
H	2.612980	-0.899216	4.505377

C	0.454521	-2.104538	0.248845
C	-0.028183	-2.345175	-1.045985
C	0.119663	-2.923121	1.335948
C	-1.020629	-3.312320	-1.193062
H	0.329519	-1.766739	-1.887541
C	-0.866704	-3.884948	1.150405
H	0.592403	-2.765552	2.297805
C	-1.448060	-4.079595	-0.107492
H	-1.458911	-3.466973	-2.173986
H	-1.176256	-4.493960	1.995223
H	-2.216414	-4.832988	-0.243125
O	1.984762	-1.500100	0.463645
S	3.124765	-1.345303	-0.655251
O	2.551990	-1.015558	-1.956992
O	4.212126	-0.569386	-0.084996
C	3.687247	-3.122013	-0.739917
F	2.686481	-3.893759	-1.163313
F	4.705618	-3.200818	-1.596431
F	4.080800	-3.522642	0.466321
C	0.308352	2.014756	-3.012183
H	-0.331931	1.273697	-2.523723
C	1.171742	1.253932	-4.027590
H	0.523612	0.667034	-4.688515
H	1.747589	1.935851	-4.664046
H	1.864442	0.571842	-3.529850
C	-0.606591	3.019466	-3.738948
H	-1.212588	2.505862	-4.495038
H	-1.287635	3.525149	-3.048539
H	-0.007571	3.784815	-4.246248
C	0.718728	3.706515	1.794092
H	0.032791	2.871957	1.964336
C	1.777607	3.621896	2.899820
H	1.284512	3.622693	3.877146
H	2.352104	2.696830	2.812159
H	2.468173	4.473555	2.881925
C	-0.058446	5.032330	1.897797
H	-0.498419	5.138190	2.896127
H	0.606571	5.887693	1.726915
H	-0.870994	5.090104	1.166621
C	-3.211489	0.010858	-2.639533
H	-2.587412	0.878893	-2.418132
C	-2.418713	-0.863050	-3.624526
H	-2.974620	-1.765141	-3.904228
H	-2.207531	-0.302063	-4.542284

H	-1.465543	-1.172562	-3.188382	C	-1.438226	2.107722	-3.424267
C	-4.505987	0.537190	-3.282604	H	-1.770003	3.955004	-2.387832
H	-5.051217	1.192895	-2.594834	H	-0.869295	0.237300	-4.294586
H	-4.278104	1.107536	-4.190345	H	-2.143065	2.344102	-4.216024
H	-5.176328	-0.284079	-3.560175	C	-4.003582	-3.512975	0.016693
C	-2.802212	-0.385361	2.449559	C	-3.961129	-3.482098	-1.378845
H	-1.789772	0.009197	2.305339	C	-3.224310	-2.487330	-2.027278
C	-3.694146	0.778352	2.924612	C	-2.537613	-1.531165	-1.280572
H	-3.715147	1.597399	2.199562	C	-2.569958	-1.569463	0.117212
H	-4.725083	0.440838	3.089452	C	-3.316971	-2.553932	0.765927
H	-3.311102	1.181445	3.868979	H	-4.573892	-4.283226	0.528767
C	-2.709738	-1.455604	3.544323	H	-4.503147	-4.224570	-1.957611
H	-3.697751	-1.814164	3.859575	H	-3.184624	-2.453410	-3.112961
H	-2.120298	-2.313923	3.209247	H	-1.987012	-0.750831	-1.793919
H	-2.219064	-1.033607	4.426124	H	-3.358912	-2.581752	1.846884
C	0.296294	0.595102	4.771925	C	-1.957255	1.071314	1.334712
H	0.517696	0.055078	5.701291	H	-1.732609	1.173008	2.390900
H	0.782029	1.575866	4.818364	H	-1.611614	1.857963	0.678467
H	-0.784769	0.758574	4.710344	C	-3.098852	0.352770	0.926909
H	0.320258	-1.185215	3.589654	H	-3.653994	-0.149976	1.710616
²TS2a				C	-3.885115	0.862516	-0.258203
C	0.701941	0.542910	0.922395	H	-3.195584	1.167122	-1.051759
C	2.421321	1.649256	-0.076489	H	-4.534530	0.086322	-0.668459
C	2.785815	1.387934	1.198554	C	-4.746264	2.087038	0.139454
N	1.718877	0.721832	1.800691	H	-4.122779	2.825209	0.654984
N	1.136164	1.134133	-0.234079	H	-5.519428	1.771777	0.851054
H	3.684117	1.610882	1.749113	Ni	-0.910174	-0.657319	0.930061
H	2.933006	2.153597	-0.878205	O	0.266818	-1.964879	0.315060
C	1.721409	0.511062	3.235272	C	0.343180	-3.372119	0.450244
C	1.293764	1.579797	4.046222	C	-0.292980	-3.937978	1.723282
C	2.263904	-0.677079	3.749300	H	0.002499	-4.988252	1.840890
C	1.459972	1.440470	5.426530	H	0.017786	-3.381781	2.604859
C	2.415068	-0.756850	5.136703	H	-1.382153	-3.894482	1.672567
C	2.026827	0.290743	5.964725	C	-0.193086	-4.105882	-0.783353
H	1.126667	2.234016	6.085946	H	0.024565	-5.179077	-0.707205
H	2.813672	-1.662479	5.577592	H	-1.274272	-3.984184	-0.875329
H	2.140338	0.197537	7.040809	H	0.275342	-3.728479	-1.695349
C	0.293738	1.461500	-1.363049	C	1.007264	-0.708908	-2.522570
C	-0.355357	2.716116	-1.340776	C	2.461304	-0.368643	-2.909245
C	0.169797	0.560937	-2.438998	C	0.456372	-1.736957	-3.518726
C	-1.235758	3.011798	-2.386205	H	1.003702	-1.174555	-1.530004
C	-0.724556	0.913027	-3.460492	H	2.947341	0.272462	-2.170736
				H	3.050725	-1.289317	-2.983073
				H	2.499147	0.137676	-3.881723

H	-0.575193	-2.017918	-3.289991
H	0.501722	-1.373622	-4.552747
H	1.063633	-2.645845	-3.471809
C	-0.051118	3.767816	-0.279523
C	-1.279312	4.554849	0.203086
C	1.012096	4.749983	-0.810977
H	0.374413	3.264922	0.590846
H	-2.078767	3.897862	0.555324
H	-0.992579	5.207171	1.034850
H	-1.688265	5.195244	-0.586172
H	1.921614	4.230913	-1.125866
H	0.626595	5.303081	-1.675075
H	1.284773	5.472851	-0.033975
C	2.659802	-1.830947	2.839633
C	2.558579	-3.189702	3.549264
C	4.081232	-1.649509	2.272866
H	1.958717	-1.835660	1.998820
H	1.611966	-3.289331	4.086421
H	2.626503	-3.996920	2.812766
H	3.376712	-3.331101	4.266236
H	4.169661	-0.749870	1.657279
H	4.816491	-1.582200	3.084109
H	4.347258	-2.507529	1.644441
C	0.694653	2.853968	3.464505
C	1.772556	3.932687	3.243803
C	-0.451799	3.427584	4.311835
H	0.269820	2.598347	2.489895
H	2.565813	3.593517	2.572195
H	1.325962	4.835504	2.808800
H	2.232714	4.211144	4.198894
H	-1.182888	2.655259	4.554287
H	-0.081422	3.862848	5.247183
H	-0.948510	4.232822	3.757070
S	-1.489481	-0.958875	4.269851
O	-0.601932	-1.664331	5.195310
O	-1.695508	0.488735	4.457715
O	-1.295256	-1.357629	2.831216
C	-3.169116	-1.683257	4.594325
F	-4.102246	-1.079307	3.822503
F	-3.189791	-2.993964	4.304084
F	-3.517838	-1.519355	5.872137
H	1.425433	-3.592793	0.510520
C	-5.368379	2.707167	-1.089143
C	-4.804851	3.847280	-1.674401

C	-6.475600	2.114771	-1.709158
C	-5.328727	4.381574	-2.852195
H	-3.952355	4.321493	-1.196248
C	-7.003126	2.644738	-2.886518
H	-6.927048	1.231055	-1.264021
C	-6.429088	3.779260	-3.464001
H	-4.881884	5.271243	-3.288142
H	-7.864677	2.173912	-3.351858
H	-6.840651	4.193782	-4.379844

²TS2b

C	0.707170	0.452770	0.857731
C	2.348240	1.695010	-0.117846
C	2.760007	1.378157	1.129158
N	1.742817	0.624735	1.714599
N	1.084128	1.129736	-0.271900
H	3.660012	1.613397	1.671809
H	2.812887	2.265569	-0.903734
C	1.822983	0.316255	3.127101
C	1.341892	1.282335	4.029958
C	2.517385	-0.835113	3.526211
C	1.622659	1.084718	5.384623
C	2.790988	-0.969612	4.890170
C	2.358962	-0.017163	5.806923
H	1.259471	1.800104	6.114486
H	3.321304	-1.846645	5.243193
H	2.571608	-0.150516	6.863725
C	0.228187	1.463896	-1.387227
C	-0.476314	2.686281	-1.319358
C	0.172077	0.613970	-2.509163
C	-1.324230	3.007260	-2.384482
C	-0.688687	0.991540	-3.549215
C	-1.439658	2.161512	-3.483269
H	-1.889001	3.933080	-2.357076
H	-0.773638	0.358142	-4.423781
H	-2.104495	2.423878	-4.301451
C	-3.877117	-3.648961	-0.281016
C	-3.899392	-3.467845	-1.665597
C	-3.258161	-2.362434	-2.231506
C	-2.599997	-1.445621	-1.412003
C	-2.558740	-1.640930	-0.026376
C	-3.215369	-2.733422	0.541061
H	-4.373644	-4.506208	0.165352

H	-4.420619	-4.179287	-2.299760	H	0.379171	5.335940	-1.457278
H	-3.278050	-2.207179	-3.307110	H	0.942065	5.448631	0.223286
H	-2.121256	-0.578409	-1.857393	C	2.933361	-1.899928	2.521372
H	-3.210517	-2.872926	1.613880	C	2.905521	-3.308494	3.135634
C	-1.970175	0.908689	1.332435	C	4.326707	-1.618566	1.927661
H	-1.794126	0.966111	2.401122	H	2.203634	-1.877995	1.704901
H	-1.568789	1.706342	0.728687	H	1.981489	-3.478954	3.693617
C	-3.130029	0.258769	0.867043	H	2.975992	-4.060107	2.342378
H	-3.476149	0.555803	-0.118052	H	3.750970	-3.469217	3.815630
C	-4.186309	-0.211083	1.830746	H	4.357911	-0.673153	1.378217
H	-4.955182	-0.784758	1.306254	H	5.084406	-1.577749	2.719767
H	-3.739140	-0.858964	2.578136	H	4.607972	-2.416661	1.230622
C	-4.835077	0.984990	2.571840	C	0.584857	2.520209	3.566259
H	-5.307971	1.663936	1.850860	C	1.531629	3.723593	3.397827
H	-4.046739	1.544467	3.085488	C	-0.587762	2.886328	4.489535
Ni	-0.892830	-0.780744	0.835901	H	0.157916	2.296222	2.584987
O	0.306278	-2.028753	0.144402	H	2.331142	3.517239	2.680002
C	0.411641	-3.437880	0.200383	H	0.976299	4.600507	3.042477
C	-0.120375	-4.071580	1.489689	H	1.995098	3.983065	4.356613
H	0.195996	-5.121266	1.537290	H	-1.224956	2.019954	4.680853
H	0.254279	-3.550250	2.368869	H	-0.235394	3.275658	5.451608
H	-1.210420	-4.042153	1.526952	H	-1.189220	3.676143	4.023226
C	-0.198918	-4.120664	-1.028030	S	-1.367954	-1.363073	4.170993
H	0.011077	-5.197870	-1.005167	O	-0.150237	-1.703931	4.906579
H	-1.281560	-3.986170	-1.056713	O	-2.043006	-0.088747	4.500061
H	0.222887	-3.712407	-1.948816	O	-1.301491	-1.621598	2.690551
C	1.044146	-0.629187	-2.620858	C	-2.568370	-2.687868	4.690531
C	2.487860	-0.243358	-3.002023	F	-3.710429	-2.637763	3.972936
C	0.511161	-1.649277	-3.634814	F	-2.025377	-3.897277	4.514114
H	1.053389	-1.117279	-1.639657	F	-2.885593	-2.532718	5.980874
H	2.957154	0.396561	-2.251185	H	1.498785	-3.640902	0.174415
H	3.101546	-1.146393	-3.094490	C	-5.851735	0.489179	3.573550
H	2.511181	0.283005	-3.964282	C	-7.218373	0.484476	3.275543
H	-0.518657	-1.942635	-3.411989	C	-5.424457	-0.032186	4.803187
H	0.555767	-1.271357	-4.663635	C	-8.145604	-0.027049	4.185413
H	1.129576	-2.551132	-3.598900	H	-7.559003	0.886283	2.323496
C	-0.271688	3.685817	-0.185278	C	-6.348702	-0.546557	5.710942
C	-1.566646	4.370937	0.283021	H	-4.364448	-0.036528	5.039193
C	0.754232	4.757110	-0.605617	C	-7.712106	-0.545679	5.406045
H	0.147417	3.153221	0.671809	H	-9.204449	-0.019539	3.940507
H	-2.352811	3.650949	0.527426	H	-6.001475	-0.950250	6.658193
H	-1.362416	4.963960	1.180981	H	-8.431391	-0.945833	6.115409
H	-1.959848	5.055434	-0.476397				
H	1.709153	4.311748	-0.897602				

²TS2c

C	0.778365	0.318039	0.950514	H	-0.737937	2.019121	2.374555
C	2.149997	1.915969	0.065388	C	-2.765728	2.420290	2.995983
C	2.651337	1.569946	1.269782	H	-2.889699	3.228891	2.268210
N	1.812713	0.590078	1.796951	H	-2.408563	2.879168	3.925769
N	1.006669	1.143996	-0.121308	Ni	-0.780496	-1.028280	0.972799
H	3.526608	1.899226	1.802939	O	0.373064	-2.312664	0.281449
H	2.495782	2.607386	-0.683592	C	0.490029	-3.717201	0.416565
C	2.145870	-0.011731	3.076421	C	0.137146	-4.226967	1.814843
C	1.921524	0.743774	4.241860	H	0.438731	-5.277482	1.915173
C	2.835633	-1.243189	3.087275	H	0.634331	-3.644406	2.590868
C	2.322652	0.188068	5.461655	H	-0.936697	-4.165340	1.995933
C	3.222646	-1.739487	4.334408	C	-0.252833	-4.517944	-0.659825
C	2.955350	-1.044837	5.509624	H	0.064066	-5.568085	-0.613123
H	2.135891	0.735046	6.379483	H	-1.332891	-4.488573	-0.519518
H	3.730001	-2.693929	4.392723	H	-0.022582	-4.140240	-1.658233
H	3.247878	-1.468540	6.465741	C	1.513975	-0.857658	-2.173767
C	0.241501	1.211536	-1.344679	C	2.912959	-0.292596	-2.489478
C	-0.625454	2.306330	-1.543246	C	1.243823	-2.088992	-3.045857
C	0.453303	0.223272	-2.328813	H	1.490868	-1.207256	-1.139119
C	-1.355931	2.348299	-2.736281	H	3.187373	0.529232	-1.823124
C	-0.309847	0.314489	-3.500060	H	3.666787	-1.078931	-2.370714
C	-1.213463	1.354093	-3.698250	H	2.962662	0.073250	-3.522494
H	-2.039626	3.171108	-2.914519	H	0.220968	-2.450785	-2.913957
H	-0.187288	-0.435989	-4.271640	H	1.410907	-1.887900	-4.111421
H	-1.794479	1.399674	-4.615050	H	1.923400	-2.895728	-2.754360
C	-3.818430	-4.002769	0.176600	C	-0.736579	3.460050	-0.552720
C	-3.874395	-3.913907	-1.215386	C	-2.176690	3.971554	-0.375518
C	-3.194092	-2.884520	-1.874647	C	0.165067	4.630797	-0.993188
C	-2.469347	-1.946050	-1.142355	H	-0.380504	3.111628	0.421437
C	-2.397028	-2.056236	0.252150	H	-2.877261	3.162687	-0.150229
C	-3.083867	-3.070934	0.916182	H	-2.214264	4.693380	0.446988
H	-4.344299	-4.800172	0.694663	H	-2.534036	4.486391	-1.273743
H	-4.448471	-4.638927	-1.785171	H	1.213113	4.332305	-1.080568
H	-3.233169	-2.808467	-2.958199	H	-0.154623	5.013182	-1.969118
H	-1.958187	-1.137843	-1.659670	H	0.106034	5.451268	-0.269232
H	-3.049351	-3.134610	1.995892	C	3.208786	-1.981255	1.805730
C	-3.029076	-0.221658	1.170512	C	3.582900	-3.451599	2.044730
H	-3.716534	-0.203061	0.337047	C	4.386016	-1.296168	1.080595
H	-3.394628	-0.675042	2.082199	H	2.334282	-1.961328	1.147792
C	-2.010081	0.737120	1.241391	H	2.813724	-3.984571	2.608213
H	-1.845344	1.293197	0.325604	H	3.710262	-3.956484	1.081723
C	-1.654027	1.444665	2.522238	H	4.533019	-3.543504	2.585333
H	-1.462008	0.726392	3.316270	H	4.155659	-0.275425	0.769266
				H	5.271610	-1.264214	1.727273

