

Supplementary Information

Ni pincer complex catalytic hydroboration of CO₂: a DFT study on the influence of borane reductants on the selective reduction

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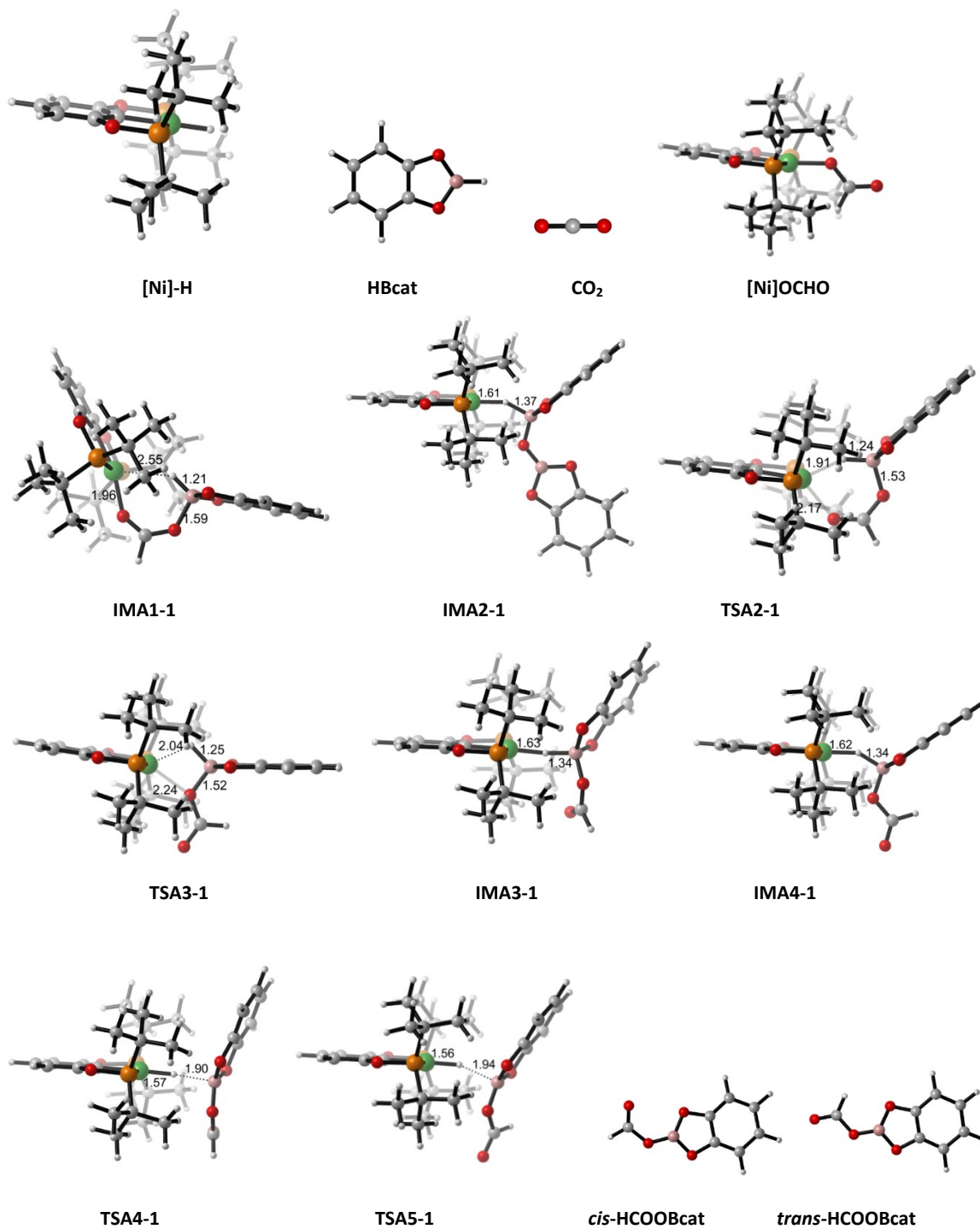
Content

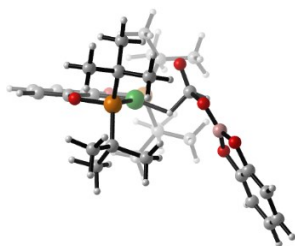
All visualized structures.....	S2-S7
Calculated energies and imaginary frequencies	S8-S10
Cartesian coordinates of all the optimized structures.....	S11-S119

All visualized structures

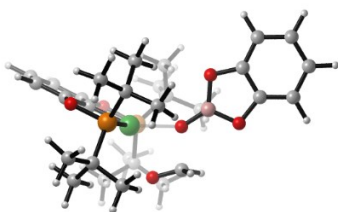
All visualized optimized intermediates and transition states, along with key bond lengths needed to understand structural changes (Å)

HBcat

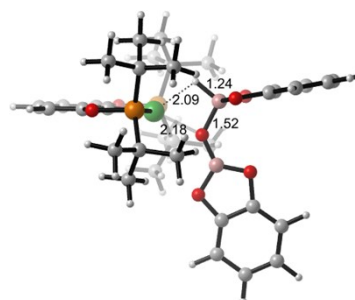




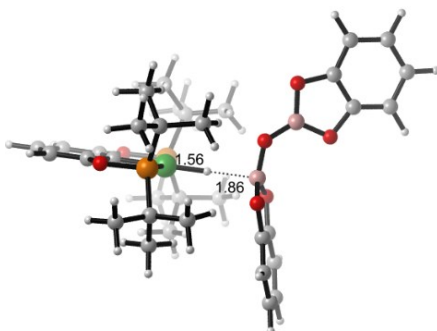
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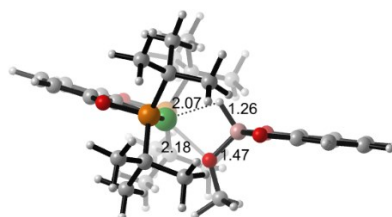
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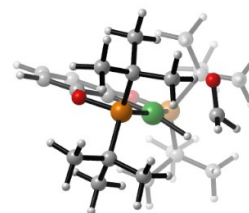
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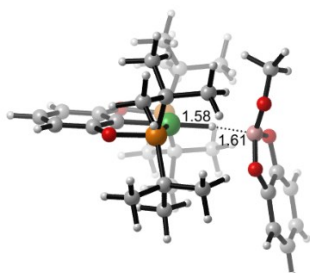
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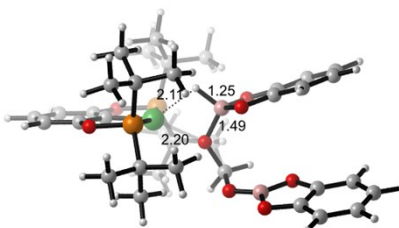
TSC1



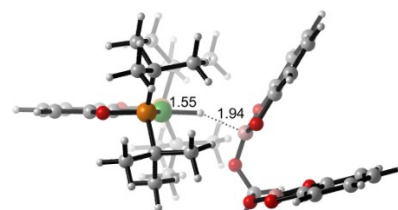
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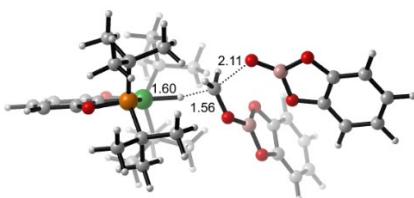
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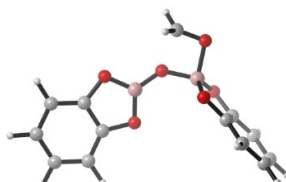
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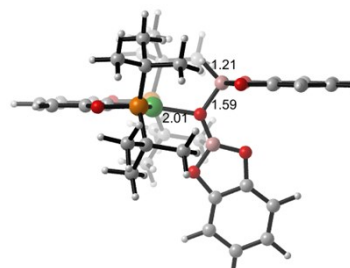
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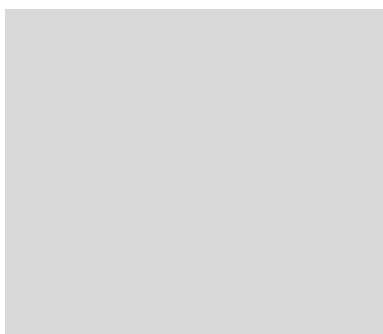
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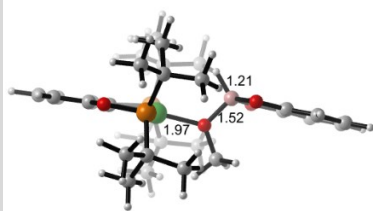
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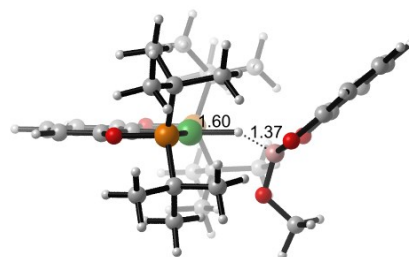
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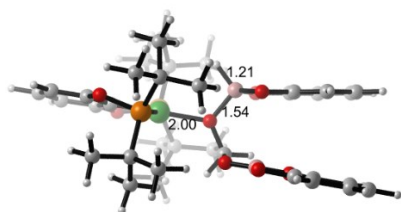
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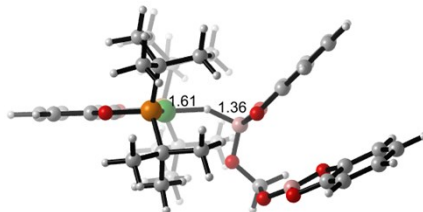
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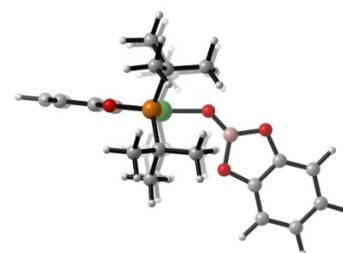
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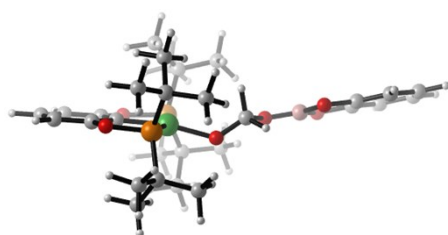
[Ni]OCH2OBcat



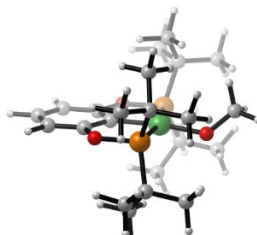
[Ni]OCH3



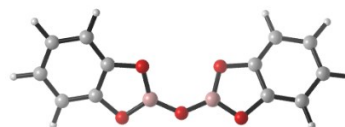
catBOCH2OBcat



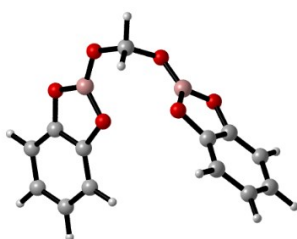
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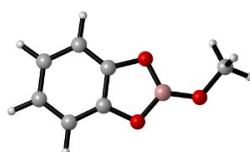
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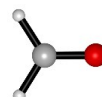
[Ni]OBcat



catBOCH2OBcat

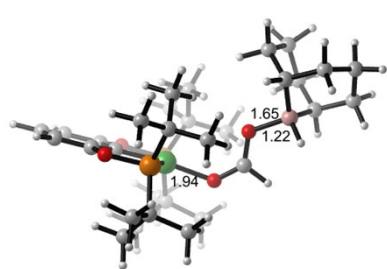


CH3OBcat

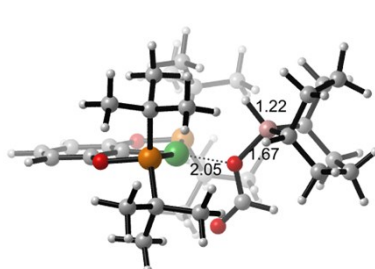


CH2O

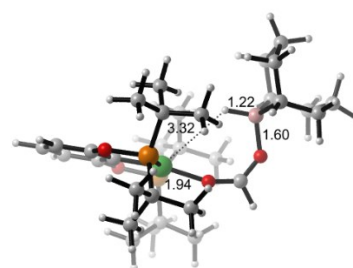
9-BBN



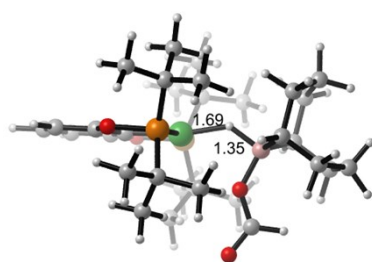
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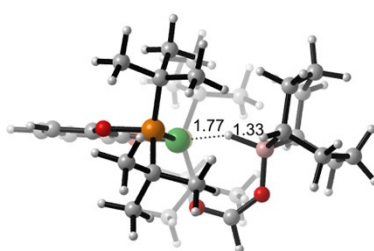
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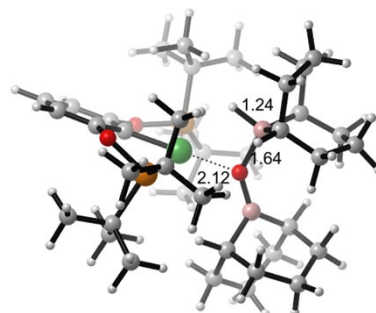
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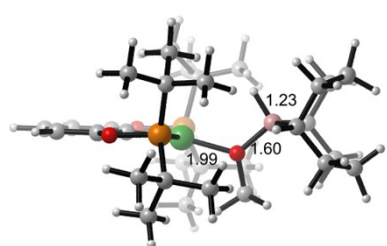
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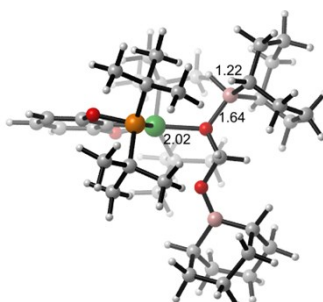
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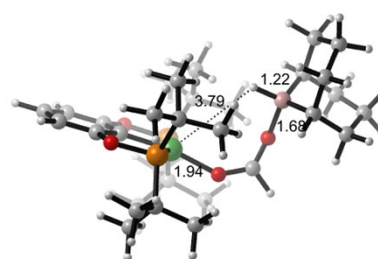
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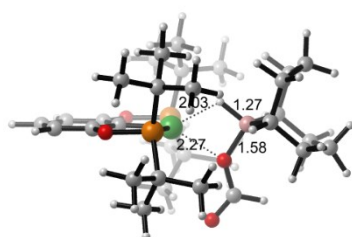
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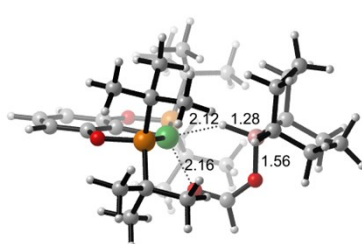
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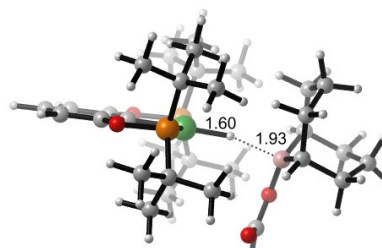
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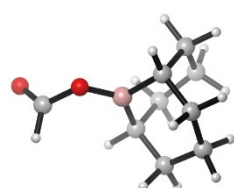
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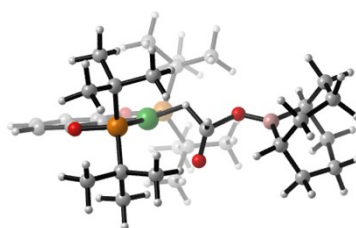
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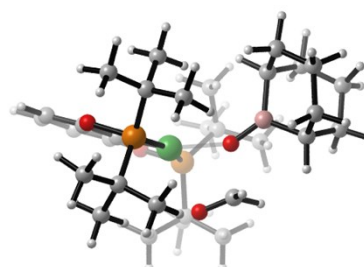
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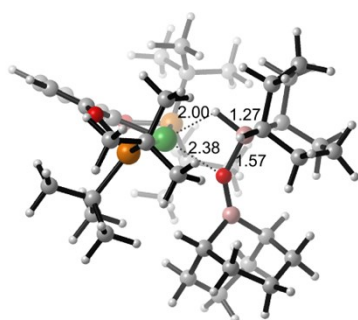
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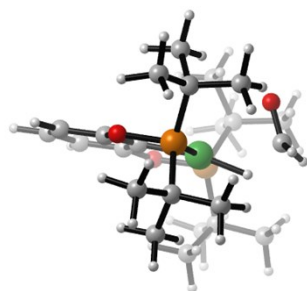
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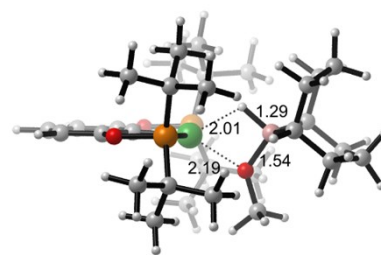
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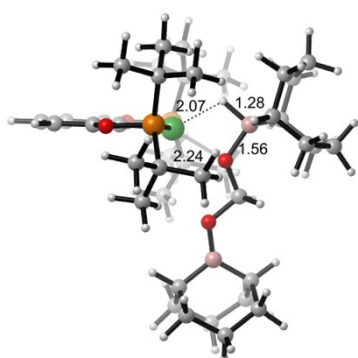
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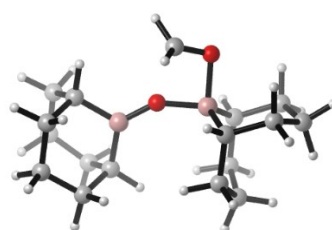
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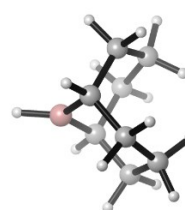
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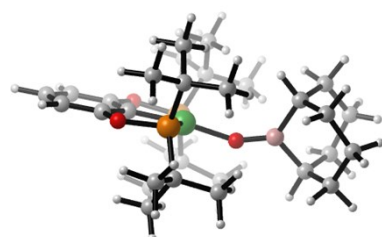
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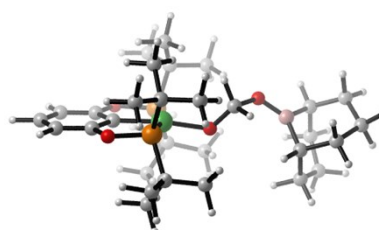
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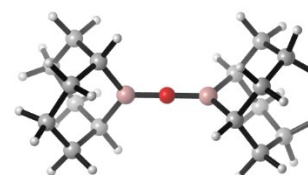
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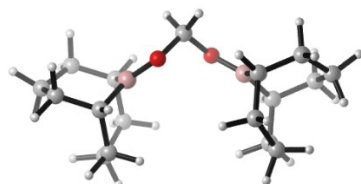
[Ni]OBBN