H	4.647424	-1.862532	0.178831	C	0.349068	0.652234	6.191253
C	1.377494	2.165657	4.226275	C	1.675393	-1.348361	5.971230
C	2.521134	3.174315	4.453074	C	0.982417	-0.443188	6.766587
C	0.264429	2.395079	5.261881	H	-0.214736	1.336186	6.815984
H	0.961134	2.364263	3.236200	H	2.123435	-2.223869	6.427005
H	3.312407	3.077357	3.702212	H	0.909716	-0.609171	7.837446
H	2.139431	4.201461	4.413634	C	0.837543	1.630173	-0.578681
H	2.979811	3.020902	5.436174	C	0.421761	2.980418	-0.509669
H	-0.494775	1.613834	5.210941	C	0.808257	0.895175	-1.782650
H	0.667494	2.397577	6.280884	C	-0.160056	3.543016	-1.650269
H	-0.201936	3.373635	5.096367	C	0.192580	1.505360	-2.885236
S	-0.948074	-1.757769	4.407292	C	-0.307421	2.802134	-2.816856
O	0.252986	-2.528071	4.734545	H	-0.501536	4.572098	-1.622045
O	-1.207177	-0.532061	5.188032	H	0.123502	0.964482	-3.820535
O	-1.217871	-1.589547	2.938323	H	-0.779997	3.246984	-3.688146
C	-2.365440	-2.872620	4.852588	C	-2.928969	-4.259003	-0.856514
F	-3.536306	-2.325019	4.466341	C	-2.762596	-3.844645	-2.179312
F	-2.249856	-4.061109	4.237383	C	-2.230124	-2.581055	-2.447670
F	-2.408938	-3.076123	6.172115	C	-1.856039	-1.742436	-1.396637
H	1.563660	-3.918275	0.259873	C	-1.988972	-2.180833	-0.074904
C	-4.090521	1.737559	3.226831	C	-2.556138	-3.423501	0.199582
C	-5.176815	1.975400	2.376640	H	-3.352484	-5.235846	-0.639502
C	-4.232542	0.792891	4.253948	H	-3.059783	-4.495361	-2.996510
C	-6.381829	1.288992	2.542760	H	-2.113125	-2.243852	-3.474031
H	-5.075863	2.704756	1.575597	H	-1.458126	-0.754139	-1.613300
C	-5.433447	0.105070	4.420013	H	-2.703467	-3.744100	1.221929
H	-3.386545	0.566881	4.896649	C	-3.087485	-0.699140	1.070505
C	-6.512008	0.349670	3.565567	H	-3.667827	-0.609258	0.160535
H	-7.214413	1.486779	1.872874	H	-3.446545	-1.417514	1.791593
H	-5.519559	-0.636156	5.208581	C	-2.322540	0.385404	1.491787
H	-7.445476	-0.190713	3.695663	H	-2.122587	0.466097	2.553523
				C	-2.280629	1.633911	0.655697
				H	-1.509586	2.296858	1.040207
				H	-2.010851	1.398247	-0.379863
				C	-3.641351	2.380105	0.631071
				H	-4.397849	1.707915	0.206438
				H	-3.544757	3.220503	-0.066508
				Ni	-0.771792	-1.106492	1.142621
				O	0.736520	-2.093340	0.656320
				C	1.075881	-3.465276	0.576751
				C	0.288198	-4.405925	1.497068
				H	0.858294	-5.330935	1.646523
				H	0.101882	-3.943677	2.463972
				H	-0.672885	-4.677513	1.059190
²TS2d							
C	0.657968	0.321799	1.575195				
C	2.596742	1.440921	1.142359				
C	2.653810	1.007272	2.419209				
N	1.461975	0.333377	2.672453				
N	1.362766	1.039231	0.635949				
H	3.401239	1.124431	3.185289				
H	3.291945	2.008847	0.548993				
C	1.160062	-0.031489	4.043185				
C	0.434284	0.892724	4.816475				
C	1.763830	-1.175756	4.587388				

C	1.042158	-3.973440	-0.869064	O	-1.154466	-2.048965	2.963911
H	1.353142	-5.025034	-0.911697	H	2.128727	-3.509516	0.910394
H	0.034584	-3.895414	-1.286490	C	-4.105540	2.891942	1.976945
H	1.723707	-3.395018	-1.498965	C	-4.622190	2.022838	2.948574
C	1.498251	-0.455714	-1.928101	C	-4.022097	4.256119	2.284309
C	3.029835	-0.289963	-1.838014	C	-5.026035	2.501219	4.193883
C	1.160877	-1.173902	-3.240662	H	-4.698147	0.960522	2.741890
H	1.192586	-1.093133	-1.091715	C	-4.429434	4.740670	3.528751
H	3.346108	0.089586	-0.864764	H	-3.645297	4.948273	1.535248
H	3.513437	-1.262727	-1.981032	C	-4.930528	3.862225	4.489631
H	3.398604	0.390793	-2.615404	H	-5.407220	1.805057	4.934978
H	0.085529	-1.313213	-3.376035	H	-4.357554	5.803365	3.743882
H	1.552783	-0.634394	-4.111725	H	-5.244788	4.234242	5.460550
H	1.618178	-2.166676	-3.240859	C	-3.167446	-3.310476	4.069246
C	0.668973	3.865517	0.710212	S	-1.918124	-1.942728	4.261114
C	-0.491935	4.807552	1.067176	O	-2.737143	-0.719535	4.362918
C	1.939042	4.711676	0.480550	O	-1.143520	-2.366103	5.426905
H	0.844070	3.225451	1.576952	F	-4.093959	-3.004415	3.129511
H	-1.414649	4.269934	1.288365	F	-3.807328	-3.523165	5.220334
H	-0.227695	5.385291	1.959061	F	-2.567597	-4.448969	3.687684
H	-0.697814	5.526490	0.266864				
H	2.804874	4.097332	0.220080				
H	1.780760	5.421194	-0.339690	²TS3			
H	2.183927	5.282322	1.383319	C	0.955210	0.496747	0.750466
C	2.459839	-2.207463	3.713643	C	2.591082	1.850251	-0.068545
C	2.199170	-3.636564	4.217937	C	2.652212	1.902252	1.283291
C	3.977260	-1.962320	3.617911	N	1.639988	1.078409	1.765288
H	2.032169	-2.119421	2.710832	N	1.544755	0.988629	-0.379155
H	1.139453	-3.791483	4.433979	H	3.305984	2.433635	1.954334
H	2.514303	-4.361732	3.460821	H	3.180084	2.330178	-0.831133
H	2.768088	-3.850062	5.130821	C	1.420752	0.937950	3.186846
H	4.212977	-1.002109	3.150220	C	0.695516	1.945464	3.841923
H	4.436846	-1.978003	4.613756	C	2.024228	-0.140492	3.850274
H	4.448828	-2.747846	3.015621	C	0.640140	1.881424	5.238042
C	-0.179583	2.153231	4.224777	C	1.945872	-0.151059	5.244329
C	0.780768	3.346091	4.393623	C	1.272642	0.854876	5.931203
C	-1.557569	2.479993	4.816059	H	0.082808	2.634360	5.784809
H	-0.323120	1.988908	3.152507	H	2.392037	-0.970455	5.797303
H	1.742620	3.167572	3.901232	H	1.209371	0.817913	7.014571
H	0.341860	4.256483	3.969420	C	1.113515	0.676174	-1.718496
H	0.975693	3.528954	5.456613	C	0.190219	1.539684	-2.340360
H	-2.210384	1.605138	4.798187	C	1.642311	-0.467213	-2.346667
H	-1.478253	2.826937	5.852931	C	-0.264081	1.181785	-3.614433
H	-2.031061	3.281101	4.240992	C	1.146999	-0.781681	-3.617863

C	0.193612	0.022878	-4.236958	H	1.842209	-3.221619	-1.953233
H	-0.984048	1.813615	-4.122971	H	3.069285	-2.863043	-3.190914
H	1.514739	-1.663821	-4.129565	H	3.561047	-3.269209	-1.545713
H	-0.181479	-0.244793	-5.220757	C	-0.236196	2.854921	-1.697681
C	-4.631653	-3.063093	-1.650496	C	-1.681395	3.264153	-2.017193
C	-4.170818	-2.793448	-2.940384	C	0.721676	3.984795	-2.127147
C	-3.430590	-1.632137	-3.173300	H	-0.157098	2.742140	-0.611444
C	-3.159505	-0.751233	-2.127781	H	-2.394279	2.468821	-1.789410
C	-3.615457	-1.008413	-0.826405	H	-1.954561	4.140020	-1.419177
C	-4.354823	-2.177535	-0.606109	H	-1.802510	3.540939	-3.070293
H	-5.207623	-3.963732	-1.454618	H	1.758964	3.765642	-1.860626
H	-4.384106	-3.481023	-3.754091	H	0.677622	4.131137	-3.212442
H	-3.058122	-1.412406	-4.170587	H	0.440033	4.926843	-1.643514
H	-2.574271	0.139985	-2.329782	C	2.734675	-1.248978	3.089665
H	-4.711177	-2.394905	0.396382	C	2.385511	-2.640944	3.635209
C	-1.901811	0.412440	0.398761	C	4.255373	-1.012678	3.073480
H	-1.756086	1.110168	1.221389	H	2.381201	-1.230389	2.056037
H	-1.562830	0.862995	-0.535734	H	1.301392	-2.764670	3.682514
C	-3.357185	-0.036561	0.308359	H	2.797804	-3.410328	2.972776
H	-3.614779	-0.526884	1.248624	H	2.801335	-2.806675	4.635800
C	-4.314532	1.178142	0.162317	H	4.505943	-0.049197	2.614471
H	-4.161103	1.660509	-0.812069	H	4.661358	-1.014137	4.092057
H	-5.344916	0.800216	0.149872	H	4.762054	-1.801405	2.504741
C	-4.179536	2.227339	1.279734	C	0.007112	3.072739	3.083397
H	-3.187533	2.687724	1.231555	C	0.853839	4.358582	3.110274
H	-4.238904	1.725501	2.251480	C	-1.410613	3.348154	3.610127
Ni	-0.472276	-0.876871	0.735612	H	-0.091978	2.759467	2.037550
O	0.697283	-2.472224	0.299124	H	1.842865	4.206688	2.665616
C	-0.402075	-3.101335	0.077603	H	0.352321	5.160269	2.555380
C	-0.839297	-3.338138	-1.356560	H	0.998745	4.700587	4.141538
H	-1.911860	-3.523523	-1.427766	H	-1.995268	2.427010	3.655436
H	-0.573240	-2.490951	-1.989961	H	-1.386019	3.792375	4.611728
H	-0.308747	-4.229482	-1.720471	H	-1.920683	4.061789	2.952512
C	-0.885272	-4.099667	1.106781	S	-1.655881	-0.970553	3.791672
H	-1.957460	-4.286510	1.019509	O	-1.114049	-1.045577	5.148209
H	-0.352113	-5.041590	0.916148	O	-2.487518	0.190384	3.432842
H	-0.645420	-3.754462	2.110280	O	-0.634982	-1.342525	2.736175
C	2.776129	-1.265529	-1.717190	C	-2.836234	-2.406617	3.717241
C	4.127560	-0.606064	-2.061804	F	-3.340716	-2.563385	2.471751
C	2.803904	-2.740620	-2.134091	F	-2.216332	-3.547763	4.052397
H	2.642951	-1.239901	-0.633601	F	-3.858301	-2.210527	4.554645
H	4.182182	0.428162	-1.711203	H	-1.567737	-1.890220	0.364015
H	4.948817	-1.161797	-1.595427	C	-5.231784	3.302408	1.165616
H	4.290105	-0.603587	-3.146066	C	-5.008503	4.441168	0.381158

C	-6.471772	3.166989	1.802551	H	-8.121712	-0.552300	1.654567
C	-5.993819	5.417564	0.233838	C	-10.557809	-2.018825	3.520420
H	-4.048331	4.561248	-0.116456	H	-11.950925	-3.485491	2.775438
C	-7.461242	4.139936	1.659773	H	-9.027256	-0.562492	3.957561
H	-6.657096	2.290720	2.419464	H	-10.963509	-2.021107	4.528465
C	-7.225725	5.269456	0.873611	C	-3.692533	-7.227254	1.939261
H	-5.799141	6.295672	-0.376510	H	-4.698790	-7.634899	1.810145
H	-8.415032	4.018701	2.166416	C	-3.784671	-6.144562	3.030064
H	-7.994181	6.029639	0.763846	H	-4.203688	-6.568886	3.951422

²TS4

C	-5.824263	-8.198855	-0.362877	H	-3.170422	-8.850760	3.286180
C	-7.131799	-8.310495	-0.025126	H	-2.738886	-9.167652	1.592819
H	-5.089198	-8.935976	-0.643225	H	-1.764221	-8.057926	2.569193
H	-7.786163	-9.163868	0.044822	C	-4.840975	-5.388692	-2.678196
C	-6.574124	-6.098301	0.113364	H	-5.775642	-5.133836	-2.167400
N	-7.571880	-7.019258	0.253934	C	-4.473498	-4.189235	-3.559720
N	-5.502598	-6.847490	-0.269307	H	-5.299045	-3.965273	-4.241521
C	-4.154232	-6.363168	-0.425054	H	-4.276126	-3.298609	-2.955653
C	-3.804940	-5.676470	-1.599033	H	-3.591641	-4.389813	-4.179219
C	-3.254288	-6.603269	0.622071	C	-5.108184	-6.632017	-3.547281
C	-2.476003	-5.263937	-1.723638	H	-5.895974	-6.421679	-4.280317
C	-1.935165	-6.170082	0.449339	H	-4.202282	-6.925013	-4.091489
C	-1.547822	-5.513926	-0.713559	H	-5.432081	-7.485732	-2.944467
H	-2.160079	-4.728756	-2.611630	C	-7.986640	-6.247566	3.051009
H	-1.212650	-6.329084	1.243739	H	-7.045860	-6.487296	2.550411
H	-0.520613	-5.179774	-0.831006	C	-7.871100	-4.801382	3.563652
C	-8.905090	-6.714680	0.692673	H	-8.776101	-4.487941	4.094845
C	-9.117501	-6.376686	2.041467	H	-7.018709	-4.711329	4.246030
C	-9.950025	-6.800133	-0.244662	H	-7.716129	-4.097628	2.738761
C	-10.438015	-6.153416	2.445963	C	-8.154517	-7.242832	4.211279
C	-11.252332	-6.573083	0.213601	H	-8.214320	-8.273821	3.844804
C	-11.495980	-6.262592	1.548749	H	-7.300757	-7.170881	4.894524
H	-10.635360	-5.884152	3.478290	H	-9.062698	-7.038569	4.789915
H	-12.081448	-6.639941	-0.484124	C	-9.700563	-7.135377	-1.707528
H	-12.513926	-6.090665	1.887770	H	-8.620223	-7.132560	-1.878568
Ni	-6.652101	-4.110098	0.414841	C	-10.225364	-8.542112	-2.045847
C	-9.517434	-2.005452	0.902268	H	-9.768028	-9.307605	-1.409128
C	-10.592028	-2.836499	1.241854	H	-11.310962	-8.599620	-1.904926
C	-8.965793	-1.192205	1.900158	H	-10.006797	-8.791683	-3.090296
C	-11.113021	-2.837219	2.535762	C	-10.305095	-6.083565	-2.647990
H	-11.018692	-3.501437	0.496874	H	-11.396936	-6.039074	-2.562662
C	-9.474576	-1.199307	3.199200	H	-9.907444	-5.087342	-2.439504

H	-10.063447	-6.321348	-3.687447	N	-5.290324	-7.088964	0.589247
C	-10.447658	-4.099807	-5.489275	C	-3.952736	-6.547412	0.641597
C	-10.504177	-3.071496	-4.549986	C	-3.281743	-6.256096	-0.554199
C	-9.337560	-2.564257	-3.959751	C	-3.335343	-6.478395	1.902468
C	-8.110562	-3.121709	-4.337074	C	-1.953770	-5.828372	-0.459175
C	-8.047598	-4.158234	-5.270555	C	-2.013709	-6.021689	1.945549
C	-9.216067	-4.649192	-5.853339	C	-1.329540	-5.697127	0.777582
H	-11.364228	-4.471252	-5.939648	H	-1.406232	-5.591281	-1.366058
H	-11.466246	-2.644302	-4.275953	H	-1.512632	-5.932353	2.904064
H	-7.194113	-2.729884	-3.904150	H	-0.301923	-5.348750	0.831375
H	-7.083680	-4.571735	-5.553920	C	-8.813806	-7.259899	1.001251
H	-9.168150	-5.448378	-6.587713	C	-9.271989	-6.827015	2.265882
C	-9.424385	-1.420850	-2.972646	C	-9.689910	-7.572628	-0.058416
H	-8.432649	-0.968334	-2.849431	C	-10.651525	-6.636311	2.408843
H	-10.058373	-0.643118	-3.416182	C	-11.058684	-7.357556	0.143913
C	-9.998881	-1.776281	-1.575573	C	-11.534002	-6.880269	1.359512
H	-10.656030	-2.650841	-1.658709	H	-11.043878	-6.288511	3.355874
H	-10.630846	-0.947412	-1.235107	H	-11.757212	-7.576486	-0.656752
C	-8.922139	-2.016753	-0.494149	H	-12.598525	-6.713298	1.497892
H	-8.226451	-1.168178	-0.554905	Ni	-6.993394	-4.424458	0.502500
C	-8.115971	-3.312818	-0.712149	C	-8.467110	-3.051486	0.254457
H	-8.798237	-4.168613	-0.634606	C	-9.703483	-3.578387	0.655531
H	-7.649088	-3.330433	-1.700230	C	-8.296883	-1.665416	0.202818
O	-4.904250	-3.804287	0.927278	C	-10.742873	-2.731977	1.035395
H	-7.079378	-2.726972	0.458984	H	-9.862623	-4.651642	0.664550
C	-4.338639	-2.532712	1.090658	C	-9.341969	-0.815331	0.576148
H	-5.008833	-1.872378	1.673997	H	-7.353557	-1.250049	-0.136282
C	-4.104371	-1.872894	-0.275600	C	-10.564653	-1.345169	0.993580
H	-3.681733	-0.864198	-0.176574	H	-11.690520	-3.155055	1.359008
H	-3.413283	-2.487111	-0.864905	H	-9.200076	0.261756	0.535956
H	-5.051117	-1.800358	-0.824611	H	-11.377203	-0.682028	1.277102
C	-3.019992	-2.662992	1.861915	C	-4.047719	-6.899073	3.179968
H	-2.337366	-3.324781	1.316710	H	-4.949251	-7.450533	2.901353
H	-2.534841	-1.687699	1.997384	C	-4.504585	-5.672041	3.979481
H	-3.199156	-3.100264	2.849692	H	-5.014085	-5.986051	4.899715
				H	-3.649075	-5.047486	4.263952
				H	-5.197154	-5.067002	3.389145
				C	-3.190625	-7.850319	4.030314
				H	-3.775120	-8.215526	4.882401
				H	-2.852612	-8.716365	3.449569
				H	-2.303426	-7.349528	4.433321
				C	-3.921294	-6.463136	-1.915773
				H	-4.976278	-6.701502	-1.754913
				C	-3.857866	-5.193159	-2.778012
²TS5a							
C	-5.470712	-8.470832	0.585270				
C	-6.796629	-8.690820	0.724533				
H	-4.632716	-9.144378	0.510216				
H	-7.367266	-9.600758	0.799333				
C	-6.473399	-6.425220	0.719397				
N	-7.396659	-7.436351	0.804549				

H	-4.392629	-5.350891	-3.722957
H	-4.314664	-4.360359	-2.235539
H	-2.822676	-4.930494	-3.026070
C	-3.286720	-7.670142	-2.629820
H	-3.774167	-7.843892	-3.596355
H	-2.219943	-7.501228	-2.816133
H	-3.379541	-8.583604	-2.030573
C	-8.323170	-6.606556	3.440043
H	-7.519753	-5.947099	3.096274
C	-8.986613	-5.894158	4.623538
H	-9.733693	-6.528444	5.117798
H	-8.221838	-5.646088	5.366397
H	-9.464317	-4.961208	4.318035
C	-7.723749	-7.937301	3.938011
H	-7.156658	-8.464115	3.168209
H	-7.042682	-7.743169	4.774201
H	-8.514819	-8.607983	4.296279
C	-9.223970	-8.220609	-1.357910
H	-8.142155	-8.082341	-1.446962
C	-9.501502	-9.737076	-1.317526
H	-9.036668	-10.217350	-0.451281
H	-10.579082	-9.926922	-1.257937
H	-9.119369	-10.221916	-2.223023
C	-9.878737	-7.616513	-2.611345
H	-10.949968	-7.839405	-2.656654
H	-9.765273	-6.531742	-2.648601
H	-9.418682	-8.039459	-3.511445
C	-12.623217	-2.446158	-5.071903
C	-11.334006	-2.523070	-4.547052
C	-10.667608	-3.752308	-4.455393
C	-11.324889	-4.903322	-4.905034
C	-12.615472	-4.831503	-5.432020
C	-13.269588	-3.602111	-5.515719
H	-13.122779	-1.483499	-5.138061
H	-10.834919	-1.619357	-4.204717
H	-10.817319	-5.862911	-4.847673
H	-13.107570	-5.735754	-5.780086
H	-14.273408	-3.543210	-5.926809
C	-9.292466	-3.835068	-3.836059
H	-8.819044	-4.788267	-4.096788
H	-8.646137	-3.042357	-4.234342
C	-9.362729	-3.697538	-2.294562
H	-10.024986	-4.470189	-1.892407
H	-9.805896	-2.731117	-2.040103

C	-7.980788	-3.827116	-1.704244
H	-7.284726	-3.016541	-1.894854
C	-7.387324	-5.074639	-1.482195
H	-8.012213	-5.957173	-1.510107
H	-6.338168	-5.194576	-1.701824
O	-5.447161	-3.599382	-0.390879
O	-6.850143	-4.019190	2.333331
C	-6.906319	-2.732084	2.902611
H	-6.924701	-1.966366	2.116112
C	-5.664360	-2.457774	3.762093
H	-5.633120	-3.133256	4.624628
H	-4.749565	-2.597343	3.182428
H	-5.683105	-1.427326	4.139999
C	-8.174946	-2.536451	3.742047
H	-8.255457	-1.497061	4.085459
H	-9.065835	-2.774961	3.158351
H	-8.149960	-3.182960	4.625908
C	-4.802181	-2.463426	0.096036
H	-5.423013	-1.946037	0.846683
C	-4.569119	-1.468214	-1.054434
H	-4.071443	-0.552195	-0.709463
H	-3.942113	-1.929466	-1.827486
H	-5.520914	-1.187213	-1.522552
C	-3.473174	-2.820410	0.773193
H	-2.773556	-3.233709	0.039680
H	-3.005219	-1.944836	1.243768
H	-3.641397	-3.583138	1.536992

²TS5b

SCF Energy:

Free Energy:

C	-5.465755	-8.467238	0.571385
C	-6.781194	-8.694590	0.782216
H	-4.626677	-9.135504	0.466806
H	-7.341196	-9.607085	0.900391
C	-6.477888	-6.426951	0.716038
N	-7.386375	-7.443459	0.873251
N	-5.296717	-7.083381	0.540058
C	-3.961376	-6.532239	0.537830
C	-3.325214	-6.267100	-0.682655
C	-3.309675	-6.424045	1.779636
C	-1.995955	-5.832969	-0.635635
C	-1.987729	-5.968123	1.773493

C	-1.336262	-5.673797	0.578803	H	-3.392456	-8.585983	-2.183289
H	-1.476374	-5.614544	-1.563416	C	-8.160614	-6.598020	3.549909
H	-1.460704	-5.851238	2.714743	H	-7.384649	-5.936729	3.152903
H	-0.307707	-5.324428	0.595087	C	-8.752808	-5.889526	4.772699
C	-8.791463	-7.271224	1.150254	H	-9.454184	-6.533648	5.318630
C	-9.175944	-6.821420	2.434026	H	-7.943520	-5.625383	5.461283
C	-9.728385	-7.610427	0.153701	H	-9.266545	-4.967537	4.497311
C	-10.544174	-6.630833	2.655873	C	-7.533349	-7.927955	4.015415
C	-11.084671	-7.405217	0.437637	H	-7.010807	-8.458385	3.217566
C	-11.488142	-6.903325	1.668617	H	-6.806648	-7.732550	4.812050
H	-10.880233	-6.268819	3.619067	H	-8.303509	-8.596596	4.420023
H	-11.828980	-7.650598	-0.312804	C	-9.344122	-8.271914	-1.164871
H	-12.543474	-6.741760	1.869889	H	-8.263469	-8.174354	-1.303448
Ni	-7.088328	-4.467158	0.401527	C	-9.665458	-9.778633	-1.111343
C	-8.640422	-3.161685	0.056596	H	-9.164867	-10.271386	-0.271579
C	-9.895860	-3.650727	0.451566	H	-10.742647	-9.939898	-0.991728
C	-8.422522	-1.782829	0.033549	H	-9.347628	-10.272540	-2.036555
C	-10.906931	-2.773801	0.839378	C	-10.032508	-7.633659	-2.383484
H	-10.088561	-4.719985	0.450436	H	-11.113191	-7.810523	-2.373693
C	-9.434318	-0.901384	0.428037	H	-9.869886	-6.553323	-2.423261
H	-7.464905	-1.397151	-0.298306	H	-9.637640	-8.071291	-3.306870
C	-10.677593	-1.393470	0.826994	C	-8.247132	-4.136305	-1.842243
H	-11.871232	-3.166919	1.151304	C	-7.449575	-5.243145	-1.505461
H	-9.250120	0.170052	0.415463	H	-7.940154	-6.195743	-1.379645
H	-11.465928	-0.706916	1.122624	H	-6.427966	-5.263131	-1.854264
C	-3.995106	-6.787520	3.089114	O	-5.626731	-3.520719	-0.514996
H	-4.881568	-7.382281	2.854843	O	-6.987276	-3.999349	2.225813
C	-4.480338	-5.526609	3.818696	C	-7.109390	-2.707950	2.767630
H	-4.967683	-5.799744	4.763428	H	-7.101889	-1.956503	1.966744
H	-3.639975	-4.862074	4.052817	C	-5.924801	-2.390796	3.691139
H	-5.200550	-4.974348	3.209462	H	-5.901683	-3.089651	4.535589
C	-3.104476	-7.657129	3.990318	H	-4.975987	-2.465889	3.156466
H	-3.676234	-7.992852	4.862850	H	-6.016486	-1.374057	4.094893
H	-2.736206	-8.542733	3.459881	C	-8.425762	-2.522916	3.535849
H	-2.236208	-7.103076	4.363708	H	-8.590936	-1.463988	3.772062
C	-4.004305	-6.488216	-2.022278	H	-9.270947	-2.878881	2.945190
H	-5.043536	-6.765624	-1.826532	H	-8.398801	-3.075512	4.481021
C	-4.012566	-5.204038	-2.867483	C	-4.925647	-2.454258	0.053547
H	-4.577477	-5.364201	-3.794475	H	-5.561919	-1.892873	0.759410
H	-4.470655	-4.388629	-2.298994	C	-4.507715	-1.466971	-1.050353
H	-2.995102	-4.908617	-3.149715	H	-3.931979	-0.627844	-0.638493
C	-3.355150	-7.663372	-2.774521	H	-3.884266	-1.978331	-1.794018
H	-3.874025	-7.843533	-3.723273	H	-5.378862	-1.055347	-1.573339
H	-2.303284	-7.455422	-3.001317	C	-3.694574	-2.933221	0.829165

H	-2.979414	-3.404475	0.148436	C	-0.658322	0.852246	-3.474855
H	-3.188903	-2.104588	1.343821	C	-1.393875	2.030529	-3.396383
H	-3.991500	-3.676144	1.570822	H	-1.832857	3.784552	-2.240581
C	-7.694995	-3.022807	-2.690956	H	-0.752473	0.233747	-4.358389
H	-6.872922	-2.561275	-2.138460	H	-2.052743	2.311919	-4.213134
H	-7.217197	-3.486929	-3.565792	C	-3.508396	-4.198166	-0.159538
C	-8.738662	-2.003811	-3.178081	C	-3.549850	-4.042500	-1.547387
H	-9.431930	-2.498017	-3.871438	C	-2.969523	-2.915019	-2.137731
H	-9.331460	-1.651453	-2.329134	C	-2.347299	-1.953119	-1.342418
C	-8.074249	-0.831541	-3.859738	C	-2.287213	-2.127843	0.044959
C	-7.789374	-0.858870	-5.229748	C	-2.888294	-3.235049	0.641123
C	-7.670508	0.285203	-3.116225	H	-3.962345	-5.070539	0.303952
C	-7.116936	0.198836	-5.843341	H	-4.039045	-4.789962	-2.165768
H	-8.099668	-1.718206	-5.820364	H	-3.006663	-2.782056	-3.216271
C	-6.996705	1.344423	-3.723790	H	-1.921663	-1.065330	-1.801426
H	-7.891487	0.321220	-2.052863	H	-2.852989	-3.324318	1.721149
C	-6.716575	1.304077	-5.090992	C	-3.032239	-0.376446	0.981638
H	-6.907084	0.160382	-6.908974	H	-3.664665	-0.317983	0.106442
H	-6.691815	2.201878	-3.130011	H	-3.432164	-0.904477	1.835973
H	-6.192593	2.128503	-5.566396	C	-2.087819	0.635163	1.199934
H	-9.318586	-4.301044	-1.903981	H	-1.867601	1.264674	0.343932

²TS5c

C	0.848976	0.250667	0.931527	C	-3.029538	2.031382	3.121669
C	2.409877	1.539464	-0.143445	H	-3.245478	2.885549	2.470410
C	2.919264	1.212852	1.061079	H	-2.717384	2.444953	4.089607
N	1.960223	0.434326	1.708539	Ni	-0.726973	-1.131811	0.974782
N	1.149256	0.952247	-0.212158	O	0.578732	-2.302305	0.239821
H	3.861079	1.443258	1.529477	C	0.765469	-3.694791	0.129480
H	2.808340	2.120866	-0.957147	C	0.232667	-4.499396	1.316432
C	2.209712	0.082485	3.090572	H	0.562267	-5.544146	1.245576
C	2.040479	1.096989	4.052732	H	0.588211	-4.090329	2.260186
C	2.778186	-1.167820	3.398975	H	-0.857523	-4.484244	1.328897
C	2.437978	0.825278	5.366300	C	0.228403	-4.289657	-1.177420
C	3.141240	-1.390901	4.732514	H	0.546353	-5.336649	-1.270873
C	2.978121	-0.408986	5.705317	H	-0.861637	-4.262890	-1.209761
H	2.315323	1.587516	6.128969	H	0.611708	-3.743483	-2.040153
H	3.566920	-2.346767	5.012795	C	1.061928	-0.801329	-2.586843
H	3.275655	-0.608673	6.730944	C	2.534199	-0.437425	-2.871516
C	0.263173	1.281210	-1.305780	C	0.571516	-1.737884	-3.699449
C	-0.437336	2.504136	-1.220004	H	1.017313	-1.347695	-1.635389
C	0.203340	0.450763	-2.443460	H	2.996667	0.106664	-2.046476
C	-1.273195	2.856433	-2.284435	H	3.115491	-1.353761	-3.023147

H	2.619498	0.171767	-3.780277
H	-0.464832	-2.052377	-3.547161
H	0.658076	-1.276510	-4.690898
H	1.191406	-2.638579	-3.714190
C	-0.275773	3.456028	-0.040213
C	-1.590686	4.136876	0.373376
C	0.780734	4.535935	-0.345630
H	0.078176	2.874888	0.814849
H	-2.407750	3.419002	0.475921
H	-1.459218	4.642580	1.336051
H	-1.897528	4.896895	-0.353679
H	1.757534	4.101242	-0.569811
H	0.472519	5.140091	-1.206672
H	0.899273	5.204479	0.515041
C	3.038197	-2.216252	2.327523
C	3.186397	-3.632430	2.901437
C	4.300029	-1.878923	1.506852
H	2.183342	-2.204523	1.642810
H	2.363445	-3.890963	3.574147
H	3.191818	-4.358837	2.083505
H	4.128472	-3.751122	3.451602
H	4.203513	-0.934710	0.966064
H	5.183807	-1.817320	2.154464
H	4.477196	-2.665435	0.764488
C	1.473930	2.469012	3.715570
C	2.580882	3.538041	3.670948
C	0.365941	2.892137	4.695513
H	1.030349	2.415186	2.718556
H	3.344855	3.297201	2.925768
H	2.157179	4.516826	3.416373
H	3.076082	3.626068	4.644693
H	-0.381051	2.103998	4.817591
H	0.773642	3.125981	5.685008
H	-0.138538	3.793188	4.327854
O	-1.335122	-1.664184	2.772422
H	1.863443	-3.844362	0.109204
C	-4.274806	1.197991	3.292810
C	-5.370041	1.353821	2.436177
C	-4.324752	0.188753	4.264219
C	-6.484310	0.517572	2.534919
H	-5.343101	2.131530	1.676197
C	-5.432121	-0.650389	4.365488
H	-3.475370	0.043706	4.925162
C	-6.516194	-0.491012	3.497599

H	-7.323094	0.651934	1.857192
H	-5.446730	-1.434607	5.117313
H	-7.377802	-1.148313	3.573163
C	-0.649293	-2.244465	3.832532
H	0.377883	-2.524419	3.539537
C	-1.374489	-3.519512	4.297971
H	-1.447200	-4.246130	3.485033
H	-0.862771	-3.996989	5.144654
H	-2.393081	-3.259116	4.613658
C	-0.524387	-1.277680	5.023307
H	-1.523017	-1.024397	5.403189
H	0.053206	-1.715346	5.846933
H	-0.027477	-0.355534	4.717901