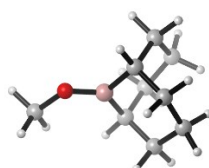
[Ni]OCH2OBBN



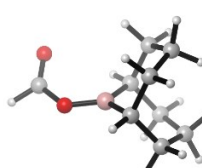
BBNOBBN



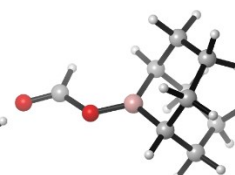
BBNOCH2OBBN



CH₃BBN

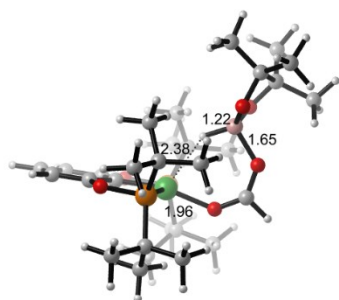


***cis*-HCOBBN**

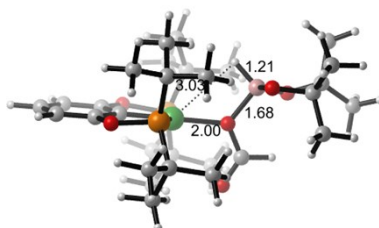


***trans*-HCOBBN**

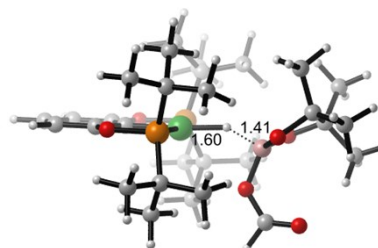
HBPIn



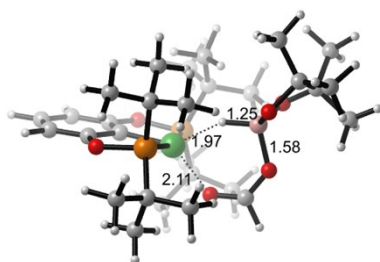
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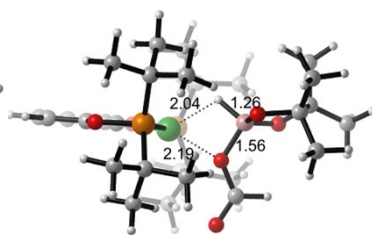
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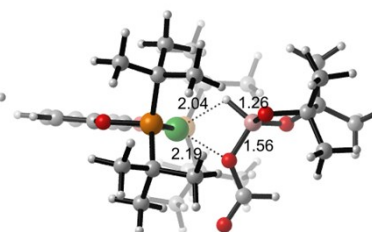
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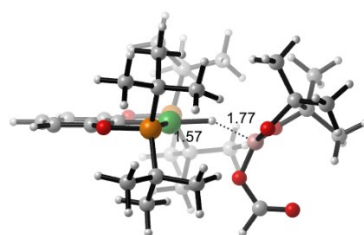
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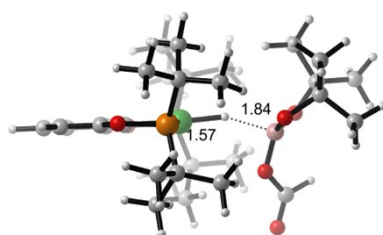
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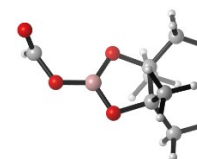
TSA3-3



TSA4-3



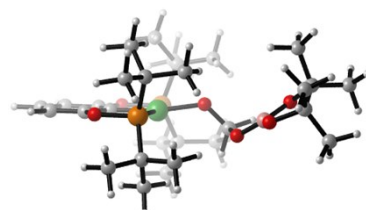
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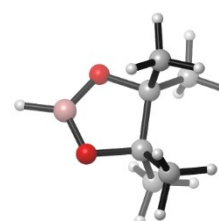
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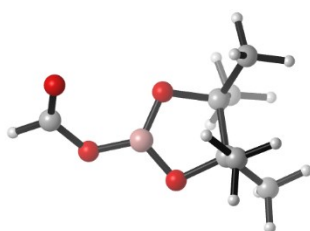
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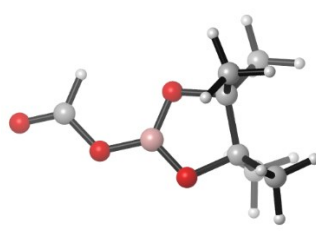
[Ni]OCH₂OBcat



HBPIn



Cis-HCOOBcat



trans-HCOOBcat

Calculated energies and imaginary frequencies

SCF energies (that is the single-point energies used for energy profiles) (in Hartrees) and thermal corrections at 298K obtained for all optimized structures and imaginary frequencies calculated for all transition states

Compound	Single-point energy	Thermal correction to Gibbs free energy	Gibbs free energy	Imaginary frequency
[Ni]-H	-1867.133516	0.519756	-1866.61376	
CO2	-188.6485802	-0.009781	-188.6583612	
HBcat	-407.1756435	0.072647	-407.1029965	
TSA1	-2055.775551	0.531536	-2055.244015	-199.0615
[Ni]OCHO	-2055.810651	0.530784	-2055.279867	
IMA1-1	-2463.002287	0.627325	-2462.374962	
IMA2-1	-2463.004561	0.631848	-2462.372713	
TSA2-1	-2462.997908	0.630311	-2462.367597	-70.2791
TSA3-1	-2462.996456	0.630004	-2462.366452	-132.3554
IMA3-1	-2463.003037	0.627314	-2462.375723	
IMA4-1	-2463.008417	0.626574	-2462.381843	
TSA4-1	-2462.994004	0.626823	-2462.367181	-138.6659
TSA5-1	-2462.997098	0.624492	-2462.372606	-126.3525
TSA6-1	-595.8426913	0.082813	-595.7598783	-127.6118
cis-HCOOBcat	-595.8468208	0.081634	-595.7651868	
trans-HCOOBcat	-595.8474434	0.082421	-595.7650224	
TSB1-1	-2462.9734004	0.629483	-2462.343917	-105.8864
[Ni]OCH2OBcat	-2463.015709	0.629953	-2462.385756	
TSB2-1	-2462.99759	0.629104	-2462.368486	-233.8000
[Ni]OBcat	-2348.469958	0.600367	-2347.869591	
HCHO	-114.54595	0.005167	-114.540783	
IMB1-1	-2755.663272	0.699223	-2754.964049	
TSB3-1	-2755.657236	0.693532	-2754.963704	-98.1044
IMB2-1	-2755.669645	0.69325	-2754.976395	

TSB4-1	-2755.659808	0.692358	-2754.96745	-116.0400
catBOBcat	-888.511802	0.149598	-888.362204	
IMD1-1	-2870.226745	0.730144	-2869.496601	
TSD1-1	-2870.220199	0.728446	-2869.491753	-121.6726
IMD2-1	-2870.235849	0.72711	-2869.508739	
TSD2-1	-2870.224512	0.724502	-2869.50001	-130.2758
catBOCH₂OBcat	-1003.078734	0.180425	-1002.898309	
TSF1-1	-1003.023778	0.176286	-1002.847492	-337.6039
TSE1-1	-2870.173778	0.719921	-2869.453857	-693.7380
TSC1	-1981.672067	0.549426	-1981.122641	-117.8851
[Ni]OCH₃	-1981.723367	0.553107	-1981.17026	
IMC1-1	-2388.941708	0.647932	-2388.293776	
TSC2-1	-2388.934044	0.647362	-2388.286682	-152.9397
IMC2-1	-2388.947209	0.647061	-2388.300148	
TSC3-1	-2388.940545	0.645739	-2388.294806	-80.1861
CH₃OBcat	-521.7997255	0.101541	-521.6981845	
9-BBN	-338.8681757	0.187	-338.6811757	
IMA1-2	-2394.719892	0.74739	-2393.972502	
IMA2-2	-2394.703579	0.748985	-2393.954594	
TSA2-2	-2394.703698	0.745677	-2393.958021	-137.0879
TSA3-2	-2394.696447	0.749563	-2393.946884	-127.9229
IMA3-2	-2394.71004	0.746694	-2393.963346	
IMA4-2	-2394.702439	0.748341	-2393.954098	
TSA4-2	-2394.700264	0.749381	-2393.950883	-74.0595
IMA5-2	-2394.704551	0.749306	-2393.955245	
TSA5-2	-2394.691286	0.744416	-2393.94687	-111.2537
cis-HCOBBN	-527.5565083	0.199034	-527.3574743	
TSA6-2	-527.5541899	0.199072	-527.3551179	-103.3168
trans-HCOBBN	-527.5557568	0.198355	-527.3574018	

TSB1-2	-2394.677899	0.745945	-2393.931954	-95.3960
[Ni]OCH₂OBBN	-2394.723855	0.74757	-2393.976285	
TSB2-2	-2394.691665	0.748267	-2393.943398	-182.9065
[Ni]OBBN	-2280.159791	0.717839	-2279.441952	
IMB1-2	-2619.031563	0.937815	-2618.093748	
TSB3-2	-2619.027888	0.937626	-2618.090262	-97.3521
BBNOBBN	-751.9225338	0.384301	-751.5382328	
IMD1-2	-2733.623304	0.965313	-2732.657991	
TSD1-2	-2733.615345	0.965334	-2732.650011	-122.7540
BBNOCH₂OBBN	-866.4946807	0.413316	-866.0813647	
TSC1	-1981.672067	0.549426	-1981.122641	-117.8851
[Ni]OCH₃	-1981.723367	0.553107	-1981.17026	
IMC1-2	-2320.629528	0.765966	-2319.863562	
TSC2-2	-2320.622284	0.767388	-2319.854896	-154.7477
CH₃OBBN	-453.5052524	0.21815	-453.2871024	
TSF1-2	-866.444936	0.412232	-866.032704	-330.5381
IMA1-3	-2467.845447	0.714358	-2467.131089	
IMA2-3	-2467.850064	0.715034	-2467.13503	
TSA2-3	-2467.8458	0.715812	-2467.129988	-44.9407
TSA3-3	-2467.840909	0.716	-2467.124909	-128.1928
IMA3-3	-2467.842201	0.718352	-2467.123849	
IMA4-3	-2467.852241	0.713822	-2467.138419	
TSA4-3	-2467.846683	0.713769	-2467.132914	-134.7775
TSA5-3	-2467.846025	0.7131	-2467.132925	-132.9905
TSA6-3	-600.7026268	0.168726	-600.5339008	-131.7447
cis-HCOOBPin	-600.7064067	0.168144	-600.5382627	
trans-HCOOBPin	-600.7082641	0.168644	-600.5396201	
TSB1-3	-2467.826696	0.716385	-2467.110311	-109.6747
[Ni]OCH₂OBPIn	-2467.873071	0.716758	-2467.156313	

Cartesian coordinates of all the optimized structures

HBcat reductant

catBOBcat

	x	y	z
H	6.69128400	0.09658000	0.31462100
C	5.62332200	0.22052400	0.16148000
C	5.12911800	1.45664200	-0.26800700
C	4.76913000	-0.86719800	0.40013200
C	3.75707200	1.66355900	-0.47926300
H	5.81974800	2.27631000	-0.44273300
C	3.41990000	-0.65021700	0.18853000
H	5.14054300	-1.83046600	0.73316100
C	2.92683000	0.58388800	-0.24064000
H	3.36169100	2.61732600	-0.81200900
O	2.36718900	-1.53243600	0.34301000
O	1.55175800	0.50445400	-0.36606800
B	1.24077900	-0.79956800	-0.00171500
O	-0.00000500	-1.34532000	0.00004800
H	-5.81980000	2.27625300	0.44275500
C	-5.12914900	1.45660700	0.26800300
C	-5.62331300	0.22050100	-0.16155800
C	-3.75710500	1.66355500	0.47924400
C	-4.76910000	-0.86720900	-0.40018700
H	-6.69126800	0.09654000	-0.31473400
C	-2.92684900	0.58389800	0.24062700
H	-3.36174400	2.61731800	0.81202500
C	-3.41987100	-0.65023000	-0.18854900
H	-5.14049600	-1.83047400	-0.73325000
O	-1.55178600	0.50447500	0.36614800
O	-2.36716500	-1.53239500	-0.34304900
B	-1.24074100	-0.79953800	0.00183200

catBOCH₂OBcat

	x	y	z
H	0.11451800	2.52258300	1.43623000
C	-0.17328900	2.96316700	0.47639300
O	-1.54198900	2.73714200	0.21938900
O	0.61621700	2.44018500	-0.57017100
C	3.51521900	-0.85464400	1.46660100
C	2.81487100	-0.04167800	0.59499200
C	2.96126100	-0.13977900	-0.79108600
C	3.81759200	-1.05676000	-1.37240400
C	4.53518000	-1.88906100	-0.49859800
C	4.38760900	-1.79068800	0.88837000
H	3.39241700	-0.76858000	2.54108300
H	3.92341400	-1.12424000	-2.44994400
H	5.21908000	-2.62427500	-0.91237100
H	4.95862400	-2.45033400	1.53510000
O	2.14265400	0.78691500	-1.40619900
O	1.90179900	0.95512300	0.88577500
B	1.49855400	1.43425800	-0.35950900
H	-0.04159400	4.04623000	0.49203500
C	-4.58004400	-0.95438500	-0.31416300
C	-3.46519700	-0.16346200	-0.10397700
C	-2.21508800	-0.71386300	0.18746100
C	-2.01539300	-2.07827500	0.28230300
C	-3.13976200	-2.89174300	0.07065200