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C	0.650578	0.188938	1.356363
C	2.620182	1.263632	0.902398
C	2.673282	0.855663	2.186039
N	1.468353	0.209038	2.450774
N	1.376951	0.875750	0.408138
H	3.426780	0.973574	2.945947
H	3.329248	1.794811	0.291916
C	1.160193	-0.131090	3.820711
C	0.473758	0.828575	4.589806
C	1.691349	-1.311808	4.368845
C	0.335733	0.580116	5.958964
C	1.534738	-1.503628	5.746777
C	0.868598	-0.569478	6.533878
H	-0.195573	1.293318	6.579608
H	1.924784	-2.405122	6.205301
H	0.755278	-0.743353	7.600394
C	0.895027	1.441768	-0.834744
C	0.501564	2.800508	-0.811541
C	0.914983	0.685347	-2.025586
C	-0.011255	3.353923	-1.988841
C	0.372944	1.290207	-3.169615
C	-0.106128	2.596231	-3.150045
H	-0.336364	4.388809	-1.994711
H	0.342234	0.734887	-4.098235
H	-0.522072	3.033840	-4.053377
C	-2.863256	-4.293570	-1.348680
C	-2.626916	-3.868949	-2.659550
C	-2.102645	-2.595410	-2.892676

C	-1.803863	-1.751867	-1.819601	H	-1.415386	4.181026	0.745278
C	-2.011890	-2.196897	-0.511292	H	-0.273657	5.217164	1.603952
C	-2.570945	-3.453395	-0.273679	H	-0.528587	5.439851	-0.126065
H	-3.277961	-5.281054	-1.162567	H	2.874496	3.875518	0.078142
H	-2.862650	-4.521334	-3.495700	H	1.925313	5.197820	-0.605582
H	-1.935868	-2.253330	-3.910881	H	2.190730	5.110906	1.147348
H	-1.413372	-0.755389	-2.007975	C	2.395068	-2.351561	3.506479
H	-2.751704	-3.747342	0.754059	C	2.199862	-3.780026	4.040522
C	-3.183719	-0.757734	0.552841	C	3.906055	-2.073785	3.379857
H	-3.694961	-0.564070	-0.384016	H	1.948422	-2.293456	2.508592
H	-3.573610	-1.533533	1.196632	H	1.152322	-3.990413	4.271200
C	-2.428335	0.260505	1.132352	H	2.531775	-4.500954	3.287217
H	-2.285632	0.230352	2.204327	H	2.792269	-3.956801	4.946703
C	-2.276686	1.581337	0.433138	H	4.114681	-1.131933	2.867798
H	-1.484216	2.155499	0.911748	H	4.380286	-2.040946	4.368624
H	-1.976912	1.430027	-0.609597	H	4.383010	-2.873835	2.802135
C	-3.589090	2.412611	0.431009	C	-0.056733	2.122549	3.984607
H	-4.374120	1.815315	-0.049501	C	0.992360	3.245062	4.108130
H	-3.433487	3.291885	-0.205547	C	-1.389760	2.584058	4.588637
Ni	-0.845041	-1.267321	0.915657	H	-0.235455	1.942630	2.920590
O	0.716457	-2.258448	0.516641	H	1.929432	2.984203	3.607828
C	1.023968	-3.627662	0.406713	H	0.614600	4.172252	3.661346
C	0.208618	-4.544016	1.323663	H	1.214217	3.444121	5.163102
H	0.688071	-5.529654	1.390372	H	-2.144615	1.795033	4.565593
H	0.137653	-4.114749	2.320316	H	-1.274069	2.914295	5.627304
H	-0.806149	-4.680091	0.951192	H	-1.781366	3.431041	4.018718
C	0.977005	-4.129177	-1.042875	O	-1.816152	-2.254960	2.324374
H	1.242015	-5.193466	-1.091310	H	2.078733	-3.717974	0.734734
H	-0.020915	-4.003758	-1.469528	C	-4.048642	2.859615	1.800883
H	1.689709	-3.578713	-1.662971	C	-4.627452	1.955729	2.704361
C	1.564680	-0.691317	-2.110100	C	-3.901448	4.193047	2.203574
C	3.090033	-0.597484	-1.894122	C	-5.024302	2.367927	3.975835
C	1.313425	-1.396969	-3.448649	H	-4.769572	0.920884	2.409299
H	1.165314	-1.310879	-1.298244	C	-4.303823	4.612573	3.473124
H	3.346067	-0.264839	-0.887557	H	-3.477332	4.914578	1.510006
H	3.537764	-1.588137	-2.030401	C	-4.861556	3.698589	4.366984
H	3.550828	0.085295	-2.619319	H	-5.464390	1.648094	4.660285
H	0.250306	-1.499673	-3.675057	H	-4.182768	5.653466	3.760799
H	1.797790	-0.870364	-4.280674	H	-5.173437	4.020290	5.356495
H	1.733937	-2.405106	-3.413032	C	-1.600562	-2.402636	3.685975
C	0.701411	3.702399	0.404054	H	-0.526982	-2.358475	3.930080
C	-0.452426	4.684364	0.663566	C	-2.117389	-3.780000	4.137097
C	2.004483	4.514007	0.247260	H	-1.615740	-4.579389	3.583936
H	0.801896	3.072932	1.290390	H	-1.957095	-3.941668	5.211462

H	-3.193526	-3.853793	3.933635
C	-2.303919	-1.300627	4.498231
H	-3.385121	-1.335207	4.308863
H	-2.132532	-1.404599	5.576979
H	-1.936161	-0.316059	4.201561

²TS6

C	0.342621	0.586191	-2.645039
C	-1.012364	0.564919	-2.540647
H	0.993488	0.772457	-3.484204
H	-1.790340	0.724406	-3.269924
C	-0.165128	0.112744	-0.472401
N	-1.299994	0.277657	-1.209816
N	0.837962	0.308283	-1.377347
C	2.224084	0.223872	-1.009284
C	2.898719	1.410137	-0.679046
C	2.824216	-1.044364	-0.936458
C	4.239019	1.303627	-0.293851
C	4.165488	-1.098221	-0.541601
C	4.867697	0.062793	-0.226951
H	4.790084	2.201021	-0.029153
H	4.661318	-2.061696	-0.474035
H	5.907814	-0.000956	0.080424
C	-2.615270	0.135277	-0.649799
C	-3.146483	-1.156857	-0.511607
C	-3.287076	1.292973	-0.220767
C	-4.411693	-1.271698	0.075874
C	-4.549111	1.125120	0.357334
C	-5.106262	-0.144032	0.503868
H	-4.851475	-2.255912	0.205074
H	-5.097004	1.993568	0.707995
H	-6.086046	-0.253709	0.960386
C	-2.635242	2.665312	-0.306478
H	-1.839538	2.615244	-1.056820
C	-1.973142	3.018802	1.039370
H	-2.728426	3.088591	1.831555
H	-1.240914	2.259794	1.332387
H	-1.461137	3.986329	0.970138
C	-3.611633	3.763556	-0.752986
H	-4.107952	3.502224	-1.694286
H	-4.388115	3.948342	-0.002380
H	-3.072004	4.705747	-0.899475
C	-2.385529	-2.398691	-0.950517

H	-1.463954	-2.076270	-1.443648
C	-1.980759	-3.254999	0.262597
H	-1.393368	-4.120824	-0.064671
H	-1.376860	-2.685455	0.976289
H	-2.864948	-3.628193	0.792678
C	-3.187787	-3.219509	-1.973988
H	-4.114468	-3.610092	-1.538609
H	-3.456919	-2.613957	-2.846685
H	-2.597278	-4.075801	-2.319040
C	2.207837	2.764754	-0.697872
H	1.166875	2.611368	-0.995632
C	2.851790	3.706001	-1.729498
H	3.898574	3.914445	-1.480106
H	2.829574	3.269624	-2.734758
H	2.318597	4.663146	-1.759557
C	2.184660	3.390608	0.706831
H	1.699327	2.712323	1.415356
H	3.198484	3.602299	1.066591
H	1.630088	4.336425	0.690511
C	2.070286	-2.322976	-1.268663
H	1.030133	-2.058608	-1.477711
C	2.642903	-2.980204	-2.536591
H	2.609919	-2.293461	-3.390152
H	3.686582	-3.281648	-2.390229
H	2.068072	-3.876942	-2.795070
C	2.059518	-3.301105	-0.081381
H	3.072737	-3.642138	0.162382
H	1.627114	-2.841677	0.813160
H	1.464704	-4.186911	-0.334032
Ni	0.121324	-0.379277	1.341660
O	0.379670	-1.741919	2.680655
C	0.876309	-0.665985	3.235651
H	0.653191	0.841942	2.142122
C	2.392585	-0.564248	3.314430
H	2.752624	-1.253687	4.093171
H	2.845931	-0.852876	2.363110
H	2.714607	0.449592	3.569065
C	0.110994	-0.076628	4.409174
H	0.439740	0.941468	4.636739
H	-0.960891	-0.071311	4.197337
H	0.284364	-0.707721	5.293902

⁴TS6

C	0.380100	0.665087	-2.447910	H	-2.328395	-4.168532	-1.881436
C	-0.973758	0.578131	-2.406158	C	2.207441	2.688298	0.013000
H	1.061282	0.853296	-3.262335	H	1.145472	2.484482	0.178429
H	-1.723617	0.685853	-3.173272	C	2.334396	3.574745	-1.240449
C	-0.201548	0.206941	-0.288968	H	3.386725	3.794061	-1.457238
N	-1.307435	0.300410	-1.087611	H	1.903152	3.088120	-2.121875
N	0.834308	0.432263	-1.151901	H	1.811989	4.526665	-1.090267
C	2.221448	0.275906	-0.807983	C	2.710491	3.423527	1.260805
C	2.900214	1.353615	-0.216281	H	2.635927	2.780777	2.142901
C	2.828289	-0.963547	-1.077500	H	3.748040	3.761421	1.153236
C	4.247031	1.159337	0.108173	H	2.094530	4.312049	1.436550
C	4.177742	-1.105394	-0.735972	C	2.035406	-2.131755	-1.650335
C	4.878666	-0.055360	-0.148705	H	1.164197	-1.725786	-2.173470
H	4.806677	1.964870	0.570545	C	2.833562	-2.948586	-2.677237
H	4.680732	-2.049063	-0.918652	H	3.243635	-2.309978	-3.467362
H	5.924568	-0.185734	0.114961	H	3.666488	-3.487554	-2.212341
C	-2.645028	0.145941	-0.586773	H	2.183857	-3.697306	-3.143677
C	-3.133733	-1.151418	-0.360451	C	1.507305	-3.033969	-0.518679
C	-3.397490	1.305414	-0.325861	H	2.338464	-3.483922	0.036853
C	-4.438778	-1.268053	0.132352	H	0.893576	-2.474177	0.192183
C	-4.701035	1.133484	0.148765	H	0.898302	-3.845585	-0.934266
C	-5.216656	-0.140320	0.377802	Ni	-0.386835	0.400168	1.734151
H	-4.847331	-2.255226	0.325175	O	0.046443	-1.195828	2.796747
H	-5.312395	2.006069	0.356424	C	1.185771	-0.677645	3.196731
H	-6.228706	-0.253586	0.756241	H	0.984150	0.980279	2.369459
C	-2.834382	2.700248	-0.553066	C	2.475307	-1.142433	2.572086
H	-1.764748	2.604132	-0.761562	H	2.791500	-2.090363	3.040843
C	-2.967676	3.580869	0.699605	H	2.352037	-1.320332	1.506338
H	-4.016690	3.766680	0.957069	H	3.279115	-0.414060	2.715342
H	-2.480830	3.103432	1.556975	C	1.241189	-0.168734	4.615193
H	-2.490181	4.552462	0.527689	H	2.150273	0.410112	4.808967
C	-3.492552	3.361337	-1.776935	H	0.362491	0.451973	4.822016
H	-3.353599	2.756744	-2.680549	H	1.218174	-1.021333	5.311640
H	-4.570705	3.486433	-1.623474				
H	-3.059820	4.351740	-1.958760	²TS7a			
C	-2.299857	-2.396136	-0.620929	C	-1.402210	0.074782	1.219401
H	-1.338501	-2.082023	-1.035741	N	-1.572732	-0.300687	-0.083877
C	-2.009296	-3.151687	0.687736	C	-0.474063	-1.002805	-0.569925
H	-1.407899	-4.044279	0.479957	C	-2.742330	0.027171	-0.848102
H	-1.457163	-2.528672	1.397658	N	-0.162542	-0.418593	1.529428
H	-2.939060	-3.479228	1.167483	C	0.417436	-1.077450	0.451540
C	-2.971510	-3.308733	-1.661293	C	0.418647	-0.296850	2.838687
H	-3.930073	-3.695782	-1.297428	C	-3.882814	-0.780810	-0.711107
H	-3.160677	-2.772826	-2.598325	C	-2.705094	1.164001	-1.671764

C	-5.017464	-0.423604	-1.447432	H	-1.879579	-2.500242	5.248548
C	-3.916477	-1.973057	0.232583	H	-0.543413	-4.709866	3.422469
C	-5.007810	0.691505	-2.281829	H	0.276392	-3.967906	4.802104
C	-3.863025	1.477079	-2.391342	H	1.025666	-3.908386	3.199352
C	-1.481835	2.065153	-1.745528	H	2.966818	3.078209	1.176238
C	-4.775378	-1.653549	1.469045	H	3.415282	1.427964	1.656130
C	-4.395444	-3.253943	-0.468928	H	3.287584	2.705323	2.875061
C	-1.759570	3.403284	-1.037694	H	0.686403	4.028132	1.807398
C	-1.007738	2.276157	-3.192196	H	0.858309	3.600797	3.522510
C	0.188285	-1.323604	3.769731	H	-0.523024	2.986966	2.585719
C	1.151597	0.860734	3.147932	H	-0.437056	-1.371555	-1.582442
C	0.724245	-1.164666	5.052031	H	1.393564	-1.530358	0.519517
C	-0.663384	-2.538271	3.432633	H	-2.985773	2.468949	2.042838
C	1.448402	-0.025114	5.391564	Ni	-2.521428	1.033833	2.419307
C	1.660291	0.974331	4.446317	C	1.306422	2.786497	7.835238
C	1.354603	1.981040	2.139744	C	0.079641	2.877975	7.178374
C	-2.017332	-2.468179	4.161209	C	-0.928128	1.926742	7.389771
C	0.069514	-3.855566	3.731944	C	-0.668990	0.876836	8.279900
C	2.843563	2.314499	1.952633	C	0.555629	0.779127	8.942228
C	0.544054	3.225713	2.541080	C	1.550561	1.734063	8.721302
H	-5.919747	-1.021161	-1.360388	H	2.071374	3.538783	7.660081
H	-5.899522	0.953494	-2.844617	H	-0.103144	3.695581	6.484505
H	-3.871928	2.353263	-3.032535	H	-1.438082	0.127123	8.451705
H	0.547580	-1.928867	5.802858	H	0.732524	-0.040998	9.633412
H	1.821238	0.101658	6.402365	H	2.503249	1.663201	9.238964
H	2.206252	1.867763	4.731825	C	-2.204653	1.971704	6.588102
H	-2.896792	-2.154785	0.584761	H	-3.024087	1.493112	7.138852
H	-0.666887	1.577833	-1.202827	H	-2.504214	3.010818	6.403275
H	-0.873552	-2.519143	2.359199	C	-2.004430	1.252367	5.228309
H	0.968539	1.643044	1.173416	H	-1.702388	0.220755	5.438667
H	-4.768048	-2.496891	2.169402	H	-1.134482	1.714022	4.745869
H	-5.815066	-1.453806	1.183700	C	-3.185636	1.270783	4.285845
H	-4.386168	-0.770581	1.989949	H	-4.014337	0.606467	4.535996
H	-4.339902	-4.104541	0.219868	C	-3.497365	2.448856	3.521552
H	-3.779210	-3.481736	-1.345800	H	-2.963268	3.372447	3.752583
H	-5.435559	-3.168787	-0.803065	H	-4.539874	2.634721	3.265972
H	-0.859616	4.030200	-1.041075				
H	-2.064296	3.230325	-0.000446				
H	-2.559882	3.956580	-1.543646				
H	-0.092690	2.879089	-3.206924				
H	-1.759313	2.802888	-3.791007				
H	-0.796747	1.320741	-3.685922				
H	-2.649655	-3.317201	3.874715				
H	-2.543207	-1.540983	3.911998				
				⁴TS7a			
				C	-0.255138	1.066580	0.287843
				N	-1.306303	0.810099	-0.559928
				C	-0.884221	0.192114	-1.733356
				C	-2.679455	1.113579	-0.266026

N	0.820505	0.535025	-0.384774	H	-2.011053	4.054859	-3.458863
C	0.455458	0.014511	-1.621254	H	-3.695032	3.621175	-3.106588
C	2.150918	0.509747	0.150038	H	-2.486785	2.348972	-3.345832
C	-3.454050	0.147770	0.405167	H	0.830009	-2.805083	3.088005
C	-3.192849	2.353515	-0.676343	H	1.678702	-1.328253	3.580979
C	-4.796777	0.456501	0.644610	H	2.587041	-2.715341	2.947884
C	-2.865618	-1.192771	0.828507	H	0.743122	-3.501211	0.656026
C	-5.337700	1.673807	0.234189	H	2.480090	-3.240556	0.391954
C	-4.544052	2.611807	-0.417917	H	1.289593	-2.392954	-0.612691
C	-2.334381	3.369554	-1.413821	H	2.967393	3.156781	-3.286854
C	-3.539329	-1.785899	2.073339	H	2.980544	1.407283	-2.989195
C	-2.922030	-2.214515	-0.324234	H	4.375711	2.393259	-2.525719
C	-2.475971	4.784458	-0.834286	H	2.655335	4.786997	-1.350571
C	-2.650211	3.345614	-2.920245	H	4.095457	4.147600	-0.545438
C	2.491671	-0.523811	1.043054	H	2.536494	4.184152	0.313764
C	3.050995	1.516407	-0.230545	H	-1.573494	-0.056921	-2.523663
C	3.798083	-0.542304	1.539092	H	1.177475	-0.424550	-2.290724
C	1.478415	-1.595866	1.419787	H	-1.455556	2.572234	2.450784
C	4.720040	0.433902	1.162394	Ni	-0.096766	2.582579	1.604338
C	4.350060	1.451262	0.289012	C	-2.151098	-3.720781	5.260359
C	2.655154	2.622767	-1.195939	C	-1.377439	-2.560362	5.205103
C	1.661962	-2.137150	2.843066	C	-1.954091	-1.299761	5.400260
C	1.499493	-2.750013	0.399773	C	-3.327345	-1.231633	5.670616
C	3.280795	2.379062	-2.581005	C	-4.105819	-2.387232	5.727345
C	3.012939	4.016407	-0.657998	C	-3.520693	-3.637597	5.516501
H	-5.426196	-0.259858	1.160948	H	-1.683025	-4.689786	5.107991
H	-6.384062	1.892255	0.429528	H	-0.310368	-2.630143	5.014248
H	-4.974619	3.559097	-0.726559	H	-3.789463	-0.259979	5.830860
H	4.100013	-1.322826	2.229072	H	-5.169341	-2.312483	5.937656
H	5.731301	0.401803	1.558404	H	-4.125466	-4.538979	5.559881
H	5.074164	2.210486	0.010488	C	-1.139612	-0.038718	5.246294
H	-1.811446	-1.022109	1.071212	H	-1.460470	0.708151	5.984040
H	-1.286754	3.081179	-1.285164	H	-0.079669	-0.240272	5.438056
H	0.486793	-1.135435	1.377484	C	-1.291267	0.564327	3.828041
H	1.567233	2.596362	-1.308414	H	-2.355478	0.714278	3.616177
H	-2.958002	-2.632605	2.451161	H	-0.921035	-0.152895	3.088292
H	-4.546096	-2.156993	1.847838	C	-0.540505	1.866593	3.695112
H	-3.620286	-1.057803	2.882240	H	-0.901384	2.660672	4.348407
H	-2.491759	-3.170802	-0.003927	C	0.837485	1.904671	3.349363
H	-2.366313	-1.874209	-1.201535	H	1.345029	0.983086	3.079047
H	-3.961019	-2.393406	-0.625386	H	1.471694	2.684985	3.760942
H	-1.783639	5.465465	-1.342316				
H	-2.233068	4.785992	0.233139				
H	-3.488624	5.183592	-0.965162				

²TS7b

C	0.304178	0.780410	-0.197872	H	-4.958505	-0.349939	1.351256
N	-0.942146	0.845639	-0.760517	H	0.809466	4.807410	-2.052622
C	-1.110031	-0.104972	-1.761673	H	0.559519	4.081766	-0.450188
C	-1.949003	1.776880	-0.336860	H	-0.474837	5.420438	-0.991584
N	0.903980	-0.239257	-0.885459	H	-0.827039	4.298487	-3.951020
C	0.058916	-0.790737	-1.842849	H	-2.159380	4.965587	-2.999051
C	2.252182	-0.657743	-0.626414	H	-2.277903	3.321167	-3.644173
C	-2.857992	1.374155	0.656120	H	0.370813	-2.341579	2.979326
C	-1.959725	3.062504	-0.901568	H	1.091550	-0.790887	2.494071
C	-3.820862	2.302105	1.064984	H	2.133334	-2.131772	3.022376
C	-2.798712	-0.005574	1.292698	H	0.513285	-4.359446	1.409987
C	-3.857474	3.584088	0.523729	H	2.275922	-4.288443	1.491674
C	-2.933208	3.959377	-0.446759	H	1.468231	-4.264761	-0.084209
C	-0.929308	3.499303	-1.931085	H	3.417007	1.711186	-4.305482
C	-2.578770	0.089928	2.811324	H	3.278102	-0.038886	-4.037351
C	-4.054744	-0.825367	0.952864	H	4.751457	0.819928	-3.561245
C	0.050407	4.514678	-1.317431	H	3.322039	3.330337	-2.323267
C	-1.590226	4.051923	-3.204063	H	4.639481	2.479464	-1.494519
C	2.464547	-1.701183	0.290075	H	3.079750	2.704768	-0.676314
C	3.300051	0.023577	-1.266891	H	-2.034286	-0.196422	-2.309279
C	3.788786	-2.063137	0.557887	H	0.370352	-1.605504	-2.476654
C	1.310197	-2.377864	1.013756	Ni	1.049226	1.867979	1.163553
C	4.849669	-1.407886	-0.063618	C	-3.704333	6.537955	3.172375
C	4.606835	-0.375915	-0.966520	C	-2.487118	5.995982	2.754463
C	3.046793	1.172881	-2.230366	C	-2.115933	4.693127	3.103445
C	1.222445	-1.877402	2.467113	C	-2.995214	3.947591	3.901798
C	1.401170	-3.910627	0.950605	C	-4.210964	4.481882	4.324416
C	3.659486	0.896796	-3.613267	C	-4.574319	5.780415	3.957139
C	3.553329	2.501831	-1.643206	H	-3.971967	7.551373	2.884538
H	-4.529195	2.031237	1.841086	H	-1.817974	6.586601	2.133059
H	-4.584133	4.302912	0.889012	H	-2.733794	2.928950	4.173420
H	-2.955266	4.969262	-0.844641	H	-4.879938	3.883101	4.937405
H	3.991861	-2.858686	1.268029	H	-5.522982	6.197389	4.283859
H	5.871597	-1.701168	0.160323	C	-0.846361	4.079683	2.565174
H	5.441658	0.133005	-1.438907	H	-1.112290	3.267233	1.876844
H	-1.934717	-0.533226	0.879684	H	-0.313450	4.824620	1.965364
H	-0.345310	2.620363	-2.219901	C	0.096517	3.495456	3.626341
H	0.380885	-2.086309	0.515117	H	-0.468189	2.818487	4.278859
H	1.965657	1.270195	-2.364556	H	0.482773	4.304559	4.263322
H	-2.493147	-0.913169	3.245674	C	1.275597	2.734687	3.028919
H	-3.412910	0.599759	3.307312	C	2.107243	3.324767	2.020618
H	-1.655840	0.638055	3.024980	H	1.849422	4.304986	1.622646
H	-3.985945	-1.830753	1.384154	H	3.174457	3.108904	2.041981
H	-4.181297	-0.925608	-0.131177	H	0.392320	1.485961	2.525392

H	1.790707	2.112397	3.761560	O	-4.370897	-1.934530	-1.528152
				C	-3.097349	-3.869831	-0.299461
				F	-2.558213	-4.195217	-1.488798
²TS8a''				F	-4.158404	-4.653003	-0.091343
Ni	0.092878	0.315313	1.036094	F	-2.184631	-4.125959	0.654913
C	-0.309271	0.919425	-0.751230	C	-4.208670	1.499439	-1.157985
C	-0.165781	1.227221	-2.991636	C	-4.684625	2.275270	-2.403637
C	-1.178000	2.007339	-2.539158	C	-5.429384	0.838845	-0.496011
N	-1.255626	1.809681	-1.161731	H	-3.531308	0.702464	-1.476665
N	0.363947	0.574358	-1.881861	H	-3.867619	2.766415	-2.940633
H	-1.839045	2.681210	-3.055245	H	-5.184171	1.592287	-3.098804
H	0.238052	1.080652	-3.979949	H	-5.400515	3.054722	-2.116631
C	-2.057041	2.592895	-0.248255	H	-5.170961	0.352743	0.447404
C	-1.383482	3.519277	0.581049	H	-6.227895	1.566994	-0.310781
C	-3.454292	2.423434	-0.213217	H	-5.822790	0.065561	-1.158249
C	-2.147508	4.233007	1.508880	C	0.097413	3.841052	0.412405
C	-4.168214	3.182141	0.725336	C	0.770287	4.355026	1.691483
C	-3.526139	4.060645	1.588767	C	0.273926	4.853732	-0.736432
H	-1.660465	4.941219	2.168786	H	0.621038	2.925961	0.132051
H	-5.243684	3.066343	0.785981	H	0.588632	3.684610	2.536979
H	-4.101951	4.623646	2.317934	H	1.852166	4.417611	1.535387
C	1.647862	-0.091727	-1.879591	H	0.423576	5.358064	1.964319
C	1.713884	-1.495638	-1.816581	H	-0.121479	4.463948	-1.679656
C	2.794952	0.723235	-1.918151	H	-0.252698	5.787679	-0.508719
C	2.989026	-2.072803	-1.799682	H	1.334287	5.087365	-0.883906
C	4.042176	0.090162	-1.921322	C	0.457943	-2.350399	-1.785157
C	4.141179	-1.293875	-1.854492	C	0.703946	-3.744357	-1.191762
H	3.084129	-3.149679	-1.733320	C	-0.161626	-2.467525	-3.191114
H	4.946646	0.687913	-1.938919	H	-0.284298	-1.848155	-1.160523
H	5.118255	-1.763015	-1.812292	H	1.221069	-3.687394	-0.226461
C	-2.301915	-0.333024	3.587010	H	-0.246640	-4.255606	-1.040685
C	-1.563839	-1.404969	4.105288	H	1.310724	-4.368815	-1.858093
C	-0.752820	-2.176278	3.272136	H	-0.401696	-1.483893	-3.605702
C	-0.664364	-1.883816	1.904708	H	0.527293	-2.971911	-3.879652
C	-1.388922	-0.780441	1.415563	H	-1.091027	-3.040996	-3.139914
C	-2.254132	-0.027816	2.227031	C	2.731034	2.243588	-1.929030
H	-2.936138	0.258114	4.241694	C	3.195583	2.808356	-3.282121
H	-1.634569	-1.645226	5.161750	C	3.540261	2.847621	-0.769300
H	-0.206300	-3.025903	3.672336	H	1.692809	2.550401	-1.789802
H	-0.102144	-2.519292	1.231426	H	3.114682	3.901370	-3.290437
H	-2.862888	0.761680	1.803962	H	4.240143	2.544069	-3.481902
O	-2.287036	-1.327331	-0.337234	H	2.589110	2.414758	-4.105002
S	-3.615025	-2.084666	-0.279253	H	3.198253	2.456569	0.192897
O	-4.309776	-1.931620	1.004369	H	4.608008	2.622537	-0.861461

H	3.430858	3.937851	-0.757807	C	-3.584030	-0.816138	-1.905011
C	1.655543	0.783706	2.153710	C	-0.693266	0.057779	4.791618
H	1.900083	1.804684	1.820638	C	0.528978	1.197643	2.969644
C	1.385831	0.792698	3.653000	C	-0.063868	0.914524	5.699378
H	1.106935	-0.205065	4.011401	C	-1.619280	-1.048801	5.287992
H	2.261633	1.117270	4.239473	C	0.841930	1.883750	5.277567
H	0.560386	1.468551	3.907698	C	1.147518	2.008157	3.928989
C	2.761145	-0.171370	1.707754	C	0.864698	1.397583	1.497993
H	2.515368	-1.197505	2.014792	C	-2.240675	-0.765842	6.660338
H	2.827796	-0.188917	0.614815	C	-0.881696	-2.401505	5.292413
C	4.172719	0.181000	2.249754	C	2.246965	0.803991	1.166863
H	4.208696	-0.030028	3.326071	C	0.816750	2.879182	1.085146
H	4.336167	1.260097	2.138379	H	-5.888047	-4.797282	2.010268
C	5.268437	-0.566359	1.528993	H	-7.425376	-3.627587	0.478617
C	6.222358	0.116608	0.764984	H	-6.696261	-1.586602	-0.702179
C	5.329049	-1.966776	1.563597	H	-0.290836	0.828272	6.755048
C	7.207388	-0.571802	0.054556	H	1.291296	2.558706	5.998115
H	6.189541	1.202900	0.727683	H	1.846656	2.773465	3.611230
C	6.307469	-2.661366	0.853870	H	-2.508353	-3.508424	2.954212
H	4.599219	-2.517564	2.151706	H	-3.485666	0.155650	-0.002263
C	7.252096	-1.966192	0.093892	H	-2.454238	-1.136808	4.590828
H	7.940119	-0.019026	-0.527694	H	0.116435	0.868586	0.899724
H	6.336135	-3.746970	0.895885	H	-3.181137	-5.238431	4.521947
H	8.018169	-2.506331	-0.455428	H	-4.714752	-5.498544	3.691005
				H	-4.411002	-3.968077	4.525712
				H	-1.926796	-5.859827	2.437893
				H	-2.188949	-4.982508	0.918218
				H	-3.442711	-6.059620	1.538313
				H	-4.914385	1.563714	-1.379678
				H	-5.821108	1.025852	0.045190
				H	-6.124496	0.294057	-1.546927
				H	-3.188448	0.038661	-2.465835
				H	-4.305120	-1.340410	-2.543216
				H	-2.754683	-1.502479	-1.701129
				H	-3.003140	-1.518927	6.872723
				H	-2.727747	0.214818	6.677072
				H	-1.496287	-0.798398	7.464870
				H	-1.563457	-3.200124	5.605485
				H	-0.035049	-2.379090	5.989043
				H	-0.494321	-2.654014	4.299528
				H	2.470594	0.916394	0.099749
				H	2.308145	-0.260357	1.417642
				H	3.031341	1.318195	1.733960
				H	0.927594	2.968684	-0.001355
²TS8a'							
C	-2.418685	-0.632021	2.274502				
N	-2.598711	-1.659232	1.388687				
C	-1.387544	-2.225901	1.007260				
C	-3.896092	-2.218005	1.092368				
N	-1.064360	-0.598720	2.459505				
C	-0.420987	-1.565520	1.689539				
C	-0.392493	0.236289	3.423172				
C	-4.272009	-3.404539	1.752476				
C	-4.739408	-1.547317	0.189085				
C	-5.557244	-3.897376	1.504330				
C	-3.309710	-4.183803	2.640721				
C	-6.424917	-3.237401	0.641394				
C	-6.015603	-2.080784	-0.017712				
C	-4.250366	-0.343311	-0.598767				
C	-3.951252	-4.745948	3.916985				
C	-2.675102	-5.334826	1.833294				
C	-5.347990	0.689407	-0.882242				

H	1.628411	3.452009	1.546448	F	-8.048361	-0.044498	5.507563
H	-0.130069	3.341420	1.372640	F	-7.873992	-1.671493	6.938774
H	-1.333684	-3.041717	0.306465	F	-6.586255	0.075892	7.118093
H	0.648452	-1.690488	1.710962				
H	-1.961584	1.859112	1.017210				
Ni	-3.866093	0.485007	3.015354	²TS8a			
C	0.868873	5.566394	5.077904	C	0.442925	0.579817	4.540838
C	-0.190089	5.270095	4.218679	C	0.745487	-0.510069	5.283013
C	-1.419891	4.819853	4.714434	H	0.076293	1.554362	4.814994
C	-1.560200	4.671763	6.101048	H	0.685043	-0.694042	6.342590
C	-0.505276	4.962105	6.965614	C	1.196927	-1.030424	3.104116
C	0.716080	5.411391	6.456850	N	1.210462	-1.476491	4.397898
H	1.812429	5.921062	4.670800	N	0.722664	0.247146	3.217572
H	-0.062622	5.383781	3.144772	C	0.525863	1.176671	2.137173
H	-2.508066	4.321882	6.503905	C	1.653406	1.733617	1.497804
H	-0.636911	4.842662	8.037890	C	-0.793762	1.521416	1.794379
H	1.536878	5.645087	7.129425	C	1.410636	2.660022	0.478548
C	-2.527990	4.405765	3.778366	C	-0.974884	2.474321	0.785044
H	-3.499251	4.775851	4.131062	C	0.114378	3.033530	0.129672
H	-2.358772	4.848208	2.789915	H	2.245032	3.103865	-0.049779
C	-2.589625	2.861847	3.660457	H	-1.981010	2.763119	0.499298
H	-2.923127	2.476129	4.633016	H	-0.042631	3.761656	-0.661032
H	-1.569771	2.496272	3.532202	C	1.651324	-2.778740	4.832548
C	-3.466706	2.333901	2.524834	C	0.687771	-3.787644	4.989927
H	-4.437567	2.845107	2.535441	C	3.022951	-2.978674	5.076592
C	-2.828350	2.515572	1.153653	C	1.132920	-5.037145	5.433432
H	-2.477810	3.548132	0.989214	C	3.416435	-4.252580	5.498663
H	-3.539455	2.298401	0.352425	C	2.481284	-5.269219	5.679962
C	-5.559775	0.910758	3.862956	H	0.419040	-5.843949	5.556437
C	-6.482428	0.589381	2.828826	H	4.464399	-4.456019	5.686338
C	-5.790303	2.025973	4.713032	H	2.810368	-6.252303	6.004603
C	-7.443151	1.536995	2.489364	Ni	1.716872	-2.071469	1.471624
H	-6.410577	-0.354996	2.302031	C	-2.009350	0.897084	2.467041
C	-6.764718	2.938119	4.354306	H	-1.674852	0.020054	3.029266
H	-5.147224	2.184170	5.571758	C	-3.052072	0.413084	1.444973
C	-7.586441	2.715596	3.231777	H	-3.837093	-0.152204	1.958530
H	-8.106167	1.339223	1.651016	H	-3.533494	1.251611	0.929799
H	-6.901467	3.835124	4.952990	H	-2.601381	-0.235807	0.690807
H	-8.357282	3.434064	2.972157	C	-2.663009	1.880222	3.455937
O	-5.000154	-0.408555	4.750777	H	-3.520298	1.411210	3.951973
S	-5.931406	-1.612298	5.196015	H	-1.963706	2.211434	4.229990
O	-6.657918	-2.201877	4.077267	H	-3.022194	2.773177	2.931412
O	-5.164914	-2.455593	6.111570	C	3.079129	1.369648	1.908175
C	-7.198719	-0.742112	6.258698	H	3.146025	0.277038	1.955645