C	-4.39233300	-2.34232800	-0.22056500
H	-5.54666700	-0.51701300	-0.54022000
H	-1.03808900	-2.49175300	0.50771200
H	-3.03077200	-3.97033900	0.13453100
H	-5.24075900	-3.00147400	-0.37903400
O	-1.29598600	0.30928800	0.34687100
O	-3.36615000	1.21415600	-0.13572100
B	-2.03181300	1.47728400	0.14339900

CH₃OBcat

	x	y	z
O	2.79495300	-0.54487700	-0.00944500
C	3.72383400	0.53763700	0.00440800
H	3.25845500	1.47605000	-0.31170500
H	4.12817400	0.65796800	1.01511700
H	4.54128400	0.28736900	-0.67713900
H	-3.73354100	1.58219500	-0.00167000
C	-2.86359200	0.93201000	-0.00093900
C	-1.58188400	1.50567000	-0.00133200
C	-3.04022000	-0.45481800	0.00049400
C	-0.51159500	0.63053800	-0.00042700
H	-1.43217800	2.58025500	-0.00229800
C	-1.94429600	-1.33249600	0.00151400
H	-4.04570400	-0.86540500	0.00083100
C	-0.68702100	-0.75606200	0.00098100
O	0.84018500	0.91817700	0.00079200
H	-2.06913000	-2.41017400	0.00260600
O	0.54479500	-1.37622800	0.00203400
B	1.46836200	-0.33194300	-0.00019600

CO₂

	x	y	z
O	0.00000000	0.00000000	-1.16916700
C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16916700

HBcat

	x	y	z
C	-0.90096700	1.43279000	-0.00002400
C	0.27152100	0.69727700	-0.00007300
C	0.27157400	-0.69739400	-0.00012200
C	-0.90103500	-1.43278100	-0.00009800
C	-2.09665400	-0.70009100	0.00004700
C	-2.09664600	0.70016300	0.00007800
H	-0.88827700	2.51749200	-0.00002700
H	-0.88838700	-2.51748800	-0.00009100
H	-3.04297200	-1.23291200	0.00013300
H	-3.04293900	1.23302400	0.00017000
O	1.57917300	-1.14682600	0.00008400
O	1.57916200	1.14677300	-0.00004400
B	2.35425000	0.00005100	0.00012300
H	3.53789200	0.00027000	0.00002500

cis-HBCOOBcat

	x	y	z
O	-3.47913000	1.12253400	0.41008500
C	-3.53671000	0.00676900	-0.02208800
O	-2.48253600	-0.83792800	-0.21032000

H	-4.46054400	-0.51158900	-0.31503100
H	4.35946000	-0.67068000	0.20182200
C	3.33229200	-0.32813000	0.11916800
C	3.07215100	1.04119600	-0.00455400
C	2.29481800	-1.27259700	0.13957800
C	1.76206600	1.53169300	-0.11386300
H	3.90096800	1.74272000	-0.01611000
C	1.00882400	-0.77572600	0.03082100
H	2.48387900	-2.33640600	0.23540500
C	0.74975200	0.59004200	-0.09323400
H	1.54696100	2.59049500	-0.20927800
O	-0.18983700	-1.46700600	0.02233000
O	-0.61801500	0.78755400	-0.18265200
B	-1.15474600	-0.48305000	-0.10946500

trans-HBCOObcat

	x	y	z
C	-1.06088400	-0.75335300	-0.00004700
C	-0.87213100	0.62938800	-0.00009800
C	-1.93057900	1.51815100	-0.00003000
C	-3.21627500	0.95544300	0.00007100
C	-3.40701600	-0.43041400	0.00015400
C	-2.32202600	-1.32030200	0.00007000
H	-1.76995200	2.59087700	-0.00008600
H	-4.08006000	1.61339400	0.00012700
H	-4.41674600	-0.82976000	0.00025800
H	-2.45733500	-2.39647200	0.00013400
O	0.48898800	0.90033000	-0.00022300
O	0.17134700	-1.38472200	-0.00005100
B	1.08807900	-0.35168400	-0.00014300
O	2.43803800	-0.58346300	-0.00014300
C	3.36031100	0.43078600	0.00021500
H	2.90391800	1.43259400	0.00060700
O	4.53555000	0.21405300	0.00012600

HCHO

	x	y	z
H	0.00012500	1.12344100	-0.93785100
C	-0.00001800	0.52895400	0.00000000
H	0.00012500	1.12344100	0.93785100
O	-0.00001800	-0.67757500	0.00000000

IMA1-1

	x	y	z
C	3.81988900	1.21447000	-2.53378600
C	2.80220400	1.18520100	-1.57982900
C	2.23823400	0.00072900	-1.08269000
C	2.80324000	-1.18325200	-1.57980600
C	3.82094200	-1.21166500	-2.53377000
C	4.31865400	0.00161300	-3.01071300
H	4.20659800	2.16674900	-2.88155800
H	4.20847600	-2.16361600	-2.88152400
H	5.10998500	0.00195600	-3.75499300
O	2.34431000	-2.39831900	-1.09464300
O	2.34222200	2.39987100	-1.09471700
P	1.14524700	-2.25932200	0.06794200
P	1.14336000	2.25998800	0.06797400
C	-0.17914700	-3.35813800	-0.74217400

C	2.00079300	-3.05460800	1.56735000
C	-0.18174800	3.35817700	-0.74178600
C	1.99835500	3.05561700	1.56749800
H	-1.40935500	-0.00236100	3.47614700
Ni	0.88448500	0.00015600	0.25383200
C	3.26279800	-2.19911000	1.82554200
H	3.01354900	-1.15003400	2.01335800
H	3.77548800	-2.58733100	2.71469000
H	3.96318300	-2.23995400	0.98606600
C	2.43924700	-4.51180700	1.32877400
H	3.09552500	-4.82106800	2.15268900
H	1.59027500	-5.20038900	1.31578200
H	2.99883400	-4.62541600	0.39538200
C	1.08546100	-2.97426300	2.80611500
H	1.63126700	-3.36794900	3.67332100
H	0.79687900	-1.94364100	3.02688400
H	0.17614100	-3.57163100	2.69356400
C	0.41668700	-4.66384800	-1.31228400
H	0.70874200	-5.37307900	-0.53546100
H	-0.35565100	-5.14869600	-1.92245800
H	1.28078100	-4.47310500	-1.95424000
C	-1.31619600	-3.68488000	0.24336600
H	-2.10885000	-4.21218500	-0.30122200
H	-0.98001500	-4.34482200	1.04993700
H	-1.78007200	-2.79282800	0.67110000
C	-0.72733900	-2.52852900	-1.92658800
H	-1.23789100	-1.62389500	-1.59491200
H	0.06794600	-2.25467200	-2.62829500
H	-1.45743000	-3.14045000	-2.47055200
C	-0.73002700	2.52829300	-1.92595900
H	0.06518100	2.25436300	-2.62773000
H	-1.24046400	1.62370400	-1.59401400
H	-1.46024300	3.14003300	-2.46995900
C	-1.31856600	3.68441700	0.24418600
H	-2.11178000	4.21115900	-0.30012700
H	-1.78169500	2.79213200	0.67225900
H	-0.98241600	4.34467600	1.05051200
C	0.41333600	4.66410500	-1.31218300
H	-0.35954700	5.14875900	-1.92182200
H	0.70569200	5.37338600	-0.53552400
H	1.27705500	4.47364700	-1.95472500
C	2.43536800	4.51334500	1.32958200
H	3.09132200	4.82287100	2.15365800
H	2.99490600	4.62785800	0.39626400
H	1.58578800	5.20117500	1.31683800
C	1.08316600	2.97372600	2.80627900
H	1.62860600	3.36752100	3.67366800
H	0.17321400	3.57019400	2.69406700
H	0.79562000	1.94270500	3.02654900
C	3.26128700	2.20134900	1.82523000
H	3.01322100	1.15185800	2.01228500
H	3.96169300	2.24353500	0.98583200
H	3.77347600	2.58952900	2.71468100
O	-0.14537300	-0.00064700	1.92538500
C	-1.31474600	-0.00158800	2.37941300
O	-2.42731600	-0.00178700	1.76999400
C	-5.93652400	-1.42463600	-0.45825600
C	-4.77038500	-0.70380500	-0.26479900

C	-4.77048600	0.70142200	-0.26430600
C	-5.93673300	1.42221300	-0.45726700
C	-7.12669000	0.69611600	-0.65430900
C	-7.12658700	-0.69857700	-0.65479200
H	-5.92532600	-2.51056400	-0.45683200
H	-5.92570000	2.50814200	-0.45509400
H	-8.05807400	1.23506100	-0.80702000
H	-8.05789400	-1.23755000	-0.80787700
O	-3.50349900	1.17333300	-0.07318700
O	-3.50332700	-1.17567200	-0.07401100
B	-2.67974000	-0.00119700	0.19624000
H	-1.59608400	-0.00092100	-0.33561800

IMA2-1

	x	y	z
Ni	0.70003300	-0.00009800	0.05050200
P	1.01494800	2.27006500	-0.00256300
P	1.01371900	-2.27041800	-0.00245800
O	-1.30935900	0.00048500	0.25435100
C	2.58862600	-0.00061600	-0.17972400
O	2.67520400	2.39622800	-0.20144400
C	0.43866800	3.21107500	-1.55318200
C	0.83045300	3.25045700	1.61424200
O	2.67397900	-2.39751000	-0.20073300
C	0.43744400	-3.21107000	-1.55330300
C	0.82808500	-3.25077100	1.61423400
C	-1.75791900	0.00071600	1.50671700
C	3.33633800	1.18261000	-0.26804900
C	3.33573500	-1.18425100	-0.26768300
C	1.35423200	4.40869200	-1.88327800
C	-1.02020200	3.68964900	-1.42058700
C	0.54647600	2.18962700	-2.70932000
C	-0.64261200	3.38970300	2.04655500
C	1.47570100	4.64808600	1.52006300
C	1.58413300	2.41649200	2.67744500
C	0.54589800	-2.18957600	-2.70933800
C	1.35265100	-4.40899400	-1.88329100
C	-1.02162800	-3.68912900	-1.42108300
C	1.58204700	-2.41741000	2.67770600
C	1.47238800	-4.64884000	1.52011200
C	-0.64520900	-3.38901700	2.04609000
O	-1.02433400	0.00059000	2.47793500
H	-2.85309900	0.00103200	1.58890200
C	4.72275300	1.21141500	-0.42429500
C	4.72213500	-1.21380700	-0.42391300
H	1.03545200	4.82547100	-2.84723800
H	2.40164400	4.10980000	-1.97182200
H	1.28569100	5.20795800	-1.14255800
H	-1.35942400	4.04568100	-2.40192600
H	-1.10671100	4.53208600	-0.72666500
H	-1.71206400	2.90296300	-1.10589600
H	1.56599400	1.80347500	-2.81796000
H	0.27764300	2.68974600	-3.64859800
H	-0.13473900	1.34562300	-2.57368000
H	-1.25011900	3.93587500	1.32117000
H	-0.67143300	3.95248800	2.98862400
H	-1.10470800	2.42033000	2.23695900
H	2.49107300	4.60927200	1.11555900

H	1.53188000	5.07318800	2.53042400
H	0.87963700	5.33627700	0.91336100
H	1.51185700	2.93464900	3.64222100
H	2.64547000	2.30725700	2.43414100
H	1.14189900	1.42325300	2.79703700
H	0.27707300	-2.68951200	-3.64871500
H	1.56558900	-1.80381000	-2.81772800
H	-0.13501500	-1.34531800	-2.57376400
H	2.40017100	-4.11044500	-1.97171500
H	1.03384000	-4.82566100	-2.84728900
H	1.28378100	-5.20824500	-1.14258400
H	-1.36075000	-4.04497000	-2.40252700
H	-1.71328100	-2.90222200	-1.10648800
H	-1.10859300	-4.53158900	-0.72724300
H	1.14049600	-1.42385700	2.79722100
H	2.64353400	-2.30893100	2.43471500
H	1.50910900	-2.93555900	3.64243500
H	2.48791500	-4.61065900	1.11594100
H	0.87604700	-5.33654400	0.91312900
H	1.52794700	-5.07409900	2.53044100
H	-0.67470700	-3.95189400	2.98808200
H	-1.25289300	-3.93466100	1.32045800
H	-1.10667400	-2.41933800	2.23646700
H	5.23902100	2.16391300	-0.48369300
C	5.40827900	-0.00138300	-0.50005900
H	5.23792100	-2.16658400	-0.48302700
H	6.48788000	-0.00167700	-0.62126700
H	-7.70483500	1.23715600	0.48865600
C	-6.79625800	0.69899600	0.23283200
C	-6.79641700	-0.69678300	0.23288600
C	-5.63703800	1.42578300	-0.09364600
C	-5.63736300	-1.42385800	-0.09353500
H	-7.70511700	-1.23471600	0.48875100
C	-4.50067500	0.70294200	-0.41868500
H	-5.62592700	2.51147300	-0.09711500
C	-4.50083500	-0.70130200	-0.41862900
H	-5.62649900	-2.50955100	-0.09691900
O	-3.26667900	1.17192400	-0.77102700
O	-3.26694500	-1.17059100	-0.77093100
B	-2.41537200	0.00056500	-0.95652700
H	-1.71628300	0.00044300	-1.93327900

IMA3-1

	x	y	z
Ni	0.57293900	0.27548200	0.13338700
P	1.97234600	-1.50913400	-0.07010600
P	-0.36648300	2.31028100	-0.03944100
O	-1.46345200	-0.04076100	3.58509100
C	2.11313700	1.23228400	-0.46014500
O	3.39822700	-0.78194700	-0.58750800
C	2.65581000	-2.37312800	1.47688100
C	1.64898300	-2.69008500	-1.53354900
O	0.93246300	3.31246000	-0.40541700
C	-0.99320100	3.18579100	1.51859100
C	-1.45051600	2.56050100	-1.57635200
C	-1.36903900	-1.24009500	3.43385900
C	3.32878500	0.59153800	-0.72727700
C	2.10953500	2.62302800	-0.63550700

C	3.94949000	-3.15380500	1.17125300
C	1.62391100	-3.31159800	2.13030800
C	2.97771900	-1.21964800	2.45699000
C	0.88736000	-3.95850400	-1.10286700
C	2.96193100	-3.08610500	-2.24024400
C	0.77322900	-1.88834000	-2.52334300
C	-0.01892900	2.73930100	2.63401700
C	-0.92302200	4.72337000	1.39912100
C	-2.42694100	2.74107500	1.86445800
C	-0.55676800	2.23195600	-2.79421200
C	-1.96720100	4.00401100	-1.71971200
C	-2.63143900	1.57387500	-1.54606100
O	-1.41053600	-1.91087700	2.29064500
H	-1.21877700	-1.93491600	4.27779900
C	4.48153200	1.26828300	-1.12951200
C	3.23155900	3.34940600	-1.03585700
H	4.38385900	-3.49888100	2.11858300
H	4.69345100	-2.53411400	0.66356500
H	3.75707200	-4.04207300	0.56129800
H	1.99769200	-3.60121400	3.12119000
H	1.47920400	-4.22989300	1.55719100
H	0.64778700	-2.84150600	2.26289200
H	3.71029900	-0.51965700	2.04331500
H	3.40080200	-1.64493200	3.37581400
H	2.07992300	-0.65503900	2.73224600
H	1.52059400	-4.63837400	-0.52518700
H	0.57940900	-4.49717300	-2.00872700
H	-0.01724800	-3.73152900	-0.53329400
H	3.51105100	-2.21371300	-2.60169900
H	2.71045600	-3.71557200	-3.10366100
H	3.62929400	-3.66342900	-1.59491600
H	0.59874800	-2.49743000	-3.41994400
H	1.26274800	-0.96146500	-2.84274000
H	-0.19959600	-1.64332800	-2.08701900
H	-0.28778900	3.25826600	3.56288000
H	1.01791100	3.00077000	2.39368900
H	-0.09188900	1.66701700	2.82577500
H	0.07392900	5.06491500	1.10911900
H	-1.15491000	5.14869900	2.38389500
H	-1.64858200	5.12896400	0.69097500
H	-2.69318600	3.16215400	2.84214900
H	-2.52711400	1.65596600	1.93808700
H	-3.15479200	3.11884000	1.13784300
H	-0.14612600	1.21871400	-2.74013500
H	0.27538800	2.93469300	-2.89423200
H	-1.16835100	2.29784600	-3.70298000
H	-1.15623500	4.73701900	-1.66966000
H	-2.71366400	4.25165100	-0.95966300
H	-2.45231200	4.10704200	-2.69905000
H	-3.24241300	1.72471600	-2.44497200
H	-3.27688400	1.71034600	-0.67581200
H	-2.29197200	0.53498400	-1.54817000
H	5.39644700	0.71598000	-1.31762500
C	4.41808100	2.65482600	-1.27829900
H	3.16700700	4.42623900	-1.15284300
H	5.30419400	3.20093000	-1.58972300
H	-5.42027900	-3.30550400	-2.74706700
C	-4.95319300	-2.71770900	-1.96169500