C	4.137358	1.836970	0.902475	H	-0.767902	-3.587589	1.521721
H	5.115953	1.455233	1.205189	H	-1.362431	-1.943563	1.541857
H	3.934813	1.459362	-0.103515	C	0.246024	-2.307564	0.126352
H	4.203795	2.931160	0.864292	H	0.528390	-3.120752	-0.555222
C	3.426334	1.921974	3.305294	C	0.092806	-1.028003	-0.689812
H	4.448370	1.632407	3.575784	H	-0.615849	-1.145627	-1.526357
H	3.373121	3.017353	3.308591	H	1.049121	-0.717431	-1.131510
H	2.758170	1.546941	4.083362	C	3.065713	-2.828762	0.303470
C	-0.781418	-3.548397	4.674461	C	4.011557	-2.594978	1.355726
H	-0.833492	-2.735214	3.943883	C	3.311659	-2.260151	-0.982181
C	-1.465775	-4.767242	4.040517	C	5.107117	-1.742565	1.120109
H	-1.598239	-5.580123	4.764505	H	3.942958	-3.160904	2.276650
H	-2.458592	-4.489049	3.677211	C	4.388290	-1.418855	-1.164740
H	-0.892686	-5.151270	3.193752	H	2.623031	-2.481608	-1.790374
C	-1.552760	-3.107171	5.933024	C	5.302313	-1.154357	-0.118968
H	-1.147722	-2.185073	6.361426	H	5.824673	-1.581044	1.919733
H	-2.606865	-2.932775	5.688742	H	4.537209	-0.956249	-2.137459
H	-1.507552	-3.885114	6.704375	H	6.157914	-0.510712	-0.295403
C	4.037274	-1.851276	4.915214	O	2.709018	-4.431040	0.084359
H	3.732284	-1.254326	4.049125	S	1.795249	-5.114468	1.148651
C	4.046907	-0.929255	6.150593	O	0.705119	-5.883378	0.562034
H	3.072848	-0.467008	6.325407	O	1.510042	-4.177784	2.258463
H	4.322087	-1.495892	7.047876	C	2.973217	-6.340118	1.906971
H	4.778862	-0.124068	6.017808	F	2.335528	-7.000380	2.876515
C	5.465336	-2.350512	4.651545	F	3.398547	-7.201975	0.985343
H	5.900162	-2.817020	5.542887	F	4.021032	-5.696974	2.430314
H	5.506571	-3.079586	3.837270				
H	6.107131	-1.503586	4.386230				
H	-0.267093	-0.195198	-0.079077				
C	-5.178479	-4.095412	2.149515	²TS8b			
C	-4.289755	-3.362545	1.360183	C	6.072807	-0.908847	5.963547
C	-3.201281	-3.983034	0.735175	C	4.844487	-0.529616	6.395111
C	-3.025514	-5.362248	0.918087	H	7.052155	-0.780085	6.393532
C	-3.913810	-6.099609	1.699603	H	4.524363	-0.006607	7.281726
C	-4.993883	-5.468391	2.321476	C	4.564803	-1.624840	4.413587
H	-6.018549	-3.595058	2.624779	N	3.938551	-0.979974	5.438562
H	-4.443483	-2.295387	1.221004	N	5.884445	-1.572745	4.754184
H	-2.168833	-5.850127	0.459599	C	6.939109	-2.219613	4.012839
H	-3.759988	-7.167765	1.828391	C	7.033105	-3.624012	4.083484
H	-5.685936	-6.041494	2.932458	C	7.824860	-1.430182	3.261911
C	-2.179004	-3.191132	-0.039895	C	8.059123	-4.232765	3.357479
H	-1.764040	-3.813878	-0.841933	C	8.836564	-2.092003	2.555948
H	-2.644897	-2.321501	-0.519095	C	8.949822	-3.476921	2.598573
C	-1.009073	-2.741797	0.874289	H	8.156598	-5.312005	3.372202
				H	9.536812	-1.514649	1.961530

H	9.734561	-3.973105	2.034666	H	9.808849	0.430313	3.864162
C	2.509266	-0.946588	5.602356	H	8.718615	1.787116	4.207498
C	1.759361	0.015753	4.903230	C	7.908840	0.677360	1.828949
C	1.928888	-1.904795	6.449179	H	8.922012	0.523949	1.441272
C	0.376404	0.018498	5.107381	H	7.200065	0.229293	1.128849
C	0.540671	-1.856424	6.621721	H	7.730396	1.758348	1.855014
C	-0.225883	-0.899774	5.965100	Ni	3.729536	-2.113941	2.665935
H	-0.239009	0.740708	4.583634	H	2.871214	0.106862	0.669246
H	0.057511	-2.582989	7.267992	H	5.072224	-0.084613	2.201018
H	-1.302727	-0.878053	6.107524	C	5.238172	-2.902580	-4.765335
C	2.750504	-2.993956	7.125713	C	5.323593	-2.499241	-3.432522
H	3.809513	-2.779156	6.965118	C	5.320442	-1.138558	-3.095864
C	2.471286	-4.364066	6.483957	C	5.229105	-0.196146	-4.127943
H	1.422065	-4.655510	6.610487	C	5.144271	-0.595957	-5.462242
H	2.691167	-4.340072	5.413317	C	5.148237	-1.953611	-5.785843
H	3.095207	-5.137190	6.947197	H	5.244863	-3.962307	-5.007830
C	2.522394	-3.029725	8.645017	H	5.394671	-3.238477	-2.640770
H	2.737170	-2.056920	9.100917	H	5.227061	0.863402	-3.880053
H	1.488839	-3.294613	8.894158	H	5.078603	0.152138	-6.248305
H	3.176446	-3.776962	9.108204	H	5.084554	-2.269086	-6.823883
C	2.436579	1.029598	3.990949	C	5.358720	-0.698270	-1.651181
H	3.283544	0.530991	3.510394	H	6.013150	-1.363704	-1.078699
C	1.525289	1.538977	2.867667	H	5.786142	0.311847	-1.585614
H	2.111414	2.139742	2.165057	C	3.956017	-0.687228	-1.011969
H	1.079045	0.707594	2.314470	H	3.588846	-1.717891	-0.965389
H	0.719411	2.175864	3.251379	H	3.277154	-0.140408	-1.681193
C	2.997801	2.205815	4.812474	C	3.921757	-0.039844	0.379212
H	2.189473	2.733068	5.332947	H	4.333081	0.979705	0.279079
H	3.719748	1.866627	5.561922	C	4.668584	-0.799841	1.474322
H	3.504505	2.921513	4.155075	H	5.524713	-1.356460	1.076663
C	6.074000	-4.444787	4.938055	C	2.301633	-2.828784	1.575569
H	5.081873	-3.996607	4.836969	C	1.316497	-2.020219	0.943667
C	6.474039	-4.380008	6.425335	C	1.940759	-3.579477	2.742327
H	7.468800	-4.816398	6.574346	C	0.095511	-1.833234	1.560563
H	6.495790	-3.353103	6.800929	H	1.550731	-1.532808	0.005915
H	5.760945	-4.946507	7.036102	C	0.679187	-3.365987	3.332769
C	5.947964	-5.907642	4.495828	H	2.583330	-4.375442	3.101162
H	5.728536	-5.986146	3.429741	C	-0.230340	-2.488845	2.768602
H	6.860963	-6.477422	4.706067	H	-0.628227	-1.164910	1.100202
H	5.133760	-6.386637	5.051202	H	0.420393	-3.921865	4.228704
C	7.745517	0.089766	3.240087	H	-1.198088	-2.327567	3.231312
H	6.755013	0.381441	3.602847	O	3.043938	-3.798188	0.358635
C	8.796487	0.693904	4.191415	S	4.486179	-4.285232	0.650974
H	8.677035	0.329450	5.217242	O	5.427391	-4.019621	-0.430063

O	4.883638	-3.954389	2.042234	H	3.330280	0.924318	4.415570
C	4.232617	-6.126674	0.699819	C	1.407950	1.687721	3.901179
F	3.795325	-6.566729	-0.477078	H	1.847992	2.530004	3.356082
F	5.398058	-6.716316	0.991488	H	1.146171	0.907911	3.179467
F	3.342724	-6.432631	1.649830	H	0.482241	2.043579	4.367524
²TS8b'				C	2.731264	2.225614	6.006685
C	6.248734	-1.047856	5.358036	H	1.837935	2.496472	6.581525
C	5.121512	-0.967653	6.107512	H	3.487225	1.863218	6.712506
H	7.289325	-0.948769	5.617989	H	3.116308	3.134720	5.531017
H	4.969127	-0.764831	7.154803	C	6.140737	-4.023855	2.974532
C	4.486341	-1.417149	3.965663	H	5.091630	-3.717949	3.045706
N	4.058689	-1.210122	5.243605	C	6.608565	-4.428434	4.386917
N	5.842682	-1.324122	4.056061	H	7.657047	-4.748323	4.363888
C	6.768054	-1.527264	2.967362	H	6.519674	-3.613722	5.110419
C	6.934396	-2.830289	2.446798	H	6.007526	-5.269309	4.752193
C	7.488264	-0.417381	2.494222	C	6.181800	-5.244004	2.047231
C	7.878020	-2.989450	1.428233	H	5.859509	-4.998964	1.033578
C	8.437062	-0.643413	1.489020	H	7.186890	-5.679491	1.999871
C	8.631034	-1.913624	0.962648	H	5.507538	-6.013499	2.430828
H	8.013759	-3.960279	0.970429	C	7.271237	0.993261	3.027021
H	9.011414	0.192204	1.102244	H	6.357532	0.993501	3.629798
H	9.343867	-2.069101	0.159639	C	8.439877	1.426804	3.931123
C	2.687638	-1.273612	5.679965	H	8.581716	0.740633	4.772749
C	1.898417	-0.117150	5.596956	H	9.377983	1.450965	3.364992
C	2.207423	-2.494226	6.191955	H	8.263007	2.429790	4.336016
C	0.605914	-0.179044	6.130917	C	7.066746	2.016565	1.896006
C	0.908214	-2.504413	6.710230	H	7.973202	2.139656	1.293520
C	0.121942	-1.353160	6.698909	H	6.253733	1.716549	1.229547
H	-0.028150	0.700797	6.092828	H	6.818929	2.995972	2.320714
H	0.504116	-3.423481	7.120411	Ni	3.345882	-1.618630	2.362396
H	-0.881696	-1.380846	7.113803	H	2.478737	0.235840	-0.323901
C	3.056787	-3.758770	6.176544	H	3.218048	0.775325	1.936908
H	3.781253	-3.660260	5.361073	C	6.402832	-4.612634	-1.984124
C	2.230779	-5.026071	5.903150	C	5.796565	-3.522996	-1.362021
H	1.597169	-5.286069	6.758435	C	6.312838	-2.228046	-1.509094
H	1.589610	-4.919102	5.024733	C	7.447718	-2.052959	-2.307852
H	2.902942	-5.871470	5.725192	C	8.063502	-3.141628	-2.930915
C	3.847667	-3.920125	7.488353	C	7.544962	-4.427199	-2.768008
H	4.509799	-3.069354	7.671143	H	5.973793	-5.601410	-1.848974
H	3.163654	-4.008237	8.340489	H	4.917823	-3.688043	-0.750615
H	4.464928	-4.824672	7.450901	H	7.859367	-1.053760	-2.434249
C	2.404410	1.159811	4.946815	H	8.946155	-2.983493	-3.545801
				H	8.021552	-5.274935	-3.253038
				C	5.688174	-1.072847	-0.763597

H	5.856085	-1.235693	0.305787	H	-2.492009	4.602230	2.482161
H	6.210782	-0.140534	-1.016491	H	-5.537042	3.106691	-0.119097
C	4.180656	-0.903636	-0.996701	H	-4.870331	4.434588	1.848600
H	3.685375	-1.854133	-0.778656	C	1.751241	-0.211124	-0.847843
H	3.998333	-0.684658	-2.057428	C	1.765223	-1.616761	-0.899603
C	3.556137	0.192540	-0.122018	C	2.872478	0.552323	-0.469059
H	3.956312	1.170432	-0.444604	C	2.965789	-2.253680	-0.563424
C	3.789274	0.024138	1.374041	C	4.048514	-0.137157	-0.154087
H	4.845638	0.164851	1.622814	C	4.095109	-1.525848	-0.197912
C	1.871533	-2.278826	1.390481	H	3.016819	-3.335507	-0.585993
C	0.991324	-1.808441	0.394969	H	4.932070	0.420469	0.139081
C	1.414046	-2.547783	2.705089	H	5.013844	-2.044963	0.059377
C	-0.262569	-1.387279	0.790224	C	-3.789930	-0.649020	3.105294
H	1.321872	-1.729721	-0.632924	C	-3.331226	-1.833432	3.694199
C	0.121699	-2.111391	3.073741	C	-2.310958	-2.577661	3.098742
H	1.971834	-3.190902	3.379205	C	-1.725218	-2.137814	1.905562
C	-0.695868	-1.513388	2.132842	C	-2.157956	-0.910656	1.384421
H	-0.928936	-0.949216	0.052044	C	-3.230285	-0.186211	1.912996
H	-0.225934	-2.294563	4.084577	H	-4.601231	-0.090577	3.563763
H	-1.695211	-1.188656	2.405859	H	-3.793971	-2.191662	4.608899
O	3.008401	-3.617869	0.788752	H	-1.993373	-3.521162	3.533808
S	2.470470	-5.016849	0.374316	H	-0.991132	-2.740665	1.384931
O	1.158255	-4.957736	-0.262472	H	-3.603492	0.703308	1.421289
O	3.555497	-5.795032	-0.224156	O	-2.459470	-1.318442	-0.814896
C	2.179003	-5.834722	2.033147	S	-3.761812	-1.987374	-1.197531
F	0.987707	-5.492490	2.540259	O	-4.797142	-1.889979	-0.156783
F	2.226014	-7.158999	1.898569	O	-4.143378	-1.721838	-2.592496
F	3.129707	-5.460619	2.917648	C	-3.331144	-3.794682	-1.208726
²TS8b''				F	-2.459375	-4.077249	-2.197495
Ni	-0.555487	0.069260	1.490259	F	-4.427425	-4.534137	-1.397708
C	-0.429282	0.805215	-0.281529	F	-2.764270	-4.170086	-0.044283
C	0.375974	1.253330	-2.347339	C	-4.009668	1.660744	-1.814512
C	-0.707922	2.044447	-2.152388	C	-4.065411	2.587287	-3.047089
N	-1.192048	1.760931	-0.877290	C	-5.390510	1.011003	-1.625130
N	0.542374	0.508408	-1.183287	H	-3.290782	0.859380	-2.005142
H	-1.175403	2.775569	-2.788023	H	-3.115651	3.092267	-3.250042
H	1.047250	1.153081	-3.184144	H	-4.338069	2.007674	-3.935224
C	-2.207423	2.514711	-0.177447	H	-4.821963	3.367914	-2.903253
C	-1.789215	3.315043	0.911005	H	-5.439441	0.417991	-0.709546
C	-3.551581	2.438580	-0.589895	H	-6.188491	1.762958	-1.607245
C	-2.776707	3.990301	1.634204	H	-5.582482	0.329821	-2.456177
C	-4.492297	3.154984	0.163637	C	-0.318645	3.564146	1.230522
C	-4.117714	3.904030	1.272206	C	-0.044029	3.846597	2.713032
				C	0.205441	4.712222	0.345821