C	-5.67313500	-1.69524800	-1.34199300
C	-3.62913000	-3.00655600	-1.58372600
C	-5.09868800	-0.91631700	-0.32095300
H	-6.69596600	-1.49522400	-1.64909000
C	-3.07330900	-2.23736200	-0.57546400
H	-3.06321200	-3.80492300	-2.05398300
C	-3.79459500	-1.20629500	0.04452800
H	-5.65213100	-0.12261800	0.17137800
O	-1.82002700	-2.32255900	-0.03442500
O	-3.02382300	-0.59363100	0.99211600
B	-1.75979600	-1.30440600	1.00205100
H	-0.76963000	-0.45410200	0.70718000

IMA4-1

	x	y	z
Ni	0.66181900	0.00001900	-0.04887500
P	0.95053800	2.22245500	-0.11536700
P	0.95146600	-2.22218100	-0.11539700
O	-1.59326800	-0.00001600	2.11473000
C	2.55791500	0.00058900	-0.22959500
O	2.61779900	2.39399200	-0.24790800
C	0.38636100	3.07322200	-1.71090800
C	0.64960100	3.23709600	1.45967200
O	2.61880100	-2.39283400	-0.24838500
C	0.38750000	-3.07352000	-1.71070800
C	0.65132800	-3.23664600	1.45985800
C	-2.45080700	-0.00096800	3.14924500
C	3.29751200	1.18800600	-0.30576600
C	3.29799000	-1.18653100	-0.30598400
C	0.79336800	4.55730300	-1.77807100
C	-1.13939300	2.92919000	-1.87594400
C	1.08448200	2.31153100	-2.86101200
C	-0.82030700	3.68572000	1.56888900
C	1.58238400	4.46348300	1.54850000
C	0.98983700	2.27820900	2.62535500
C	1.08494800	-2.31146200	-2.86098600
C	0.79549200	-4.55733800	-1.77776500
C	-1.13836300	-2.93053900	-1.87557400
C	0.99121500	-2.27734700	2.62530800
C	1.58469200	-4.46257100	1.54882500
C	-0.81838000	-3.68590100	1.56930500
O	-2.08657100	-0.00070700	4.29877700
H	-3.51394200	-0.00207900	2.85221500
C	4.68611700	1.21694900	-0.43922800
C	4.68660900	-1.21488600	-0.43943900
H	0.57312000	4.93907800	-2.78344400
H	1.86305600	4.69682200	-1.59377800
H	0.23158800	5.17056400	-1.06745500
H	-1.43054200	3.37022800	-2.83801800
H	-1.70139700	3.43933500	-1.09042500
H	-1.45321600	1.88210700	-1.87602600
H	2.17346400	2.40065100	-2.81027400
H	0.75175900	2.73549000	-3.81677900
H	0.82666000	1.24695200	-2.85995400
H	-1.06121100	4.47058700	0.84390400
H	-0.98181200	4.10642200	2.56943400
H	-1.52932700	2.86519500	1.43528400
H	2.63437300	4.17980800	1.46662300

H	1.43209200	4.93488300	2.52817800
H	1.36788700	5.21636800	0.78656000
H	0.89081000	2.82584100	3.57125900
H	2.02097000	1.91268100	2.56054200
H	0.31369000	1.42042500	2.66260600
H	0.75233400	-2.73569100	-3.81667100
H	2.17399500	-2.39988500	-2.81042500
H	0.82643600	-1.24704700	-2.85994200
H	1.86531600	-4.69612800	-1.59371800
H	0.57524400	-4.93940900	-2.78302600
H	0.23428800	-5.17086400	-1.06692100
H	-1.42926800	-3.37157700	-2.83772100
H	-1.45295000	-1.88368900	-1.87538500
H	-1.69992300	-3.44131100	-1.09014000
H	0.31464900	-1.41988200	2.66243400
H	2.02215200	-1.91130300	2.56031000
H	0.89254800	-2.82481900	3.57134100
H	2.63653700	-4.17840600	1.46676000
H	1.37046900	-5.21569400	0.78703800
H	1.43475200	-4.93387200	2.52860400
H	-0.97967900	-4.10632100	2.57000200
H	-1.05893700	-4.47112900	0.84459900
H	-1.52778100	-2.86574300	1.43542700
H	5.20770800	2.16710000	-0.49056900
C	5.37026900	0.00117600	-0.50259900
H	5.20858700	-2.16481600	-0.49094400
H	6.45193700	0.00140300	-0.60445900
H	-6.72658800	1.23423500	-2.15279000
C	-5.93323300	0.69682500	-1.64085200
C	-5.93275100	-0.69908400	-1.64100200
C	-4.92282900	1.42485200	-0.98713800
C	-4.92183900	-1.42654700	-0.98744300
H	-6.72573300	-1.23693400	-2.15305600
C	-3.93105700	0.70093300	-0.34688600
H	-4.91823000	2.51038600	-0.97495000
C	-3.93057500	-0.70207200	-0.34703900
H	-4.91647800	-2.51208100	-0.97548700
O	-2.85773800	1.16873600	0.36006200
O	-2.85692700	-1.16928500	0.35981800
B	-2.08131500	-0.00005500	0.74723900
H	-0.95911700	0.00064700	0.02014300

IMB1-1

	x	y	z
Ni	1.10802200	0.00054700	-0.07650300
P	1.44835400	2.27065600	-0.12551100
P	1.44502700	-2.26971400	-0.15023100
C	2.97368400	-0.00272900	0.28696000
O	3.06213300	2.39552400	0.31442300
C	1.50431100	3.11582100	-1.83375200
C	0.67733300	3.35918200	1.22557600
O	3.05954700	-2.40125300	0.28523200
C	1.49651900	-3.09481600	-1.86840600
C	0.67672200	-3.37340600	1.19037200
C	3.70469500	1.17996700	0.47389900
C	3.70338000	-1.18841400	0.45936700
C	2.52846800	4.27030400	-1.87127300
C	0.11420800	3.62780700	-2.25915900

C	1.97625200	2.02704100	-2.82390400
C	-0.85566900	3.43370400	1.08011300
C	1.26318400	4.78485100	1.23789700
C	1.02748600	2.66306100	2.56162400
C	1.96928300	-1.99539500	-2.84639100
C	2.51789400	-4.25109500	-1.92161700
C	0.10453300	-3.59871600	-2.29750300
C	1.02759300	-2.69015700	2.53286600
C	1.26557800	-4.79786700	1.18746200
C	-0.85630100	-3.44958500	1.04658100
C	5.05812100	1.20581800	0.81284500
C	5.05678200	-1.21992100	0.79793200
H	2.58330400	4.64240000	-2.90235000
H	3.52693700	3.93792700	-1.57655500
H	2.24533600	5.11091600	-1.23501900
H	0.16671200	3.93624900	-3.31139800
H	-0.18638900	4.50859000	-1.68210100
H	-0.67234700	2.87080400	-2.18047900
H	2.94241800	1.60035200	-2.53304900
H	2.09680900	2.48214800	-3.81541600
H	1.24820900	1.21735000	-2.91202000
H	-1.17303100	3.92181900	0.15616600
H	-1.25720600	4.01610600	1.91920400
H	-1.32265100	2.44856100	1.11599300
H	2.35695600	4.77975400	1.25809400
H	0.91269100	5.29903200	2.14215900
H	0.92805000	5.37407600	0.37957500
H	0.59251300	3.24594200	3.38368000
H	2.10875500	2.61189100	2.72064300
H	0.61439800	1.65170300	2.61486300
H	2.08381800	-2.43837500	-3.84409000
H	2.93859800	-1.57691200	-2.55417100
H	1.24474100	-1.18122500	-2.92140300
H	3.51746800	-3.92490100	-1.62375000
H	2.57087100	-4.61017700	-2.95739900
H	2.23323500	-5.09903400	-1.29588000
H	0.15453700	-3.89431200	-3.35354600
H	-0.68056100	-2.84133900	-2.20831300
H	-0.19656900	-4.48600400	-1.73078900
H	0.61291500	-1.68008000	2.59674700
H	2.10900100	-2.63872900	2.69087900
H	0.59482700	-3.28203100	3.34964400
H	2.35936200	-4.79036300	1.20412700
H	0.92886500	-5.37996900	0.32490500
H	0.91918500	-5.32124700	2.08802700
H	-1.25533400	-4.04056600	1.88085800
H	-1.17401700	-3.93001400	0.11873300
H	-1.32541700	-2.46586700	1.09254000
H	5.56298500	2.15720600	0.94445900
C	5.72613900	-0.00846700	0.97487000
H	5.56057000	-2.17342000	0.91787700
H	6.77973700	-0.01067500	1.23980900
H	-3.81867200	-0.04755700	5.94214000
C	-3.70701800	-0.03902600	4.86185600
C	-4.84705300	-0.03431300	4.05116800
C	-2.41620400	-0.03296100	4.30825400
C	-4.75099100	-0.02333600	2.65048000
H	-5.83013600	-0.03925900	4.51277100

C	-2.33640600	-0.02214000	2.92763000
H	-1.52498800	-0.03660000	4.92750400
C	-3.47417700	-0.01749000	2.11777300
H	-5.62599600	-0.01963900	2.00944300
O	-1.21159300	-0.01470900	2.12253500
O	-3.09388900	-0.00716300	0.79458500
B	-1.70255800	-0.00568000	0.80404500
O	-0.89024900	0.00270900	-0.27337500
H	-6.77892300	-1.20766200	-3.06286000
C	-5.86327200	-0.67087100	-2.82877600
C	-5.86267000	0.72375200	-2.81691900
C	-4.69246100	-1.39967200	-2.54533800
C	-4.69119800	1.44657600	-2.52118400
H	-6.77783200	1.26526400	-3.04186000
C	-3.54401800	-0.68177900	-2.25941200
H	-4.68215700	-2.48565900	-2.55080900
C	-3.54342800	0.72287900	-2.24748900
H	-4.67988300	2.53249300	-2.50826400
O	-2.29976700	-1.15738800	-1.96370100
O	-2.29875200	1.19232800	-1.94370200
B	-1.44327000	0.01544600	-1.75958100
H	-0.43513000	0.02073400	-2.42784500

IMB2-1

	x	y	z
Ni	-1.37412500	-0.00072500	0.09424300
P	-1.66144500	-2.21749400	0.17278500
P	-1.66392300	2.21552600	0.18267000
C	-3.03029900	-0.00339600	1.03854400
O	-3.08789600	-2.39653600	1.04779400
C	-2.15075300	-3.02865600	-1.46973200
C	-0.50110900	-3.26993600	1.24329200
O	-3.09041900	2.38953500	1.05855700
C	-2.15410200	3.03274100	-1.45656500
C	-0.50468900	3.26494200	1.25740400
C	-3.67735900	-1.19197300	1.39953400
C	-3.67867100	1.18280900	1.40485600
C	-2.51608300	-4.51761100	-1.32275800
C	-1.01798800	-2.85425600	-2.50055700
C	-3.39508100	-2.25742500	-1.96530000
C	0.74770200	-3.70793100	0.45433900
C	-1.21148900	-4.50587600	1.83461600
C	-0.08185300	-2.34228800	2.40825400
C	-3.39764100	2.26217900	-1.95520200
C	-2.52107100	4.52068800	-1.30358800
C	-1.02117300	2.86365100	-2.48809200
C	-0.08381000	2.33276600	2.41815600
C	-1.21670200	4.49725300	1.85438600
C	0.74323900	3.70841400	0.47012800
C	-4.88852200	-1.22321300	2.09191300
C	-4.88987000	1.20964000	2.09734900
H	-2.93365600	-4.87486000	-2.27310300
H	-3.26956700	-4.67860700	-0.54554200
H	-1.64246500	-5.13687600	-1.09897300
H	-1.34801400	-3.27694300	-3.45838400
H	-0.09696200	-3.36394500	-2.20938600
H	-0.77293700	-1.80130700	-2.66348000
H	-4.24500400	-2.36753600	-1.28569400

H	-3.68814800	-2.65513900	-2.94514800
H	-3.18887200	-1.18887500	-2.08620900
H	0.50960600	-4.47063300	-0.29485400
H	1.46290400	-4.15644200	1.15578200
H	1.24910700	-2.87785800	-0.04922500
H	-2.10957100	-4.22985700	2.39233100
H	-0.51771300	-4.99895400	2.52758800
H	-1.48996100	-5.23837200	1.07356800
H	0.56110900	-2.90701400	3.09560700
H	-0.94997600	-1.99222700	2.97805600
H	0.48027500	-1.47357300	2.05645500
H	-3.69085000	2.66319300	-2.93365500
H	-4.24781800	2.36899500	-1.27538200
H	-3.19039700	1.19427200	-2.07990500
H	-3.27441000	4.67763100	-0.52541400
H	-2.93949200	4.88119800	-2.25232900
H	-1.64811800	5.14015400	-1.07775600
H	-1.35179600	3.28946900	-3.44432100
H	-0.77476900	1.81163500	-2.65500300
H	-0.10080100	3.37347400	-2.19508400
H	0.48034200	1.46693700	2.06251300
H	-0.95139500	1.97816100	2.98595900
H	0.55767200	2.89564900	3.10839500
H	-2.11393700	4.21746300	2.41157700
H	-1.49682700	5.23246400	1.09656200
H	-0.52320000	4.98853600	2.54890400
H	1.45799600	4.15465500	1.17346900
H	0.50371700	4.47430400	-0.27535000
H	1.24573200	2.88151200	-0.03753900
H	-5.34512800	-2.17368900	2.34819600
C	-5.48395800	-0.00788200	2.43737300
H	-5.34751100	2.15846500	2.35786500
H	-6.42654200	-0.00961400	2.97780000
H	7.63934100	-0.01047800	4.12715800
C	6.95684800	-0.00822300	3.28209000
C	7.47109700	-0.00531300	1.98164700
C	5.57276800	-0.00828300	3.52117000
C	6.62499800	-0.00233300	0.86057300
H	8.54697300	-0.00535000	1.83217500
C	4.74940000	-0.00533600	2.40928200
H	5.16252900	-0.01051800	4.52575700
C	5.26402600	-0.00242200	1.10884900
H	7.01122000	-0.00005800	-0.15329200
O	3.37306600	-0.00469500	2.35444100
O	4.22302600	0.00011300	0.20715100
B	3.06238300	-0.00131400	0.98785400
O	1.79577800	0.00018900	0.54742900
H	3.19526100	1.25288700	-5.96896700
C	2.89042300	0.71273400	-5.07684500
C	2.89031600	-0.68300400	-5.08052800
C	2.50324700	1.43707500	-3.93489700
C	2.50304300	-1.41330200	-3.94241500
H	3.19507200	-1.21848500	-5.97548900
C	2.12387000	0.71070100	-2.81858400
H	2.50809700	2.52265200	-3.91903800
C	2.12377100	-0.69277700	-2.82227700
H	2.50772800	-2.49894800	-3.93228300
O	1.71724300	1.17585500	-1.60042700

O	1.71705600	-1.16429900	-1.60660800
B	1.36198700	0.00373100	-0.81586700
H	-0.00268400	0.00394100	-0.74066700

IMC1-1

	x	y	z
Ni	0.67408100	0.05102300	0.15539400
P	0.60942100	2.33675100	0.03487300
P	1.34247700	-2.13087100	0.00627100
C	2.53929100	0.36227900	-0.05266200
O	2.23967400	2.73733100	0.09080700
C	0.12075500	3.12441300	-1.63064500
C	0.00473900	3.29950600	1.55153700
O	3.00034500	-1.98628500	-0.21670800
C	0.87797900	-3.07925300	-1.57638900
C	1.34737300	-3.19987300	1.58142200
C	3.09099000	1.65146000	-0.03005100
C	3.46558300	-0.68139600	-0.18805700
C	0.85473300	4.46005100	-1.87215700
C	-1.40177500	3.33799300	-1.74751600
C	0.57951800	2.11511300	-2.70890000
C	-1.53747900	3.31630100	1.62094200
C	0.54732000	4.74181000	1.60110100
C	0.57530100	2.52252600	2.76185100
C	0.87882100	-2.01033300	-2.69412300
C	1.91834900	-4.16018900	-1.93450400
C	-0.52602500	-3.70832300	-1.47809500
C	1.88651900	-2.26595800	2.69101800
C	2.28976800	-4.41440200	1.46435200
C	-0.06791900	-3.67687500	1.95832300
C	4.45935900	1.90766900	-0.12820000
C	4.84301500	-0.48312100	-0.29192900
H	0.62702700	4.79600100	-2.89191000
H	1.93898400	4.35550600	-1.78263600
H	0.52683000	5.24817000	-1.18975200
H	-1.63690000	3.56921100	-2.79453900
H	-1.73601900	4.19016300	-1.14826300
H	-1.99260900	2.46423500	-1.46069500
H	1.65487200	1.91471600	-2.65540400
H	0.36792500	2.53984400	-3.69859500
H	0.04201200	1.16653100	-2.62808900
H	-1.95992800	4.08395400	0.96775900
H	-1.84495200	3.55559200	2.64691400
H	-1.99606500	2.36473800	1.34009800
H	1.63457500	4.77577400	1.48854200
H	0.29261200	5.17844100	2.57560400
H	0.09595500	5.37748300	0.83488800
H	0.28437500	3.03938000	3.68508900
H	1.66880300	2.47346800	2.73506800
H	0.18636100	1.50126400	2.81431200
H	0.67250300	-2.50476700	-3.65194100
H	1.84804500	-1.50701000	-2.78100800
H	0.10274400	-1.25705700	-2.53307500
H	2.93421700	-3.75759000	-1.96130700
H	1.67993300	-4.54908800	-2.93276100
H	1.89834100	-5.00658700	-1.24392700
H	-0.81302100	-4.06457200	-2.47585500
H	-1.29919300	-3.00715600	-1.15039600

H	-0.53582500	-4.57792500	-0.81375900
H	1.24983000	-1.38716200	2.83614700
H	2.90062900	-1.91659900	2.47346500
H	1.91648800	-2.81942900	3.63810300
H	3.27794600	-4.13123000	1.09203900
H	1.87904000	-5.19150000	0.81440800
H	2.41671100	-4.85833900	2.46037600
H	-0.03241200	-4.12956500	2.95773200
H	-0.44580700	-4.43592700	1.26953800
H	-0.79318900	-2.86172300	1.99014900
H	4.82107900	2.93042900	-0.10494700
C	5.32970400	0.82452800	-0.25876800
H	5.50621900	-1.33610100	-0.39222400
H	6.39877000	1.00130100	-0.33727900
H	-0.93802800	-0.59507700	2.52956800
H	-2.33402900	0.43603700	2.12927600
C	-1.76313500	-0.44784600	1.82782500
H	-2.42541900	-1.31878800	1.86160700
O	-1.23516000	-0.29276700	0.51000200
C	-5.68083300	0.81381300	0.06718100
C	-4.45782200	0.22247300	-0.20530000
C	-4.33810200	-1.17102200	-0.35836400
C	-5.43974400	-2.00384700	-0.24223400
C	-6.68594700	-1.40818100	0.03034200
C	-6.80440100	-0.02694900	0.18188900
H	-5.76259800	1.89090300	0.18185300
H	-5.33703000	-3.07835500	-0.36348200
H	-7.56698600	-2.03821400	0.12085200
H	-7.77683300	0.41174600	0.38984600
O	-3.04664200	-1.51143400	-0.61554300
O	-3.24553900	0.82206400	-0.35947100
B	-2.25683100	-0.25786200	-0.61882300
H	-1.60160700	-0.08814200	-1.62748800

IMC2-1

	x	y	z
Ni	0.62101600	0.00038700	0.02324800
P	0.90183100	2.21452800	-0.06554600
P	0.90369900	-2.21367600	-0.06566400
O	-1.54075700	-0.00161600	2.31318100
C	2.51136600	0.00122700	-0.22765100
O	2.56608900	2.39399800	-0.24792900
C	0.28532700	3.05477500	-1.64750500
C	0.64187700	3.24222300	1.50842000
O	2.56816000	-2.39150000	-0.24810100
C	0.28827100	-3.05481900	-1.64754400
C	0.64504100	-3.24150700	1.50842900
C	3.24685400	1.18886000	-0.32838900
C	3.24786700	-1.18577100	-0.32843200
C	0.67874100	4.54145400	-1.73292900
C	-1.24325500	2.89541700	-1.76702500
C	0.95641100	2.29450300	-2.81442900
C	-0.82142900	3.70504300	1.64438400
C	1.58837000	4.45913400	1.57537500
C	0.98883000	2.28285800	2.67173900
C	0.95867700	-2.29392600	-2.81445600
C	0.68326500	-4.54109500	-1.73277000
C	-1.24046700	-2.89720500	-1.76738900

C	0.99178600	-2.28186400	2.67157700
C	1.59239300	-4.45777200	1.57522100
C	-0.81790000	-3.70532600	1.64482900
C	4.63053400	1.21864400	-0.50759100
C	4.63157900	-1.21435500	-0.50761800
H	0.41914600	4.92000700	-2.73021000
H	1.75379900	4.68762800	-1.58874000
H	0.14023300	5.15291900	-1.00299300
H	-1.56670800	3.32407000	-2.72447100
H	-1.78712000	3.40759500	-0.97020500
H	-1.54643800	1.84536500	-1.74719000
H	2.04564700	2.39272000	-2.79487500
H	0.59289200	2.71183400	-3.76193400
H	0.70792200	1.22793300	-2.80151200
H	-1.07190500	4.48280200	0.91505500
H	-0.95522600	4.14226800	2.64242900
H	-1.53838800	2.88736500	1.53764500
H	2.63605900	4.16406800	1.47979300
H	1.45696300	4.94004900	2.55335700
H	1.37086100	5.20834200	0.81042200
H	0.90681900	2.83431500	3.61786600
H	2.01611000	1.90850000	2.59506900
H	0.30239200	1.43210400	2.70842700
H	0.59582300	-2.71180800	-3.76197300
H	2.04802400	-2.39085900	-2.79468600
H	0.70893000	-1.22764200	-2.80172800
H	1.75841200	-4.68621000	-1.58820200
H	0.42438900	-4.91993700	-2.73013000
H	0.14508800	-5.15306600	-1.00301300
H	-1.56317900	-3.32623800	-2.72491400
H	-1.54486200	-1.84751200	-1.74759200
H	-1.78389700	-3.41005000	-0.97069500
H	0.30478500	-1.43158400	2.70848300
H	2.01879900	-1.90686400	2.59449900
H	0.91048400	-2.83335100	3.61774800
H	2.63983800	-4.16200400	1.47910700
H	1.37506200	-5.20731800	0.81055400
H	1.46174300	-4.93853400	2.55337700
H	-0.95114900	-4.14262900	2.64291300
H	-1.06800400	-4.48326500	0.91556500
H	-1.53545700	-2.88816000	1.53823800
H	5.15073200	2.16849900	-0.57712600
C	5.31217700	0.00243700	-0.59338700
H	5.15259100	-2.16376200	-0.57717300
H	6.38994300	0.00290400	-0.73139200
H	-6.69565300	1.23395200	-1.96228000
C	-5.90980400	0.69599500	-1.43903500
C	-5.90873200	-0.69967700	-1.44022400
C	-4.90852600	1.42298300	-0.76969900
C	-4.90633400	-1.42626200	-0.77213000
H	-6.69375500	-1.23794500	-1.96438800
C	-3.92453100	0.70105200	-0.11381200
H	-4.90507600	2.50876400	-0.75689600
C	-3.92344400	-0.70394000	-0.11501300
H	-4.90120300	-2.51205700	-0.76116500
O	-2.86544900	1.16886000	0.60581300
O	-2.86363800	-1.17135400	0.60378900
B	-2.07817000	-0.00099000	1.00627400

H	-0.97364400	0.00082900	0.19125400
C	-2.47546500	-0.00302500	3.38383000
H	-3.11456300	-0.89558100	3.35687700
H	-1.91155000	-0.00132700	4.32202600
H	-3.11836300	0.88675300	3.35593400

IMD1-1

	x	y	z
C	5.76956200	0.62770000	-0.40337000
C	4.46047700	0.14390100	-0.41238000
C	3.35313800	0.89613500	0.00420500
C	3.64254700	2.19284800	0.45075400
C	4.93278600	2.72470600	0.48770800
C	5.99293700	1.92761700	0.05312300
H	6.58341500	-0.00853400	-0.73544600
H	5.08921900	3.73808500	0.84268300
H	7.00458300	2.32328600	0.07203400
O	2.59755400	2.99482900	0.86717700
O	4.25154700	-1.15619000	-0.84015800
P	1.08090800	2.40124700	0.44865700
P	2.71917000	-1.73680100	-0.46937100
C	0.17447800	2.83396100	2.05400200
C	0.65312600	3.57745900	-1.01213200
C	3.12571400	-2.88745400	1.00174300
C	2.37280600	-2.66543800	-2.08409000
H	-1.79005600	-1.27938300	-1.27218800
C	-1.11058700	-0.42473000	-1.22511000
O	-0.27373600	-0.53693200	-0.11194700
O	-1.85265900	0.78993200	-1.16991300
C	-6.53620200	-0.42715400	-1.18571400
C	-5.32105000	0.22669800	-1.09631800
C	-5.23131400	1.58483500	-0.77943200
C	-6.35436000	2.35711200	-0.54414300
C	-7.59559300	1.70688100	-0.63704800
C	-7.68410700	0.34632400	-0.94906200
H	-6.58896500	-1.48511600	-1.41828300
H	-6.27309800	3.41072300	-0.29841200
H	-8.50408500	2.27483000	-0.45896600
H	-8.66040900	-0.12581800	-1.00816500
O	-3.90197600	1.96090700	-0.75095000
O	-4.05105200	-0.28104400	-1.28746500
B	-3.20119600	0.79448500	-1.05274400
H	-0.49758000	-0.37714600	-2.12825900
Ni	1.57769200	0.20812300	-0.03760500
C	0.99353900	2.80610700	-2.30706600
H	0.33634100	1.94146400	-2.44024200
H	0.84928800	3.47091000	-3.16883600
H	2.03238800	2.46033900	-2.31964700
C	-0.83133500	3.98553700	-1.05205200
H	-1.10382000	4.63635100	-0.21654000
H	-1.00622400	4.55438900	-1.97491000
H	-1.50141000	3.12631000	-1.06130700
C	1.52605500	4.84921800	-0.94774700
H	1.25551200	5.49108100	-1.79618800
H	1.36363400	5.42210500	-0.03082600
H	2.59251000	4.62316700	-1.02009600
C	0.34890200	4.32469300	2.40995000
H	-0.17549500	4.98408100	1.71220700

H	-0.07867000	4.49808800	3.40586600
H	1.40319700	4.61446500	2.44085200
C	-1.32021700	2.46483200	1.98614500
H	-1.76359900	2.66028900	2.97120600
H	-1.87333500	3.05949600	1.25611500
H	-1.48275400	1.40910000	1.76117900
C	0.85171600	1.97636100	3.14898900
H	0.74745600	0.90546100	2.94862900
H	1.91399300	2.21572500	3.25682600
H	0.35930500	2.18367800	4.10742500
C	3.03913800	-2.00990100	2.27187100
H	3.72332700	-1.15602000	2.22839200
H	2.02533000	-1.63488900	2.43605600
H	3.32010400	-2.62058800	3.13975200
C	2.12113900	-4.05086300	1.12036000
H	2.29654200	-4.55888700	2.07763600
H	1.07797100	-3.72203600	1.10500500
H	2.26729900	-4.79660300	0.33152100
C	4.56125600	-3.44314300	0.89189900
H	4.75150500	-4.06841900	1.77369400
H	4.70865000	-4.06654100	0.00698400
H	5.30838900	-2.64606400	0.87376100
C	1.00632600	-3.37839800	-2.03327600
H	0.73290200	-3.68877200	-3.04981900
H	1.03339800	-4.27447900	-1.41028300
H	0.21066400	-2.74230200	-1.64156200
C	3.48247900	-3.67699600	-2.43178200
H	3.49032700	-4.53003300	-1.74702500
H	3.29790300	-4.07112400	-3.43978200
H	4.47339400	-3.21363900	-2.42792700
C	2.34154400	-1.57110200	-3.17678500
H	1.56397800	-0.82276100	-2.98849300
H	3.30059600	-1.05127500	-3.25868900
H	2.12506500	-2.04128700	-4.14421400
C	-2.81465600	-4.34471100	0.92501100
C	-2.23397900	-3.09072300	1.02334300
C	-2.98460200	-1.96534500	1.40140900
C	-4.33423400	-2.06542000	1.69520200
C	-4.93013400	-3.33746100	1.60241700
C	-4.18590000	-4.45459800	1.22395000
H	-2.22522700	-5.20902700	0.63295900
H	-4.90598900	-1.18970100	1.98680100
H	-5.98628900	-3.44626000	1.83464400
H	-4.66614100	-5.42766000	1.16277600
O	-2.19686900	-0.85166700	1.41458400
O	-0.93731100	-2.73802600	0.79204600
B	-0.81739300	-1.29467500	1.11493600
H	-0.01097400	-1.05364100	1.98933800

IMD2-1

	x	y	z
C	5.79793500	1.11193500	-0.63539800
C	4.56616900	0.47412500	-0.48441200
C	3.38143200	1.15399100	-0.17485900
C	3.49701300	2.54025600	-0.01004400
C	4.70302800	3.22870400	-0.14871000
C	5.84987800	2.49731600	-0.46540100
H	6.68424700	0.53433700	-0.87709000

H	4.73393000	4.30470200	-0.01150200
H	6.79867200	3.01436500	-0.57939600
O	2.35939900	3.26400400	0.30785200
O	4.51359800	-0.90196300	-0.64536800
P	0.98027600	2.31421600	0.47856100
P	2.98780500	-1.55333900	-0.36620200
C	0.55401400	2.64793800	2.29482000
C	-0.17154200	3.18150500	-0.75602700
C	3.33077400	-2.63078200	1.15570500
C	2.77010800	-2.53456300	-1.97563700
H	-2.42605000	-1.94655800	-2.07921100
C	-1.86877300	-1.08446000	-2.46241600
O	-0.76243400	-0.79012200	-1.67083600
O	-2.73359000	0.04984700	-2.56117500
C	-6.77641000	-1.09485600	-0.16304400
C	-5.76059300	-0.45796300	-0.85231900
C	-5.81822800	0.90323400	-1.16672600
C	-6.89930900	1.68973800	-0.81081400
C	-7.93962500	1.05436700	-0.11301800
C	-7.87911800	-0.30622200	0.20427200
H	-6.71416400	-2.14968700	0.08198500
H	-6.93465600	2.74476500	-1.06169300
H	-8.80760400	1.63512200	0.18568400
H	-8.70012900	-0.76581600	0.74694900
O	-4.67381000	1.26635200	-1.84487300
O	-4.58119400	-0.98646900	-1.33402200
B	-3.92278000	0.09223500	-1.92948400
H	-1.51206000	-1.28423600	-3.47594400
Ni	1.71525000	0.24901300	0.01611500
C	0.17595600	2.56489100	-2.13159400
H	-0.05703800	1.49751600	-2.16721800
H	-0.42246600	3.06756000	-2.90216200
H	1.23304700	2.70794400	-2.38434500
C	-1.65156500	2.90742700	-0.42688500
H	-1.97878500	3.46183200	0.45936300
H	-2.26950300	3.24125300	-1.26898100
H	-1.86184700	1.84732400	-0.27043500
C	0.08409000	4.70169300	-0.81951600
H	-0.55551200	5.12115400	-1.60670500
H	-0.16553600	5.21266100	0.11331100
H	1.12348700	4.92913200	-1.06849200
C	0.26947700	4.13524900	2.57748300
H	-0.66628700	4.47098700	2.12171800
H	0.17385100	4.27790300	3.66180000
H	1.08188400	4.77886000	2.22593600
C	-0.64301000	1.77827200	2.72595800
H	-0.82339200	1.93583000	3.79720700
H	-1.56186000	2.02866200	2.19170100
H	-0.44941400	0.71333800	2.57096800
C	1.79634000	2.21687300	3.10743100
H	2.03424100	1.15904600	2.95385700
H	2.68020800	2.80881500	2.85296500
H	1.58569300	2.36083700	4.17475400
C	3.92413500	-1.68147100	2.22156000
H	4.88699200	-1.26664000	1.91000400
H	3.25038400	-0.84813200	2.44639600
H	4.08016100	-2.24736000	3.14864200
C	2.00705500	-3.21383700	1.69001900