H	0.251283	2.669330	0.977915	C	6.425304	2.120259	4.657314
H	-0.467519	3.065502	3.351855	H	4.386031	2.349574	4.004016
H	1.036886	3.876112	2.885648	C	7.351011	1.292666	5.296967
H	-0.449038	4.813359	3.031644	H	7.655039	-0.601936	6.279646
H	0.095163	4.478044	-0.718162	H	6.731509	3.094786	4.285918
H	-0.347650	5.636782	0.547168	H	8.379782	1.617963	5.423769
H	1.266604	4.898587	0.545389				
C	0.541987	-2.409833	-1.327205	²TS9a			
C	0.547015	-3.846481	-0.787221	C	0.821943	0.611983	4.567203
C	0.403771	-2.410644	-2.862046	C	1.002962	-0.523640	5.281599
H	-0.349721	-1.912259	-0.938619	H	0.658878	1.634622	4.866813
H	0.729249	-3.870545	0.294067	H	1.037403	-0.708531	6.342852
H	-0.417264	-4.315753	-0.981519	C	1.115595	-1.099026	3.073742
H	1.315769	-4.462238	-1.269027	N	1.174558	-1.550489	4.360236
H	0.338846	-1.392686	-3.258072	N	0.888845	0.242029	3.227395
H	1.261476	-2.908101	-3.331240	C	0.773349	1.195910	2.159201
H	-0.510415	-2.935864	-3.149287	C	1.895582	1.987719	1.858985
C	2.861564	2.074785	-0.428330	C	-0.459574	1.320057	1.493574
C	3.661451	2.651588	-1.610481	C	1.754362	2.935332	0.839666
C	3.384469	2.630343	0.906149	C	-0.547586	2.286135	0.484954
H	1.830721	2.418052	-0.536354	C	0.547929	3.083924	0.161594
H	3.614859	3.746496	-1.607234	H	2.597565	3.560503	0.569522
H	4.714979	2.355855	-1.552084	H	-1.477914	2.415731	-0.056185
H	3.268476	2.296002	-2.568830	H	0.459644	3.826288	-0.626816
H	2.794899	2.255750	1.746974	C	1.409819	-2.903267	4.794907
H	4.429837	2.357792	1.084680	C	0.317485	-3.779300	4.871730
H	3.324649	3.724357	0.905191	C	2.712284	-3.255348	5.168097
C	0.719133	0.305453	2.956027	C	0.562347	-5.060824	5.371448
H	1.263038	1.231354	2.725291	C	2.908533	-4.550492	5.658734
C	1.646316	-0.914257	2.936598	C	1.845044	-5.442244	5.763067
H	1.237754	-1.695647	3.592001	H	-0.253231	-5.771997	5.446262
H	1.686108	-1.361138	1.930296	H	3.906212	-4.867077	5.946860
H	0.210939	0.446187	3.917173	H	2.016221	-6.445392	6.144043
C	3.102259	-0.601944	3.325066	Ni	1.276838	-2.161448	1.353655
H	3.718066	-1.507152	3.235420	C	-1.654493	0.453209	1.873072
H	3.507913	0.110673	2.598141	H	-1.273722	-0.545768	2.111039
C	3.266096	-0.012254	4.735693	C	-2.675176	0.295367	0.738708
H	2.976353	-0.761027	5.484112	H	-3.414976	-0.461439	1.017464
H	2.575593	0.832252	4.849039	H	-3.217426	1.228336	0.546636
C	4.682207	0.451871	4.976549	H	-2.200575	-0.018915	-0.196888
C	5.619963	-0.367045	5.615814	C	-2.357285	0.993490	3.133793
C	5.104914	1.700969	4.500304	H	-3.203650	0.350043	3.400358
C	6.943282	0.047316	5.776738	H	-1.681290	1.028847	3.991715
H	5.307487	-1.338619	5.991836	H	-2.739702	2.005581	2.955856

C	3.215955	1.798474	2.597087	H	-2.024910	-3.654288	-1.580444
H	2.979666	1.530526	3.632906	C	-0.788813	-3.017176	0.095996
C	4.028110	0.633692	1.999325	H	-0.693285	-3.336064	1.141142
H	4.946254	0.484200	2.579591	H	-1.302097	-2.048838	0.105493
H	3.464092	-0.300338	2.005224	C	0.588580	-2.883851	-0.577172
H	4.303346	0.843639	0.961868	H	1.132775	-3.824592	-0.509575
C	4.066282	3.075344	2.648187	C	0.448387	-2.486094	-2.045113
H	4.924573	2.918824	3.310170	H	-0.131445	-3.248263	-2.581514
H	4.464729	3.336730	1.661325	H	1.417672	-2.397723	-2.538965
H	3.495757	3.932218	3.023983	C	2.102423	-1.509843	-0.247034
C	-1.075087	-3.338544	4.444462	C	3.371769	-2.062821	-0.506288
H	-0.951617	-2.586239	3.658641	C	1.817189	-0.225077	-0.742372
C	-1.911712	-4.473932	3.845721	C	4.335285	-1.331625	-1.200077
H	-2.203788	-5.210472	4.603808	H	3.603121	-3.057952	-0.141745
H	-2.831751	-4.074217	3.409356	C	2.783732	0.499235	-1.439011
H	-1.363994	-4.995822	3.058202	H	0.837011	0.213227	-0.590477
C	-1.826997	-2.672369	5.612183	C	4.047414	-0.047765	-1.674596
H	-1.287137	-1.802184	5.998554	H	5.315031	-1.769624	-1.375498
H	-2.819261	-2.337725	5.286611	H	2.543151	1.496781	-1.796756
H	-1.961190	-3.381921	6.437363	H	4.795794	0.514229	-2.226499
C	3.882566	-2.299854	4.992415	O	2.045742	-3.756630	2.063281
H	3.481018	-1.307941	4.765363	C	2.275888	-4.985436	1.459350
C	4.725582	-2.166479	6.269692	H	2.472741	-4.879950	0.369437
H	4.114646	-1.849349	7.122989	C	1.062308	-5.920150	1.609065
H	5.207026	-3.113839	6.537054	H	1.226154	-6.889969	1.119767
H	5.519712	-1.425442	6.122441	H	0.865569	-6.092379	2.673024
C	4.736493	-2.723124	3.784678	H	0.167750	-5.463721	1.173276
H	5.229040	-3.683691	3.977041	C	3.527660	-5.648875	2.054618
H	4.101380	-2.843139	2.903265	H	3.400171	-5.774971	3.135216
H	5.513199	-1.974484	3.586324	H	3.715622	-6.632200	1.603640
H	-0.074289	-1.529277	-2.156917	H	4.407579	-5.018862	1.888918
C	-5.013647	-3.791568	1.264422				
C	-3.914595	-3.474609	0.466804				
C	-2.908880	-4.418799	0.216788				
C	-3.040053	-5.694000	0.778027	²TS9b			
C	-4.141720	-6.019412	1.570948	C	5.977625	-1.399283	6.245894
C	-5.130684	-5.067834	1.821079	C	4.709046	-1.172463	6.667528
H	-5.783523	-3.045907	1.445062	H	6.903549	-1.511355	6.786503
H	-3.838365	-2.485882	0.021858	H	4.293760	-1.046346	7.654296
H	-2.266066	-6.435444	0.597012	C	4.645206	-1.357399	4.396795
H	-4.223338	-7.015403	1.997404	N	3.913708	-1.142285	5.523277
H	-5.987173	-5.317689	2.440832	N	5.917033	-1.513522	4.859801
C	-1.702202	-4.055575	-0.613436	C	7.030186	-1.879856	4.025538
H	-1.116518	-4.957999	-0.823490	C	7.504813	-3.197225	4.101855
				C	7.573427	-0.916581	3.154692

C	8.579967	-3.542394	3.274670	H	5.835055	-6.132132	4.918425
C	8.635488	-1.316627	2.339229	C	7.051021	0.514815	3.140230
C	9.135869	-2.617027	2.399276	H	5.965414	0.469253	3.267735
H	8.967705	-4.556043	3.304263	C	7.618340	1.310587	4.330939
H	9.079393	-0.607754	1.649445	H	7.364761	0.838464	5.284978
H	9.960353	-2.907768	1.754382	H	8.710625	1.377343	4.264175
C	2.488843	-0.939877	5.521972	H	7.212989	2.329278	4.339497
C	2.002602	0.341560	5.837338	C	7.314151	1.253733	1.822822
C	1.655854	-2.026832	5.190727	H	8.380458	1.458488	1.673403
C	0.615879	0.523138	5.824781	H	6.951660	0.681252	0.962897
C	0.278669	-1.782091	5.181787	H	6.796568	2.219367	1.831636
C	-0.235078	-0.527506	5.496844	Ni	4.070249	-1.504738	2.467159
H	0.197348	1.494578	6.062702	H	2.450010	0.394066	-0.422080
H	-0.402130	-2.580889	4.914890	H	4.345187	0.537160	1.258724
H	-1.309269	-0.365988	5.478144	C	3.693472	-5.195858	-3.625127
C	2.223856	-3.408999	4.879599	C	3.903726	-4.175017	-2.699521
H	3.063720	-3.290457	4.188056	C	4.383668	-2.921598	-3.105958
C	1.227561	-4.335490	4.173861	C	4.640999	-2.719080	-4.466426
H	0.401152	-4.634917	4.830983	C	4.431584	-3.737871	-5.397972
H	0.810195	-3.861894	3.281367	C	3.957329	-4.981374	-4.979894
H	1.748115	-5.246116	3.860675	H	3.325787	-6.161303	-3.287485
C	2.754598	-4.091102	6.156062	H	3.695357	-4.349807	-1.648645
H	3.527104	-3.497485	6.652821	H	5.012880	-1.752196	-4.798127
H	1.942717	-4.260282	6.874466	H	4.640727	-3.559390	-6.449493
H	3.193753	-5.062556	5.902135	H	3.795585	-5.776944	-5.702001
C	2.951786	1.500418	6.131579	C	4.584753	-1.811997	-2.099752
H	3.809366	1.105593	6.685326	H	5.190973	-2.182504	-1.265837
C	3.507099	2.104510	4.827812	H	5.153837	-0.995750	-2.564032
H	4.243935	2.885291	5.050481	C	3.254260	-1.252906	-1.564074
H	3.991649	1.342462	4.211406	H	2.686651	-2.053811	-1.079656
H	2.699489	2.555722	4.240171	H	2.648945	-0.921522	-2.417434
C	2.327895	2.597916	7.003938	C	3.422825	-0.075592	-0.597598
H	1.544549	3.147169	6.469559	H	4.045744	0.685702	-1.095171
H	1.889003	2.185497	7.918796	C	4.091492	-0.394811	0.739844
H	3.095301	3.325325	7.290021	H	5.013989	-0.973316	0.577292
C	6.892415	-4.238825	5.027103	C	2.361677	-0.980092	1.782304
H	6.056925	-3.778555	5.559219	C	1.731851	0.200904	2.208916
C	7.910719	-4.707588	6.080172	C	1.560147	-2.034321	1.308248
H	8.767872	-5.205231	5.612171	C	0.341380	0.306096	2.215333
H	8.297699	-3.867010	6.668842	H	2.329257	1.040925	2.545736
H	7.445268	-5.421939	6.768826	C	0.169104	-1.920385	1.311149
C	6.301343	-5.413296	4.233300	H	2.021667	-2.953251	0.968203
H	5.548494	-5.028888	3.541336	C	-0.448645	-0.752654	1.764311
H	7.072559	-5.946074	3.663878	H	-0.123388	1.218977	2.578148

H	-0.433190	-2.753245	0.956032
H	-1.531597	-0.667786	1.761355
O	4.555019	-3.342841	2.330288
C	4.562896	-3.967039	1.083841
H	4.022256	-3.350223	0.338022
C	3.833007	-5.317567	1.154429
H	2.807786	-5.172119	1.512557
H	3.795474	-5.818215	0.177671
H	4.341852	-5.985995	1.858375
C	5.999312	-4.133472	0.563801
H	6.508684	-3.163044	0.555845
H	6.568235	-4.792198	1.228611
H	6.023694	-4.553303	-0.450319

BP1

O	-0.093291	0.379344	0.337456
C	-1.019453	0.029918	1.042820
C	-1.775971	-1.263164	0.790133
H	-2.838512	-1.055526	0.611918
H	-1.353114	-1.777883	-0.074540
H	-1.723517	-1.916086	1.670294
C	-1.484567	0.862203	2.225672
H	-1.408584	0.282570	3.154173
H	-0.876473	1.765032	2.306482
H	-2.540190	1.137477	2.108937

Cl

Cl	0.000000	0.000000	0.000000
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HOTf

H	-0.077231	-0.334926	0.085746
S	-2.009811	-0.648626	-0.784682
O	-3.308498	-0.240822	-0.294044
O	-1.382266	-0.097362	-1.976737
O	-0.957268	-0.539992	0.457241
C	-2.038442	-2.504071	-0.980185
F	-2.504906	-3.068858	0.127651
F	-2.823802	-2.805929	-2.009953
F	-0.797717	-2.934413	-1.218021

[(IPr)NiCl]₂

C	2.846007	10.429711	5.773207
C	1.568660	10.758776	5.449004
H	3.578057	10.927765	6.388693
H	0.955409	11.601387	5.725953
C	2.046694	8.784500	4.407031
N	1.100263	9.749311	4.611931
N	3.117574	9.222251	5.135030
C	4.332437	8.460088	5.229340
C	4.557628	7.709727	6.397721
C	5.191812	8.418982	4.119454
C	5.701527	6.907778	6.438519
C	6.322134	7.598756	4.210468
C	6.575162	6.850145	5.354857
H	5.901977	6.305856	7.318585
H	7.003013	7.538185	3.366899
H	7.452415	6.210782	5.400928
C	-0.186894	9.696938	3.974596
C	-0.406215	10.513976	2.850604
C	-1.132945	8.768365	4.438147
C	-1.632314	10.388413	2.191617
C	-2.343833	8.680586	3.741953
C	-2.591944	9.478851	2.630536
H	-1.832412	10.993400	1.313559
H	-3.093883	7.967343	4.069909
H	-3.533970	9.387003	2.097036
Ni	1.910663	7.229802	3.370929
C	4.929291	9.204936	2.843608
H	3.999028	9.763781	2.971808
C	4.735871	8.266200	1.640194
H	4.495499	8.843221	0.739949
H	5.640856	7.683869	1.434413
H	3.917847	7.560978	1.818920
C	6.048341	10.227588	2.581958
H	5.820037	10.819210	1.687760
H	6.165074	10.914715	3.427820
H	7.012627	9.732790	2.417514
C	3.551745	7.695644	7.541616
H	2.962313	8.616022	7.489122
C	2.570710	6.519219	7.376664
H	1.819190	6.536129	8.175812
H	2.060861	6.558636	6.411288
H	3.103497	5.562710	7.423515
C	4.217711	7.668267	8.925301

H	3.458124	7.778154	9.707396	C	-1.910291	2.601908	4.452377
H	4.736874	6.721160	9.109577	H	-0.446936	1.345402	5.397684
H	4.945897	8.479423	9.037338	H	-3.170347	3.911545	3.311245
C	0.679337	11.437191	2.312243	H	-2.594288	2.565276	5.295894
H	1.370916	11.663712	3.129340	Ni	1.744449	5.335821	2.101353
C	1.492447	10.724444	1.214833	C	4.947266	3.484122	1.214063
H	0.851972	10.472095	0.362123	H	4.022568	3.315330	1.772233
H	2.301934	11.374019	0.859183	C	5.937818	4.123044	2.196318
H	1.924294	9.790856	1.582619	H	6.035425	3.487068	3.082778
C	0.128540	12.778797	1.806550	H	6.938443	4.233194	1.760413
H	-0.483995	13.274814	2.567820	H	5.583348	5.101558	2.530246
H	0.956378	13.446640	1.543130	C	5.456768	2.117896	0.718403
H	-0.485543	12.655027	0.907638	H	5.668822	1.457026	1.567172
C	-0.882090	7.862964	5.634796	H	4.716637	1.622830	0.080449
H	0.116551	8.078257	6.022913	H	6.379913	2.234026	0.137685
C	-1.886567	8.146335	6.764911	C	1.574255	5.189394	-2.220115
H	-1.850198	9.196820	7.075378	H	0.937888	4.588047	-1.564814
H	-2.913808	7.925354	6.452415	C	0.968713	6.601844	-2.256426
H	-1.661703	7.522221	7.637632	H	-0.069373	6.553820	-2.606113
C	-0.902361	6.379891	5.226139	H	0.976936	7.052380	-1.259978
H	-1.885323	6.080189	4.845810	H	1.516916	7.260404	-2.940144
H	-0.164643	6.178529	4.442915	C	1.561671	4.535096	-3.612550
H	-0.666118	5.743341	6.086489	H	0.543017	4.507526	-4.016577
C	1.948027	2.234145	-0.569141	H	2.189280	5.095841	-4.315309
C	0.934326	1.786409	0.216949	H	1.941653	3.507795	-3.573373
H	2.414970	1.810684	-1.443715	C	1.535171	1.239116	3.524166
H	0.345965	0.883766	0.179942	H	2.132948	1.533167	2.656966
C	1.605929	3.798349	1.054923	C	2.322371	1.664911	4.774243
N	0.740303	2.754832	1.200356	H	1.814607	1.357298	5.695830
N	2.344074	3.461739	-0.041224	H	3.313440	1.195777	4.770118
C	3.341713	4.347581	-0.575266	H	2.453513	2.750396	4.797959
C	2.978581	5.191660	-1.636062	C	1.349029	-0.286808	3.466190
C	4.609971	4.384401	0.033929	H	0.835380	-0.590358	2.546724
C	3.957523	6.056544	-2.138900	H	2.319702	-0.795059	3.499354
C	5.549714	5.270754	-0.500235	H	0.752245	-0.642985	4.314182
C	5.231255	6.092048	-1.580727	C	-1.725521	4.249331	0.995966
H	3.711888	6.718745	-2.963397	H	-0.786265	4.597458	0.558157
H	6.538782	5.329193	-0.059537	C	-2.439058	3.372348	-0.049833
H	5.977498	6.774891	-1.977657	H	-1.820704	2.517165	-0.343277
C	-0.179876	2.690675	2.302236	H	-3.385205	2.984994	0.347268
C	0.195567	1.953776	3.435927	H	-2.660970	3.955306	-0.951514
C	-1.377161	3.427091	2.228667	C	-2.545677	5.504822	1.319956
C	-0.704271	1.910936	4.507289	H	-3.557199	5.259177	1.666307
C	-2.237810	3.358414	3.328064	H	-2.046581	6.115042	2.076941