H	2.21979600	-3.79196300	2.59867800
H	1.29016200	-2.43024600	1.95064400
H	1.51840600	-3.88008800	0.97548900
C	4.34102600	-3.76189500	0.88547800
H	4.59355200	-4.24539200	1.83818700
H	3.93128700	-4.53439600	0.22824900
H	5.26990300	-3.38375800	0.44723000
C	1.70154200	-3.63407700	-1.82484200
H	1.49449600	-4.05533800	-2.81719300
H	2.05050300	-4.45674600	-1.19187800
H	0.75941200	-3.26054600	-1.41669700
C	4.09605600	-3.15139100	-2.46813300
H	4.46621400	-3.94009500	-1.80950800
H	3.91778500	-3.60194700	-3.45308700
H	4.87912400	-2.39717500	-2.57635400
C	2.29727200	-1.49053100	-3.01495300
H	1.32550600	-1.06763800	-2.74609300
H	3.02031700	-0.67452300	-3.12662900
H	2.20163000	-1.98382800	-3.99134100
C	-2.04321600	-3.64707500	1.95035800
C	-1.74655900	-2.54237100	1.16884100
C	-2.39447100	-1.31273500	1.36358600
C	-3.36025800	-1.14971300	2.34260000
C	-3.66650900	-2.26678500	3.14069600
C	-3.02136200	-3.48960500	2.94882500
H	-1.54261800	-4.59668000	1.78743200
H	-3.86397500	-0.19761100	2.47750100
H	-4.41910400	-2.17170700	3.91857300
H	-3.27640600	-4.33702700	3.57930000
O	-1.93182200	-0.39369200	0.46386800
O	-0.85637100	-2.44440900	0.13841800
B	-0.84224600	-1.04010400	-0.26744700
H	0.31371200	-0.51648200	0.21726800

TSA1

	x	y	z
C	1.10341100	3.73677000	-0.33295600
C	1.10758700	2.34579900	-0.22457200
C	-0.06391600	1.58168400	-0.13787300
C	-1.26807300	2.29924800	-0.14884300
C	-1.32617600	3.68892100	-0.25487300
C	-0.12656800	4.39792900	-0.34880500
H	2.04177500	4.27773300	-0.39859400
H	-2.28738400	4.19247300	-0.26228000
H	-0.15064300	5.48080900	-0.43245000
O	-2.46011500	1.59510100	-0.04948000
O	2.33028100	1.69178400	-0.19528200
P	-2.24141200	-0.06792200	0.04760500
P	2.20068700	0.02986300	0.01569300
C	-3.11257700	-0.44386200	1.69020100
C	-3.19410900	-0.62364500	-1.49595000
C	3.08918300	-0.18772900	1.67820700
C	3.17827000	-0.58749600	-1.48759100
H	-0.08144000	-1.86525800	0.83196600
Ni	-0.02055700	-0.30262200	0.02071200
C	-2.25808100	-0.29841700	-2.68426300
H	-1.32985900	-0.87057900	-2.62428100
H	-2.77184100	-0.56828800	-3.61600500

H	-2.01872200	0.76941100	-2.73413600
C	-4.51415500	0.15206800	-1.68226200
H	-4.93151300	-0.11287400	-2.66214000
H	-5.26372800	-0.10059000	-0.92915500
H	-4.35564800	1.23376300	-1.66435600
C	-3.45818500	-2.14143600	-1.46386100
H	-3.87758300	-2.44244900	-2.43253500
H	-2.53543900	-2.70778800	-1.31093800
H	-4.18890500	-2.41808000	-0.69685500
C	-4.59803700	-0.03601000	1.69533200
H	-5.21015000	-0.70374800	1.08243100
H	-4.97886000	-0.09804200	2.72294400
H	-4.74202200	0.99138300	1.34727600
C	-2.97273500	-1.93827100	2.04562600
H	-3.41791100	-2.10690700	3.03448700
H	-3.49004800	-2.59085500	1.33742000
H	-1.92667700	-2.25542200	2.09671400
C	-2.35959700	0.39237200	2.75064000
H	-1.29469500	0.13948000	2.78517200
H	-2.45073400	1.46627300	2.56379000
H	-2.78866200	0.18058800	3.73808300
C	2.21344400	0.57084100	2.70270800
H	2.12563000	1.63509700	2.46348700
H	1.20541900	0.14788700	2.76392300
H	2.67636200	0.48346200	3.69370300
C	3.15464200	-1.67549600	2.08075300
H	3.47010000	-1.73832300	3.13030200
H	2.19611000	-2.19374800	1.98420300
H	3.88528800	-2.23095700	1.48747300
C	4.50120000	0.42822800	1.67657500
H	4.88391700	0.44150300	2.70536200
H	5.20280000	-0.15947100	1.07785300
H	4.49800800	1.45733900	1.30469900
C	4.41912600	0.28439600	-1.77102200
H	4.87098400	-0.05737000	-2.71095000
H	4.15697900	1.33961700	-1.88452100
H	5.18024300	0.20076100	-0.99159200
C	3.59462800	-2.06340600	-1.31822700
H	3.96005700	-2.43226500	-2.28505800
H	4.41276900	-2.17474000	-0.59970100
H	2.76956100	-2.71143600	-1.00858300
C	2.20126000	-0.46468600	-2.68100500
H	1.34113100	-1.12822900	-2.56042500
H	1.84424700	0.56324100	-2.81059000
H	2.73210000	-0.74993700	-3.59848200
O	-0.12045600	-2.38667000	-1.16362400
C	0.23087800	-2.69252700	0.00219000
O	0.82240800	-3.63656700	0.50740500

TSA2-1

	x	y	z
Ni	0.74557800	-0.00004900	0.27384100
P	0.96801100	-2.26204800	0.00398400
P	0.96846200	2.26190600	0.00395100
O	0.11807000	0.00006200	2.34592000
C	2.37901000	-0.00022200	-0.71778400
O	2.46274600	-2.39408100	-0.74466100
C	1.32140800	-3.32527000	1.53804900

C	-0.11925900	-3.15490300	-1.29027100
O	2.46313700	2.39362200	-0.74487000
C	1.32225900	3.32501900	1.53800500
C	-0.11874200	3.15501300	-1.29017300
C	-1.02830000	0.00016400	2.82058700
C	3.04650200	-1.18268100	-1.06618300
C	3.04669200	1.18209900	-1.06628900
C	1.82465000	-4.73322500	1.16335500
C	0.08583000	-3.43739900	2.45249700
C	2.44034300	-2.57690000	2.30057200
C	-1.35519300	-3.82049700	-0.65543400
C	0.69483300	-4.21054600	-2.07038000
C	-0.58223700	-2.06653400	-2.28494300
C	2.44108100	2.57636000	2.30040900
C	1.82581000	4.73285700	1.16328800
C	0.08679700	3.43743800	2.45257400
C	-0.58195400	2.06676700	-2.28487200
C	0.69545600	4.21057100	-2.07028700
C	-1.35452800	3.82076500	-0.65521300
O	-2.14935000	0.00022300	2.18996600
H	-1.15187900	0.00021100	3.91476400
C	4.28017100	-1.21220100	-1.71807100
C	4.28036500	1.21136100	-1.71818100
H	2.16793600	-5.23728400	2.07624100
H	2.66592800	-4.69397000	0.46548800
H	1.03487200	-5.35295100	0.72844900
H	0.36446800	-4.01059000	3.34633400
H	-0.75153800	-3.95345600	1.97846500
H	-0.25694500	-2.45690200	2.78518600
H	3.34938100	-2.48431600	1.69892300
H	2.69166500	-3.14689500	3.20446900
H	2.11995300	-1.57741800	2.60885800
H	-1.08252700	-4.67653600	-0.03059700
H	-1.99177800	-4.20111100	-1.46488700
H	-1.96078800	-3.11937900	-0.07543300
H	1.55419200	-3.76990200	-2.58079900
H	0.03571700	-4.65161100	-2.82907600
H	1.05713000	-5.02293100	-1.43609900
H	-1.14256800	-2.54737900	-3.09721400
H	0.26420600	-1.53467800	-2.73309200
H	-1.24178400	-1.33803600	-1.80833600
H	2.69264100	3.14628600	3.20428400
H	3.35003500	2.48354600	1.69866900
H	2.12046700	1.57695900	2.60872200
H	2.66699600	4.69341200	0.46532000
H	2.16932700	5.23680700	2.07614700
H	1.03613500	5.35279100	0.72849000
H	0.36566200	4.01055600	3.34638700
H	-0.25617800	2.45702100	2.78528800
H	-0.75049100	3.95370400	1.97862900
H	-1.24161000	1.33836400	-1.80827100
H	0.26437600	1.53478300	-2.73308400
H	-1.14223600	2.54774600	-3.09709800
H	1.55472800	3.76982600	-2.58076400
H	1.05789300	5.02288900	-1.43600100
H	0.03636100	4.65175000	-2.82893600
H	-1.99111600	4.20151100	-1.46460100
H	-1.08168100	4.67673500	-0.03036100

H	-1.96018700	3.11971400	-0.07519800
H	4.74003800	-2.16566300	-1.95662600
C	4.89134700	-0.00048400	-2.04130900
H	4.74038600	2.16472800	-1.95682000
H	5.85182600	-0.00058400	-2.54889400
H	-7.41142600	-1.23569000	-1.31255200
C	-6.52655600	-0.69687400	-0.98463300
C	-6.52644500	0.69785600	-0.98466700
C	-5.39693200	-1.42337500	-0.56343500
C	-5.39670500	1.42419900	-0.56350600
H	-7.41122900	1.23679700	-1.31261400
C	-4.28981900	-0.70160000	-0.15129300
H	-5.38821500	-2.50918100	-0.55692400
C	-4.28970800	0.70226700	-0.15132800
H	-5.38781500	2.51000400	-0.55705000
O	-3.08384500	-1.17387200	0.28473400
O	-3.08365800	1.17437000	0.28467400
B	-2.30035800	0.00019700	0.66729500
H	-1.16566000	0.00009600	0.15655300

TSA3-1

	x	y	z
Ni	0.65966500	0.00000000	0.02719400
P	0.96119200	2.25720100	-0.07675500
P	0.96119700	-2.25720000	-0.07675500
O	-1.27108300	-0.00000200	1.16844800
C	2.54967600	0.00000300	-0.15969400
O	2.63016500	2.39623700	-0.16711400
C	0.47394900	3.12538900	-1.70059700
C	0.63968200	3.27655900	1.48897400
O	2.63017100	-2.39623100	-0.16711700
C	0.47395600	-3.12539000	-1.70059600
C	0.63969300	-3.27655700	1.48897500
C	-1.84182500	-0.00000200	2.37669000
C	3.29729000	1.18505200	-0.21225000
C	3.29729300	-1.18504400	-0.21225100
C	1.37171200	4.34490300	-1.99611000
C	-1.00741400	3.54940500	-1.70354900
C	0.70332600	2.07323800	-2.81039400
C	-0.86915500	3.49777900	1.71959700
C	1.36922900	4.63494500	1.46286500
C	1.22168100	2.42230900	2.64153300
C	0.70333600	-2.07324100	-2.81039500
C	1.37171600	-4.34490600	-1.99610500
C	-1.00740900	-3.54940300	-1.70355000
C	1.22168700	-2.42230300	2.64153300
C	1.36924600	-4.63494000	1.46287000
C	-0.86914400	-3.49778400	1.71959700
O	-1.21339300	-0.00000100	3.41128900
H	-2.94342600	-0.00000300	2.34310600
C	4.68909300	1.21280400	-0.30771600
C	4.68909600	-1.21279300	-0.30771700
H	1.12913300	4.71521300	-3.00049200
H	2.43323900	4.08553000	-1.97626500
H	1.20455300	5.16739800	-1.29689700
H	-1.28176800	3.84214900	-2.72545500
H	-1.18078200	4.41889900	-1.06248200
H	-1.68680700	2.75113100	-1.39103200

H	1.73708700	1.71195400	-2.82863200
H	0.49271400	2.53517600	-3.78344000
H	0.03850700	1.21276000	-2.69511100
H	-1.27279700	4.27197200	1.06184900
H	-1.02095300	3.83142800	2.75359800
H	-1.46018100	2.59248900	1.56914700
H	2.43060400	4.52602200	1.22306700
H	1.29247500	5.08923800	2.45903200
H	0.91828300	5.33479900	0.75378500
H	1.12679200	2.99055700	3.57561000
H	2.28463300	2.20675600	2.49084500
H	0.68341600	1.48010400	2.77393100
H	0.49272500	-2.53518100	-3.78344000
H	1.73709700	-1.71195800	-2.82863100
H	0.03851800	-1.21276200	-2.69511500
H	2.43324400	-4.08553600	-1.97625600
H	1.12913900	-4.71521600	-3.00048700
H	1.20455200	-5.16740000	-1.29689200
H	-1.28176200	-3.84214800	-2.72545600
H	-1.68680100	-2.75112700	-1.39103500
H	-1.18078000	-4.41889400	-1.06248100
H	0.68341700	-1.48010000	2.77393000
H	2.28463700	-2.20674400	2.49084500
H	1.12680000	-2.99054900	3.57561000
H	2.43062200	-4.52601100	1.22307600
H	0.91830700	-5.33479600	0.75378800
H	1.29248900	-5.08923200	2.45903600
H	-1.02094100	-3.83143100	2.75359800
H	-1.27278000	-4.27198100	1.06185000
H	-1.46017500	-2.59249800	1.56914400
H	5.20757100	2.16539200	-0.34200200
C	5.37752400	0.00000600	-0.35401100
H	5.20757600	-2.16538000	-0.34200400
H	6.46136200	0.00000800	-0.42725600
H	-7.52799800	1.23606300	-0.62664100
C	-6.58759500	0.69775400	-0.54681000
C	-6.58759300	-0.69776600	-0.54681000
C	-5.38743600	1.42445100	-0.44505500
C	-5.38743300	-1.42446100	-0.44505600
H	-7.52799600	-1.23607700	-0.62664200
C	-4.21018200	0.70169000	-0.34617500
H	-5.37634400	2.51013300	-0.44288300
C	-4.21018100	-0.70169800	-0.34617500
H	-5.37633900	-2.51014300	-0.44288400
O	-2.93174500	1.17420800	-0.23748200
O	-2.93174300	-1.17421300	-0.23748200
B	-2.06089000	-0.00000200	-0.13402300
H	-1.12474500	-0.00000100	-0.95763800

TSA4-1

	x	y	z
Ni	0.61746700	0.21896500	0.10057700
P	1.84111200	-1.63952400	-0.04551000
P	-0.10363500	2.30452100	-0.06498800
O	-2.34150800	0.28187800	3.67601500
C	2.27633800	1.03878000	-0.43721700
O	3.34525900	-1.09149400	-0.58225800
C	2.41510600	-2.50804600	1.54338000

C	1.42463400	-2.84514100	-1.46032700
O	1.28960200	3.21131800	-0.36085700
C	-0.72611100	3.21558000	1.47725100
C	-1.09786100	2.70123600	-1.63317700
C	-1.85389700	-0.81721900	3.62669700
C	3.42684900	0.28806500	-0.69843200
C	2.40949600	2.42398800	-0.58443800
C	3.57076500	-3.49470300	1.28952600
C	1.25468700	-3.22782000	2.25426100
C	2.92008200	-1.36309800	2.45337800
C	0.48065000	-3.96948900	-0.99468400
C	2.68568500	-3.45835900	-2.10236000
C	0.70145100	-1.98322500	-2.52061500
C	0.07339100	2.59901100	2.64828600
C	-0.43066000	4.72957800	1.43480700
C	-2.23241700	2.97853800	1.69582100
C	-0.21108700	2.26192300	-2.82107300
C	-1.41701300	4.19988700	-1.78763700
C	-2.39458500	1.87200100	-1.65498500
O	-1.72229400	-1.59819600	2.53737800
H	-1.43369400	-1.34322900	4.49770700
C	4.64822200	0.85376500	-1.06910900
C	3.60265200	3.04813600	-0.95224500
H	3.96924100	-3.83144000	2.25571000
H	4.38786200	-3.03015200	0.73050200
H	3.23747500	-4.38626700	0.74886400
H	1.60552500	-3.57009500	3.23709100
H	0.91098400	-4.10919200	1.70750500
H	0.39524400	-2.57339600	2.41246900
H	3.76345900	-0.82725500	2.00801400
H	3.25563600	-1.78941200	3.40769400
H	2.12806400	-0.63686800	2.66725600
H	0.99616900	-4.69675200	-0.35953500
H	0.12222300	-4.51268900	-1.87943300
H	-0.39442200	-3.59167600	-0.45937000
H	3.37104500	-2.68994400	-2.46686800
H	2.37489700	-4.07521300	-2.95589400
H	3.23512300	-4.10412400	-1.41272100
H	0.45240500	-2.61031300	-3.38697400
H	1.33385700	-1.16160900	-2.87516500
H	-0.22796400	-1.55832700	-2.12773700
H	-0.21842800	3.09629600	3.58200900
H	1.15257100	2.73569100	2.51565300
H	-0.13549200	1.53220200	2.75917000
H	0.63070800	4.93074300	1.27128800
H	-0.71680900	5.16157200	2.40260600
H	-1.00163300	5.25032200	0.66289300
H	-2.51317100	3.38797600	2.67432000
H	-2.50025800	1.91967800	1.70488300
H	-2.83610800	3.49435200	0.94157700
H	0.06754800	1.20570200	-2.75276900
H	0.70615100	2.85388300	-2.88640500
H	-0.77493800	2.40386300	-3.75210200
H	-0.51702900	4.81716400	-1.70651700
H	-2.14843400	4.54695400	-1.05187600
H	-1.85073000	4.36913400	-2.78211100
H	-2.92951700	2.06915500	-2.59329600
H	-3.06797000	2.11957600	-0.83068600

H	-2.18850600	0.79951600	-1.60731500
H	5.51059500	0.22157500	-1.25527900
C	4.72032800	2.24389400	-1.19019400
H	3.64796000	4.12803600	-1.05079900
H	5.66066700	2.70711300	-1.47688100
H	-5.14129200	-2.86111300	-3.22462400
C	-4.78252600	-2.32806900	-2.34893400
C	-5.41992300	-1.14874100	-1.95091600
C	-3.68858800	-2.84372000	-1.63495300
C	-4.98875400	-0.42947800	-0.82432900
H	-6.26747300	-0.77984000	-2.52121000
C	-3.27437100	-2.12748400	-0.52485700
H	-3.19445500	-3.76415000	-1.92821600
C	-3.90528800	-0.94299000	-0.13271500
H	-5.47910100	0.48354600	-0.50331300
O	-2.26267400	-2.42045600	0.35868200
O	-3.29418700	-0.44830400	0.99762300
B	-2.24567200	-1.34115200	1.26199200
H	-0.73793800	-0.41000200	0.57729500

TSA5-1

	x	y	z
Ni	0.64387100	0.10973500	-0.02014400
P	0.44097100	2.29910100	-0.13507600
P	1.40212000	-1.96617600	-0.10490200
O	-1.84418400	-0.86883000	2.45110400
C	2.49633600	0.52587800	-0.32693300
O	2.01389000	2.86583500	-0.36615000
C	-0.39757900	2.98314800	-1.69197100
C	-0.00130000	3.25765500	1.44289500
O	3.07004700	-1.79330700	-0.31059200
C	0.97702000	-2.93402500	-1.68217300
C	1.40415800	-3.03942000	1.46463500
C	-2.16547400	-0.10058900	3.52113000
C	2.95018000	1.84250500	-0.45921000
C	3.47315900	-0.47034900	-0.43020300
C	-0.34863500	4.51883200	-1.79108500
C	-1.85539800	2.48663700	-1.76031500
C	0.38330800	2.38273400	-2.88349100
C	-1.52826100	3.35408500	1.62125500
C	0.62365500	4.66727500	1.48429500
C	0.60635400	2.42359600	2.59457300
C	1.43658100	-2.04167300	-2.85770600
C	1.70363000	-4.28761000	-1.77574200
C	-0.54728800	-3.13136100	-1.78382900
C	1.54824600	-2.03686300	2.63363000
C	2.59791300	-4.01632900	1.51064500
C	0.08388000	-3.81809700	1.61724700
O	-1.53874200	-0.13241600	4.54472000
H	-3.05077300	0.53324400	3.35395900
C	4.28739800	2.17617600	-0.67838400
C	4.82496600	-0.19898400	-0.64835000
H	-0.71064100	4.82438900	-2.78160800
H	0.67008600	4.90102300	-1.67433300
H	-0.99112300	5.00118600	-1.04837900
H	-2.29667300	2.80748200	-2.71299300
H	-2.47564100	2.89133800	-0.95593800
H	-1.91239000	1.39552800	-1.71156000

H	1.42376000	2.71932700	-2.90131400
H	-0.09535100	2.70305400	-3.81779100
H	0.37798100	1.28799200	-2.86129300
H	-1.97539100	4.06230600	0.91552200
H	-1.74657800	3.72156600	2.63240400
H	-2.03154400	2.39080900	1.49718100
H	1.70580800	4.63116100	1.33835600
H	0.42607200	5.10605000	2.47109900
H	0.19919000	5.33970800	0.73523300
H	0.40119300	2.92313600	3.55000600
H	1.69276100	2.32847600	2.49233300
H	0.18302400	1.41647200	2.64330600
H	1.16741100	-2.53343000	-3.80145300
H	2.51867300	-1.88336100	-2.85295100
H	0.94790500	-1.06201800	-2.83747000
H	2.78276100	-4.17874400	-1.63084300
H	1.54011400	-4.71302300	-2.77480700
H	1.32326600	-5.01105900	-1.04875800
H	-0.77739900	-3.62665300	-2.73662400
H	-1.07668900	-2.17502000	-1.76103300
H	-0.94819200	-3.75253000	-0.97907000
H	0.68054400	-1.37787100	2.71499400
H	2.44958700	-1.42238700	2.53088300
H	1.63207400	-2.59668700	3.57409900
H	3.55132700	-3.49384900	1.40335900
H	2.54314600	-4.79077500	0.74195300
H	2.59219600	-4.52010300	2.48606500
H	0.05769700	-4.27247500	2.61602000
H	0.00028400	-4.63111900	0.88825200
H	-0.79636600	-3.17780600	1.52630300
H	4.58567400	3.21542600	-0.77324000
C	5.21758200	1.13685800	-0.76953800
H	5.54251400	-1.01014400	-0.71995900
H	6.26504600	1.37180100	-0.93870600
H	-6.42280100	0.34433800	-2.51867800
C	-5.65964200	-0.14959300	-1.92451200
C	-5.33093500	-1.48151200	-2.19407900
C	-5.02308100	0.56580000	-0.89706500
C	-4.35274400	-2.15912500	-1.44851500
H	-5.84313600	-2.00715800	-2.99464100
C	-4.06022600	-0.11210800	-0.17106300
H	-5.27308100	1.59816300	-0.67585800
C	-3.73256000	-1.44527100	-0.43746600
H	-4.09636100	-3.19492500	-1.64434800
O	-3.30028400	0.34211900	0.88761300
O	-2.76899100	-1.86982300	0.44862700
B	-2.45597700	-0.73490400	1.20884800
H	-0.85617100	-0.21300900	0.24716100

TSA6-1

	x	y	z
C	-1.04561800	-0.76187600	-0.01904500
C	-0.80193200	0.60980900	0.07470900
C	-1.82380900	1.54050000	0.06810400
C	-3.12890500	1.03464100	-0.03744200
C	-3.37386300	-0.33916700	-0.13121400
C	-2.32596800	-1.27291100	-0.12396500
H	-1.62092100	2.60364500	0.13995600

H	-3.96447000	1.72810200	-0.04699800
H	-4.39672000	-0.69470400	-0.21212100
H	-2.50339900	-2.34050800	-0.19694800
O	0.56467700	0.82318200	0.16753500
O	0.15802200	-1.44535000	0.01207300
B	1.11404700	-0.45104700	0.12339600
O	2.44440700	-0.72522000	0.19946600
C	3.44209600	0.21739000	0.28156200
H	3.66197600	0.47939300	1.32770200
O	4.03305400	0.63601200	-0.66717600

TSB1-1

	x	y	z
C	4.78046900	-0.15331400	-1.54591900
C	3.55552600	-0.45434300	-0.95011000
C	2.61189500	0.51949100	-0.59643100
C	2.94892200	1.84039100	-0.92030000
C	4.16050600	2.19572500	-1.51471200
C	5.07380100	1.18438900	-1.81856200
H	5.47568100	-0.95037000	-1.78871100
H	4.36920900	3.23727500	-1.73660000
H	6.02272300	1.44097800	-2.28119700
O	2.03268100	2.84354200	-0.65300800
O	3.25714100	-1.78698900	-0.70282500
P	0.56687000	2.28496100	-0.04712800
P	1.76706800	-2.00875400	0.03719800
C	0.44665900	3.37161500	1.50562800
C	-0.61472500	2.79705200	-1.44144200
C	2.34298700	-2.82468500	1.65416200
C	0.92989000	-3.17546600	-1.20087400
H	-1.26445600	-1.61403800	1.58418200
C	-0.94091600	-0.55659600	1.64731200
O	-0.05882300	-0.22435200	2.49276600
O	-2.20011500	0.24164800	1.71832800
C	-5.30144000	-2.08266100	-1.17801900
C	-4.68780200	-1.21799300	-0.28996300
C	-5.37095800	-0.14814000	0.29604700
C	-6.70319400	0.10401800	0.01928100
C	-7.33828900	-0.76656100	-0.88142900
C	-6.65360200	-1.83570900	-1.46725700
H	-4.75981000	-2.91011900	-1.62468600
H	-7.22542500	0.93558100	0.48071200
H	-8.38410400	-0.60369900	-1.12530900
H	-7.17490500	-2.49065700	-2.15931400
O	-4.52019000	0.54032100	1.13131700
O	-3.38448700	-1.22776700	0.16454700
B	-3.29782900	-0.13661100	1.04857700
H	-0.66295100	-0.34593100	0.43164000
Ni	0.92915200	0.06743200	0.15526100
C	-0.04705800	2.16490300	-2.73237400
H	0.06819900	1.07994800	-2.63813700
H	-0.74399300	2.35979200	-3.55740700
H	0.92445300	2.58965400	-3.00035700
C	-2.01354700	2.20590700	-1.17492600
H	-2.46002400	2.56863400	-0.24537900
H	-2.68104600	2.48971400	-1.99874300
H	-1.98227100	1.11235800	-1.13579900
C	-0.71214400	4.32098900	-1.63774500

H	-1.28909000	4.52521700	-2.54921500
H	-1.22995400	4.81072600	-0.80830400
H	0.27393100	4.78035000	-1.75695600
C	0.94857000	4.80888500	1.25326500
H	0.28814200	5.38398300	0.60091200
H	0.98512400	5.32666500	2.22029500
H	1.95486800	4.82045800	0.82709300
C	-0.99181000	3.39789000	2.05625200
H	-0.98449400	3.92721200	3.01784800
H	-1.67598500	3.94044600	1.39430500
H	-1.38830500	2.39480200	2.23083900
C	1.37845700	2.69704100	2.54009800
H	1.02249400	1.69587200	2.79491700
H	2.40915800	2.63134600	2.17239100
H	1.38931600	3.31187000	3.44966200
C	2.98943000	-1.67610500	2.46612200
H	3.84251500	-1.23503700	1.93999700
H	2.26013700	-0.89474300	2.69329400
H	3.35985300	-2.08876900	3.41366500
C	1.15644100	-3.39018100	2.45615400
H	1.53715300	-3.77900000	3.40950500
H	0.42964700	-2.60820900	2.68942200
H	0.66014600	-4.22172100	1.94484900
C	3.40245000	-3.91887400	1.41206500
H	3.82867600	-4.20303500	2.38265900
H	2.98277400	-4.82276400	0.96457400
H	4.21827200	-3.56153500	0.77776100
C	-0.51244000	-3.48474900	-0.75095200
H	-0.99613500	-4.09707900	-1.52320700
H	-0.54874900	-4.05360000	0.18275000
H	-1.11594000	-2.58032800	-0.62600400
C	1.70307100	-4.48664200	-1.43710000
H	1.63457500	-5.16435300	-0.58176800
H	1.26397200	-5.00564000	-2.29902900
H	2.75943600	-4.30600900	-1.65839800
C	0.87588500	-2.38304000	-2.52773400
H	0.33173900	-1.43959600	-2.41309700
H	1.87612600	-2.15887300	-2.90988500
H	0.35129900	-2.98658200	-3.27924000

TSB2-1

	x	y	z
Ni	-0.77945600	0.00004200	0.22102900
P	-1.05586700	2.24571700	0.05182700
P	-1.05649300	-2.24555400	0.05184300
C	-2.24172600	0.00023300	-1.00108500
O	-2.30744300	2.39928600	-1.05607700
C	-1.82536800	3.12951700	1.54571500
C	0.27486200	3.25595600	-0.85037200
O	-2.30818500	-2.39880800	-1.05596800
C	-1.82603100	-3.12924400	1.54575400
C	0.27396700	-3.25602400	-0.85048700
C	-2.81410500	1.18426900	-1.49061900
C	-2.81447800	-1.18365000	-1.49055900
C	-2.34559600	4.53990900	1.20918000
C	-0.83232900	3.18869000	2.72270100
C	-3.01962600	2.23718800	1.95920800
C	1.47387700	3.54082900	0.07505100