H	-2.648299	6.117572	0.417898
Cl	0.666042	7.185806	1.513091
Cl	2.986746	5.353744	3.942331

(IPr)]NiCl

C	1.096506	-0.533975	0.024055
C	1.753875	0.653501	-0.033603
H	1.449964	-1.552210	0.000762
H	2.802238	0.890423	-0.117765
C	-0.470956	1.116433	0.140424
N	0.782253	1.644809	0.038318
N	-0.255743	-0.230259	0.130250
C	-1.321829	-1.190571	0.217389
C	-1.723321	-1.628743	1.490170
C	-1.942564	-1.608712	-0.971032
C	-2.782879	-2.539819	1.550126
C	-2.997371	-2.520465	-0.857261
C	-3.411602	-2.983431	0.389101
H	-3.127637	-2.894512	2.516390
H	-3.507189	-2.860358	-1.753387
H	-4.236756	-3.686616	0.456989
C	1.030381	3.060360	0.007558
C	1.035429	3.709976	-1.237898
C	1.207277	3.734215	1.227027
C	1.247135	5.092556	-1.239275
C	1.415574	5.116355	1.171736
C	1.438053	5.788311	-0.047866
H	1.248512	5.631067	-2.181811
H	1.547960	5.672924	2.094325
H	1.594893	6.862969	-0.069430
C	1.127991	3.015982	2.565364
H	1.053979	1.941794	2.371169
C	-0.143800	3.431480	3.326285
H	-0.125406	4.499680	3.570901
H	-1.040729	3.239748	2.728262
H	-0.228093	2.869718	4.263813
C	2.390420	3.242997	3.412588
H	3.292318	2.929878	2.874830
H	2.510493	4.298291	3.681766
H	2.329638	2.669166	4.344155
C	0.766112	2.964985	-2.536355
H	0.752383	1.893075	-2.316970
C	-0.621025	3.336370	-3.091096

H	-0.837569	2.757855	-3.996734
H	-1.406786	3.132639	-2.356269
H	-0.669531	4.400838	-3.347620
C	1.870675	3.204630	-3.577983
H	1.914897	4.255448	-3.884981
H	2.855517	2.928601	-3.184940
H	1.679549	2.606649	-4.476093
C	-1.082274	-1.098458	2.763506
H	-0.202887	-0.511130	2.482429
C	-0.600307	-2.231763	3.683068
H	-1.436069	-2.838786	4.048267
H	0.095893	-2.898606	3.162289
H	-0.088062	-1.816279	4.558090
C	-2.049728	-0.151497	3.496504
H	-2.363464	0.671659	2.846212
H	-2.950656	-0.684743	3.820872
H	-1.568085	0.274697	4.384290
C	-1.531882	-1.066250	-2.331342
H	-0.641624	-0.444933	-2.195456
C	-1.159704	-2.193749	-3.307776
H	-0.360895	-2.824407	-2.901773
H	-2.018492	-2.838979	-3.523998
H	-0.814741	-1.772723	-4.258848
C	-2.635962	-0.162500	-2.908665
H	-3.556408	-0.729905	-3.087640
H	-2.874584	0.655933	-2.221553
H	-2.313643	0.271340	-3.862340
Ni	-2.111185	2.031938	0.263633
Cl	-3.974998	3.072598	0.402015

(IPr)]NiOi-Pr (2CAT1)

C	1.095228	-0.543903	0.045975
C	1.772805	0.632341	0.005176
H	1.432897	-1.567166	0.009307
H	2.825117	0.852526	-0.075440
C	-0.445326	1.132089	0.183218
N	0.816389	1.641319	0.089194
N	-0.251654	-0.220514	0.160635
C	-1.338884	-1.160950	0.225250
C	-1.705264	-1.672357	1.481581
C	-2.020071	-1.482556	-0.959982
C	-2.777587	-2.568927	1.524947
C	-3.083893	-2.386138	-0.864024

C -3.456589 -2.927640 0.362790
 H -3.095184 -2.976686 2.479288
 H -3.634122 -2.655468 -1.759994
 H -4.291397 -3.620638 0.416640
 C 1.084892 3.050830 0.023623
 C 1.099568 3.666983 -1.239342
 C 1.272701 3.754884 1.223953
 C 1.318806 5.048018 -1.276697
 C 1.488369 5.134323 1.133370
 C 1.512018 5.774017 -0.103523
 H 1.327857 5.561766 -2.232702
 H 1.629016 5.714047 2.040220
 H 1.676388 6.846734 -0.153523
 C 1.185197 3.065729 2.577045
 H 1.209896 1.984759 2.408024
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 H -0.244207 4.468420 3.451155
 H -0.998905 3.095403 2.619930
 H -0.245311 2.863024 4.210462
 C 2.371952 3.414140 3.488892
 H 3.327547 3.186413 3.003872
 H 2.377708 4.475567 3.760516
 H 2.313463 2.838259 4.419236
 C 0.829659 2.883852 -2.515836
 H 0.911010 1.817709 -2.282703
 C -0.607764 3.136779 -3.006925
 H -0.814638 2.543695 -3.905389
 H -1.339648 2.861664 -2.239714
 H -0.755046 4.194621 -3.254332
 C 1.857861 3.187622 -3.616735
 H 1.788754 4.224835 -3.962895
 H 2.881715 3.017787 -3.265517
 H 1.680647 2.541437 -4.483597
 C -1.031238 -1.202871 2.761638
 H -0.098807 -0.698237 2.489821
 C -0.665856 -2.361554 3.701350
 H -1.556857 -2.874806 4.079468
 H -0.039930 -3.104488 3.194634
 H -0.114434 -1.982779 4.569246
 C -1.925026 -0.165842 3.467364
 H -2.152116 0.669055 2.796278
 H -2.875090 -0.617006 3.775901
 H -1.426552 0.229504 4.360549
 C -1.649277 -0.873020 -2.302592

H -0.888649 -0.107152 -2.128269
 C -1.036150 -1.931244 -3.235582
 H -0.146175 -2.389470 -2.788595
 H -1.753186 -2.732409 -3.449465
 H -0.745255 -1.477383 -4.190032
 C -2.855368 -0.170734 -2.949617
 H -3.628588 -0.892489 -3.239121
 H -3.300563 0.552291 -2.258726
 H -2.537964 0.353990 -3.858553
 Ni -2.166923 1.886616 0.203776
 O -3.913885 1.749437 -0.160542
 C -4.786183 0.980687 0.635735
 H -4.257022 0.102587 1.049104
 C -5.927590 0.456492 -0.241663
 H -6.478794 1.296690 -0.680849
 H -5.522048 -0.149883 -1.058151
 H -6.629190 -0.160819 0.334423
 C -5.316966 1.802197 1.815502
 H -6.003324 1.217703 2.442731
 H -4.482822 2.146208 2.438724
 H -5.848986 2.686925 1.445509

⁴CAT1

C 0.795608 -0.492415 0.319760
 C 1.473433 0.670787 0.156395
 H 1.127524 -1.517902 0.326317
 H 2.518072 0.871576 -0.018783
 C -0.727692 1.207199 0.476539
 N 0.536593 1.692586 0.247080
 N -0.544217 -0.154368 0.498509
 C -1.605262 -1.119081 0.578897
 C -2.040742 -1.541172 1.844982
 C -2.145195 -1.620542 -0.621028
 C -3.033134 -2.527763 1.891372
 C -3.129042 -2.608831 -0.521107
 C -3.565872 -3.061739 0.721803
 H -3.389644 -2.880378 2.853822
 H -3.565871 -3.022092 -1.424123
 H -4.334510 -3.827370 0.777867
 C 0.822535 3.091688 0.112821
 C 0.569988 3.708881 -1.124589
 C 1.322929 3.787706 1.227215
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C	1.590165	5.151798	1.066613
C	1.344914	5.791536	-0.145612
H	0.645630	5.590348	-2.166299
H	1.984230	5.720038	1.903067
H	1.549660	6.853707	-0.246927
C	1.608029	3.088178	2.547483
H	1.112254	2.113044	2.523622
C	1.031983	3.851088	3.749596
H	1.507311	4.829945	3.881280
H	-0.046094	3.998638	3.627343
H	1.197513	3.277458	4.668782
C	3.119971	2.848922	2.712990
H	3.525631	2.257866	1.884118
H	3.665533	3.799426	2.741676
H	3.324790	2.312192	3.646417
C	-0.004887	2.934000	-2.300260
H	0.095326	1.866924	-2.079037
C	-1.506089	3.233552	-2.454394
H	-1.942161	2.619874	-3.251726
H	-2.043430	3.024524	-1.526355
H	-1.667907	4.287675	-2.709536
C	0.755909	3.199432	-3.608470
H	0.645075	4.237502	-3.940900
H	1.826253	2.994194	-3.496780
H	0.364824	2.557677	-4.406057
C	-1.431642	-0.988768	3.124185
H	-0.875708	-0.080971	2.869545
C	-0.433779	-1.997254	3.720941
H	-0.935599	-2.934036	3.990794
H	0.362142	-2.237130	3.006757
H	0.031208	-1.588137	4.625191
C	-2.499810	-0.580539	4.149401
H	-3.200377	0.140555	3.715326
H	-3.070880	-1.442456	4.513367
H	-2.023216	-0.108688	5.015600
C	-1.655078	-1.136711	-1.979123
H	-1.205403	-0.149297	-1.834685
C	-0.567297	-2.076902	-2.532351
H	0.287295	-2.148470	-1.853235
H	-0.969011	-3.086586	-2.677597
H	-0.201483	-1.713692	-3.499795
C	-2.786782	-0.976242	-3.006002
H	-3.208296	-1.943383	-3.302281
H	-3.598207	-0.356065	-2.615998

H	-2.397802	-0.500091	-3.912973
Ni	-2.149205	2.274427	1.440206
O	-3.750628	2.309076	0.629490
C	-4.227747	1.529155	-0.440189
H	-3.372380	1.105188	-0.991596
C	-5.031212	2.414266	-1.396767
H	-5.894711	2.840888	-0.873944
H	-4.415113	3.240066	-1.765676
H	-5.394604	1.838351	-2.257523
C	-5.072284	0.374489	0.105005
H	-5.434912	-0.272110	-0.703690
H	-4.483052	-0.235759	0.794281
H	-5.937326	0.772488	0.648039

NaO*i*Pr

O	0.874979	-0.194830	-0.019979
C	1.083924	-0.039716	-1.311349
H	1.163683	1.051606	-1.689731
C	-0.066770	-0.635022	-2.203135
H	-1.018304	-0.178535	-1.897207
H	0.062596	-0.479065	-3.291095
H	-0.147007	-1.716779	-2.011062
C	2.433790	-0.679260	-1.803800
H	2.655220	-0.524623	-2.877005
H	3.257830	-0.254386	-1.214037
H	2.412813	-1.762129	-1.602604

[•]O*i*Pr

O	0.874979	-0.194830	-0.019979
C	1.083924	-0.039716	-1.311349
H	1.163683	1.051606	-1.689731
C	-0.066770	-0.635022	-2.203135
H	-1.018304	-0.178535	-1.897207
H	0.062596	-0.479065	-3.291095
H	-0.147007	-1.716779	-2.011062
C	2.433790	-0.679260	-1.803800
H	2.655220	-0.524623	-2.877005
H	3.257830	-0.254386	-1.214037
H	2.412813	-1.762129	-1.602604

[•]OTf

O	-0.766821	0.279633	-0.002299
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S	-0.914580	-1.001662	0.724810
O	-0.206252	-2.158040	0.130561
O	-0.858611	-0.908105	2.201231
C	-2.702924	-1.428955	0.418708
F	-2.970228	-1.561777	-0.899478
F	-3.051469	-2.593326	1.011185
F	-3.536891	-0.478424	0.896407

PI

C	-2.419768	0.226335	-0.181145
C	-2.724511	-0.050849	1.158795
C	-3.235624	-0.327947	-1.173307
C	-3.811176	-0.856441	1.494805
H	-2.105853	0.366458	1.948909
C	-4.325438	-1.134974	-0.843231
H	-3.013183	-0.123280	-2.218135
C	-4.617228	-1.402273	0.493889
H	-4.029355	-1.058915	2.539994
H	-4.945545	-1.553597	-1.631390
H	-5.464625	-2.029888	0.755162
H	-2.324040	2.953246	-0.238212
C	4.219824	-1.406818	-0.780811
C	3.094315	-0.661742	-1.131326
C	2.609513	0.348006	-0.291126
C	3.281459	0.592678	0.912410
C	4.407339	-0.149595	1.268747
C	4.880536	-1.152973	0.422152
H	4.583230	-2.183333	-1.448556
H	2.583782	-0.862278	-2.070748
H	2.917850	1.375648	1.574366
H	4.917296	0.058172	2.205618
H	5.759127	-1.730339	0.695924
C	1.358478	1.115948	-0.647178
H	1.415266	2.123904	-0.221137
H	1.291675	1.236493	-1.736680
C	0.089235	0.405285	-0.143539
H	0.136746	0.319304	0.950195
H	0.084697	-0.621986	-0.528289
C	-1.229690	1.094042	-0.552217
H	-1.223694	1.188654	-1.647360
C	-1.362136	2.508779	0.037096
H	-1.305706	2.487059	1.131802
H	-0.568447	3.169916	-0.325560

PI'

H	-0.530091	0.130910	0.088298
H	0.592437	-0.879307	1.991524
C	-0.934772	-4.906318	-4.004104
C	-0.460233	-4.188056	-2.908196
C	0.477749	-3.159559	-3.075261
C	0.925727	-2.868232	-4.367677
C	0.453525	-3.585142	-5.468494
C	-0.478528	-4.607174	-5.289885
H	-1.659793	-5.702203	-3.855429
H	-0.820245	-4.420864	-1.908266
H	1.653736	-2.072979	-4.511749
H	0.816024	-3.345944	-6.464727
H	-0.846094	-5.167919	-6.144806
C	0.947585	-2.365000	-1.879845
H	1.175986	-3.054869	-1.059654
H	1.881729	-1.839906	-2.117275
C	-0.109017	-1.348047	-1.412965
H	-1.061163	-1.871388	-1.267125
H	-0.278076	-0.622015	-2.218337
C	0.257662	-0.603512	-0.123989
H	1.183587	-0.030528	-0.269899
C	0.431971	-1.515378	1.111356
H	1.338651	-2.120822	1.001804
C	-0.752402	-2.426971	1.343333
C	-1.995315	-1.900560	1.720078
C	-0.651990	-3.808828	1.143957
C	-3.105203	-2.727753	1.883750
H	-2.092919	-0.829973	1.885262
C	-1.760112	-4.642760	1.305229
H	0.306691	-4.237561	0.862531
C	-2.992480	-4.103639	1.673209
H	-4.059480	-2.298858	2.177448
H	-1.657629	-5.712873	1.146291
H	-3.857112	-4.749014	1.799394

SP-alkene

C	-2.086318	0.790278	0.190691
H	-3.034987	0.317376	0.429908
H	-1.195807	0.194385	0.361871
C	-3.343847	2.749311	-0.629764

H	-3.229630	3.832973	-0.517621
H	-4.112615	2.443454	0.088240
C	-0.763680	2.720954	-0.619071
C	-0.706349	3.785456	-1.534959
C	0.435595	2.339563	0.009888
C	0.498868	4.420106	-1.832605
H	-1.609175	4.121404	-2.032505
C	1.639134	2.972268	-0.284332
H	0.418312	1.555702	0.760039
C	1.679512	4.015124	-1.212412
H	0.511643	5.234920	-2.551312
H	2.547715	2.658664	0.222458
H	2.618262	4.512239	-1.439324
C	-3.866384	2.435711	-2.054334
H	-4.053144	1.357718	-2.119833
H	-3.087439	2.660446	-2.791332
C	-2.044860	2.033914	-0.312262
C	-5.121548	3.209826	-2.374805
C	-6.379995	2.715774	-2.010364
C	-5.051654	4.464266	-2.992700
C	-7.537885	3.453046	-2.256412
H	-6.450384	1.741071	-1.532486
C	-6.206042	5.206515	-3.241137
H	-4.081551	4.859599	-3.286592
C	-7.454182	4.702514	-2.872793
H	-8.505919	3.050483	-1.970577
H	-6.131391	6.176187	-3.725901
H	-8.355125	5.277283	-3.068005

SP-bz

C	-1.213445	-0.733449	-0.017786
C	-2.021809	-0.014849	0.864621
C	-0.301001	-0.061546	-0.833504
C	-1.918021	1.375883	0.931612
H	-2.732147	-0.537541	1.499480
C	-0.197179	1.328906	-0.766561
H	0.327955	-0.621054	-1.520623
C	-1.005765	2.047684	0.116079
H	-2.547602	1.935151	1.618343
H	0.512979	1.852112	-1.401127
H	-0.924524	3.130009	0.168131
H	-1.294156	-1.815836	-0.070196