C	-0.26368700	4.57523700	-1.43998900
C	0.72662600	2.35479400	-2.02429300
C	-3.02027100	-2.23686900	1.95920400
C	-2.34627400	-4.53964600	1.20929700
C	-0.83298500	-3.18835600	2.72273900
C	0.72594600	-2.35482500	-2.02429100
C	-0.26490800	-4.57509900	-1.44026900
C	1.47288200	-3.54129700	0.07494300
C	-3.87282800	1.21290200	-2.39925800
C	-3.87320900	-1.21199800	-2.39919600
H	-2.97113800	4.88835000	2.04137500
H	-2.95807900	4.55019000	0.30269500
H	-1.53287600	5.26243800	1.09368300
H	-1.34463600	3.62997000	3.58802300
H	0.03877200	3.81505800	2.50872600
H	-0.50677300	2.18249300	2.99745900
H	-3.77036800	2.16157300	1.16634900
H	-3.50180400	2.68537200	2.83763200
H	-2.68569700	1.23276800	2.23171100
H	1.24524200	4.31584100	0.81299600
H	2.31517700	3.90345400	-0.52910900
H	1.80889000	2.64690000	0.60899100
H	-1.16456400	4.41229600	-2.03776700
H	0.50542400	5.00212800	-2.09687000
H	-0.48602700	5.32044800	-0.67323300
H	1.47423800	2.89838400	-2.61663500
H	-0.10893000	2.10888400	-2.68804500
H	1.18628600	1.42526000	-1.68245500
H	-3.50239100	-2.68494000	2.83771600
H	-3.77105600	-2.16135400	1.16637700
H	-2.68633800	-1.23240800	2.23155600
H	-2.95880700	-4.54995700	0.30284500
H	-2.97176600	-4.88806700	2.04153700
H	-1.53355100	-5.26216900	1.09377300
H	-1.34525100	-3.62969900	3.58805400
H	-0.50751800	-2.18213000	2.99750200
H	0.03817500	-3.81463700	2.50875200
H	1.18582800	-1.42544600	-1.68233800
H	-0.10955700	-2.10862900	-2.68800700
H	1.47342300	-2.89851900	-2.61670900
H	-1.16579000	-4.41188000	-2.03796100
H	-0.48736000	-5.32037300	-0.67360600
H	0.50406700	-5.00205900	-2.09726300
H	2.31419300	-3.90386200	-0.52923900
H	1.24408300	-4.31648000	0.81266000
H	1.80793800	-2.64754600	0.60915000
H	-4.26750300	2.16584700	-2.73656500
C	-4.39670700	0.00052300	-2.84971800
H	-4.26818000	-2.16483600	-2.73645900
H	-5.22124700	0.00063500	-3.55717200
H	1.44917400	-0.91696700	2.84474600
H	7.48190200	-0.00066100	-2.26024500
C	6.72624500	-0.00056700	-1.47997800
C	7.12023100	-0.00038900	-0.13872900
C	5.36881700	-0.00062700	-1.84204600
C	6.17511600	-0.00026400	0.90069500
H	8.17796700	-0.00034700	0.10835400
C	4.44758500	-0.00050300	-0.80982400

H	5.05092300	-0.00076500	-2.87968500
C	4.84127600	-0.00032500	0.53243300
H	6.46981800	-0.00012600	1.94503700
O	3.07266700	-0.00052500	-0.88208400
O	3.72564200	-0.00023200	1.33766500
B	2.62331900	-0.00035900	0.45672700
O	1.34850600	-0.00033000	0.83841800
C	0.90551900	-0.00013400	2.55391000
H	1.44949100	0.91654400	2.84464000
O	-0.36333600	0.00008300	2.54164800

TSB3-1

	x	y	z
Ni	1.14689800	-0.00019000	-0.04298200
P	1.48399600	2.26056300	-0.05947700
P	1.48177900	-2.26122500	-0.06086200
C	2.94613000	-0.00125200	0.56023400
O	3.02919500	2.39575500	0.57977300
C	1.74961100	3.10172200	-1.75028100
C	0.53454200	3.33206300	1.18385700
O	3.02663700	-2.39833900	0.57882300
C	1.74717200	-3.10127500	-1.75228000
C	0.53112100	-3.33298500	1.18135800
C	3.64707900	1.18322000	0.82987800
C	3.64581900	-1.18657000	0.82942400
C	2.75881000	4.26563000	-1.65621500
C	0.42230200	3.60133300	-2.35324800
C	2.35026100	2.01605300	-2.67210000
C	-0.94812600	3.47537800	0.78292400
C	1.16265500	4.72807300	1.36497000
C	0.63510900	2.56656700	2.52495800
C	2.34854100	-2.01528000	-2.67324700
C	2.75572600	-4.26580000	-1.65890900
C	0.41967400	-3.59969000	-2.35580300
C	0.63219000	-2.56880500	2.52316900
C	1.15801800	-4.72970600	1.36123600
C	-0.95162300	-3.47473500	0.78017200
C	4.94547700	1.21028000	1.34034100
C	4.94418900	-1.21521200	1.33987600
H	2.94379600	4.64037700	-2.67114500
H	3.71377800	3.94518400	-1.23252000
H	2.38430400	5.10200100	-1.06217000
H	0.60224900	3.88556000	-3.39820200
H	0.05437700	4.49336100	-1.83667000
H	-0.36655700	2.84299700	-2.34543600
H	3.27367700	1.59228500	-2.26267600
H	2.59281600	2.47192500	-3.64067200
H	1.64380400	1.20136800	-2.85003600
H	-1.08298800	4.16556500	-0.05310700
H	-1.50564500	3.87916100	1.63749100
H	-1.40484300	2.52592400	0.49813800
H	2.23503900	4.67164100	1.57336500
H	0.67876900	5.22086300	2.21815600
H	1.00582800	5.36708200	0.49134600
H	0.11723500	3.14892900	3.29778600
H	1.67467200	2.43911200	2.84277600
H	0.15896900	1.58374000	2.47780400
H	2.59110700	-2.47063300	-3.64206100

H	3.27205100	-1.59218100	-2.26334700
H	1.64248600	-1.20016400	-2.85080600
H	3.71088200	-3.94611500	-1.23506200
H	2.94046800	-4.64006900	-2.67406100
H	2.38079900	-5.10230100	-1.06531300
H	0.59959700	-3.88322100	-3.40094900
H	-0.36873100	-2.84088500	-2.34751000
H	0.05116800	-4.49189900	-1.83995100
H	0.15719700	-1.58538500	2.47676200
H	1.67181500	-2.44282400	2.84136500
H	0.11344800	-3.15126500	3.29534100
H	2.23045600	-4.67439600	1.56963700
H	1.00059800	-5.36779800	0.48704500
H	0.67372500	-5.22281800	2.21400300
H	-1.50938600	-3.87946900	1.63413300
H	-1.08692500	-4.16356400	-0.05690300
H	-1.40779500	-2.52459400	0.49681600
H	5.43008800	2.16261000	1.52920300
C	5.58654800	-0.00285500	1.59397500
H	5.42779300	-2.16812900	1.52835500
H	6.59758400	-0.00346600	1.99142300
H	-5.05320200	-0.00078500	5.63987000
C	-4.74415700	-0.00060700	4.59863300
C	-5.71503000	-0.00086100	3.59190200
C	-3.37344400	-0.00012500	4.29243500
C	-5.36144500	-0.00064400	2.23294500
H	-6.76651200	-0.00123300	3.86405300
C	-3.03865100	0.00008500	2.95046700
H	-2.61134000	0.00007500	5.06495500
C	-4.00844100	-0.00016900	1.94406800
H	-6.10429300	-0.00083400	1.44240400
O	-1.78545700	0.00055000	2.37041800
O	-3.39023300	0.00011500	0.71320000
B	-2.02253800	0.00057300	0.98687400
O	-1.02993600	0.00094700	0.08083300
H	-5.81699500	-1.23335800	-4.36216200
C	-5.01946300	-0.69464800	-3.85738700
C	-5.01911700	0.70031600	-3.85704400
C	-3.99978400	-1.42094000	-3.21436600
C	-3.99907900	1.42578800	-3.21366700
H	-5.81638300	1.23966600	-4.36155500
C	-2.99975800	-0.69986000	-2.58470300
H	-3.99122000	-2.50683800	-3.20749900
C	-2.99941000	0.70390500	-2.58435700
H	-3.98997400	2.51167800	-3.20626900
O	-1.91244700	-1.17385400	-1.90810500
O	-1.91187600	1.17703000	-1.90750700
B	-1.17156700	0.00128800	-1.43400100
H	0.01520900	0.00105900	-1.80070800

TSB4-1

	x	y	z
Ni	-1.38268300	-0.18455100	-0.15264100
P	-2.09628200	1.72117900	-1.02039900
P	-1.17506000	-2.29803900	0.46621800
C	-3.14247700	-0.77514200	-0.65449300
O	-3.68078800	1.39162200	-1.50289600
C	-2.43080000	3.20265900	0.12878000

C	-1.35070600	2.22424500	-2.68894500
O	-2.68802800	-2.97788600	0.14993400
C	-1.03338100	-2.72379100	2.31471800
C	-0.08550900	-3.39168000	-0.63550600
C	-4.06652200	0.08007400	-1.26395300
C	-3.57405000	-2.08898200	-0.44366300
C	-3.67843800	4.00339900	-0.29888000
C	-1.21527600	4.14428500	0.21512800
C	-2.69620700	2.58078700	1.51915000
C	0.14508600	2.56258600	-2.53631900
C	-2.10405000	3.39361700	-3.35062000
C	-1.48163900	0.97448500	-3.59029400
C	-1.71096500	-1.54540700	3.05147600
C	-1.78238500	-4.02318800	2.67609300
C	0.43641300	-2.82931100	2.76291500
C	-0.61850700	-3.19610200	-2.07357700
C	-0.17160100	-4.88667800	-0.27642300
C	1.37564700	-2.90377200	-0.58421300
C	-5.34932200	-0.31948500	-1.64277300
C	-4.84322000	-2.54740900	-0.80054100
H	-3.84795800	4.79838600	0.43929200
H	-4.57118800	3.37528500	-0.33627300
H	-3.55752400	4.47987400	-1.27514400
H	-1.38568800	4.86252000	1.02841700
H	-1.08233500	4.72516500	-0.70317800
H	-0.28590300	3.61087600	0.42861100
H	-3.52858000	1.86883500	1.49214400
H	-2.95995400	3.37790000	2.22666600
H	-1.81322600	2.06287800	1.90622100
H	0.31420600	3.46470000	-1.94334900
H	0.56834400	2.74056800	-3.53377800
H	0.70457100	1.74394200	-2.07664500
H	-3.17817000	3.19625100	-3.41959100
H	-1.72094300	3.53338800	-4.37001100
H	-1.95473800	4.33669600	-2.81639400
H	-1.05109300	1.20225900	-4.57384500
H	-2.52519600	0.68042600	-3.73564800
H	-0.93667700	0.11979500	-3.17590400
H	-1.70405600	-1.74415000	4.13122600
H	-2.75427400	-1.42090700	2.74094100
H	-1.18552900	-0.60157700	2.87699300
H	-2.83838900	-3.97178000	2.40182500
H	-1.71643700	-4.16978700	3.76229400
H	-1.34961600	-4.90498500	2.19727400
H	0.46482100	-2.88875300	3.85915300
H	1.03137100	-1.96471000	2.45928400
H	0.91671100	-3.73528600	2.37950700
H	-0.58568500	-2.14527900	-2.37940500
H	-1.64739600	-3.55162600	-2.18033000
H	0.01340800	-3.76783000	-2.76521900
H	-1.20769900	-5.23880000	-0.25840100
H	0.29025400	-5.10954300	0.69000400
H	0.36730100	-5.46792800	-1.03623800
H	1.96948900	-3.48791600	-1.29933900
H	1.82910300	-3.03099000	0.40237300
H	1.45547100	-1.84942500	-0.86226500
H	-6.02732300	0.38612400	-2.11226200
C	-5.72425700	-1.64392300	-1.40106900

H	-5.12671000	-3.57838300	-0.61407500
H	-6.71814600	-1.97784700	-1.68698000
H	8.28748100	-1.04499800	-3.40129800
C	7.56331800	-0.73770800	-2.65246200
C	7.99878400	-0.43088800	-1.35918700
C	6.20689900	-0.65673900	-3.00670400
C	7.09785400	-0.02886700	-0.35989700
H	9.05561700	-0.50368400	-1.11965800
C	5.32926500	-0.26016400	-2.01370000
H	5.85775700	-0.89168900	-4.00669200
C	5.76500600	0.04674800	-0.72157100
H	7.42310500	0.21219200	0.64659700
O	3.96077000	-0.09864700	-2.08407100
O	4.67951600	0.40949300	0.04984100
B	3.58296600	0.31355900	-0.80705200
O	2.30468700	0.58753300	-0.48814300
H	1.40508000	1.44412100	6.25973200
C	1.39628300	1.64015900	5.19142700
C	1.07549600	2.91919600	4.72801100
C	1.71200600	0.59943200	4.30242100
C	1.05646900	3.21477400	3.35495100
H	0.83851200	3.70344300	5.44115600
C	1.68829600	0.90119800	2.95145800
H	1.97123500	-0.39393400	4.65315300
C	1.36784600	2.18157500	2.48737100
H	0.81803300	4.20701600	2.98664200
O	1.96826200	0.08337100	1.88230800
O	1.44189900	2.20434100	1.11500900
B	1.73726500	0.87626900	0.73802800
H	0.03998700	0.30186400	0.25369200

TSC1

	x	y	z
Ni	-0.00000400	-0.38367100	0.16923600
P	-2.21625900	-0.10378100	0.10621600
P	2.21625700	-0.10378800	0.10622600
C	0.00000600	1.43299200	-0.39982000
O	-2.39268600	1.51488300	-0.32049500
C	-3.17993900	-0.90971000	-1.32018000
C	-3.12077600	-0.09875600	1.77502500
O	2.39269900	1.51487100	-0.32049700
C	3.17995700	-0.90969400	-1.32017100
C	3.12072400	-0.09876200	1.77506200
C	-1.18599800	2.16211900	-0.55069800
C	1.18601400	2.16211400	-0.55069500
C	-4.60104100	-0.33465100	-1.47543900
C	-3.23327900	-2.44334600	-1.17284700
C	-2.35972300	-0.57374200	-2.58945500
C	-3.28003500	-1.53866200	2.30083800
C	-4.48695700	0.61372100	1.74328300
C	-2.18584500	0.68123500	2.72878800
C	2.35956300	-0.57400600	-2.58940600
C	4.60093500	-0.33437600	-1.47563000
C	3.23360000	-2.44330000	-1.17266700
C	2.18609200	0.68186200	2.72860000
C	4.48722900	0.61308600	1.74322800
C	3.27932100	-1.53862300	2.30120600
C	-1.21578100	3.51309600	-0.89919200

C	1.21580200	3.51309200	-0.89918600
H	-5.00254600	-0.66171700	-2.44325000
H	-4.60962000	0.75930100	-1.46266400
H	-5.28335400	-0.70181800	-0.70375100
H	-3.78276900	-2.85112200	-2.03179300
H	-3.76339200	-2.76524900	-0.27108800
H	-2.22573200	-2.86839900	-1.19060100
H	-2.29761700	0.50467000	-2.76551100
H	-2.86298400	-1.02642900	-3.45361500
H	-1.35160600	-0.99129500	-2.52824200
H	-4.01650400	-2.10959200	1.72762000
H	-3.62978200	-1.50368800	3.34067900
H	-2.33171200	-2.08768200	2.28819800
H	-4.41671500	1.60508600	1.28649700
H	-4.84214100	0.74244800	2.77414500
H	-5.24513800	0.03782500	1.20814500
H	-2.64520200	0.72070600	3.72496100
H	-2.02596900	1.70993500	2.39054500
H	-1.20902900	0.19640500	2.82256600
H	2.86285800	-1.02664600	-3.45357100
H	2.29721700	0.50438100	-2.76554000
H	1.35154400	-0.99177700	-2.52807100
H	4.60929300	0.75957800	-1.46295000
H	5.00239500	-0.66144700	-2.44345700
H	5.28340500	-0.70133200	-0.70398400
H	3.78305300	-2.85108200	-2.03163300
H	2.22613200	-2.86854300	-1.19024500
H	3.76388900	-2.76499700	-0.27093600
H	1.20899600	0.19758500	2.82232500
H	2.02683000	1.71059900	2.39018800
H	2.64534500	0.72121300	3.72482500
H	4.41751100	1.60431100	1.28605400
H	5.24521800	0.03662600	1.20842100
H	4.84233900	0.74205000	2.77408600
H	3.62911000	-1.50357000	3.34103100
H	4.01551000	-2.11003100	1.72810600
H	2.33074900	-2.08721300	2.28870700
H	-2.16603400	4.02475100	-1.01325400
C	0.00001200	4.17688300	-1.07944700
H	2.16605700	4.02474400	-1.01324700
H	0.00001400	5.22883500	-1.35151100
H	-0.00001600	-1.79339200	0.92893600
H	-0.91002100	-3.34371600	0.58531300
C	0.00004100	-2.91658000	0.10999500
H	0.91006000	-3.34368600	0.58541600
O	0.00010800	-2.70178700	-1.15153900

TSC2-1

	x	y	z
Ni	0.64159500	0.00003700	0.11936400
P	0.93925800	2.24969500	-0.02386000
P	0.93977800	-2.24954100	-0.02387000
O	-1.22970900	-0.00030300	1.23875000
C	2.52759400	0.00025300	-0.12729200
O	2.60842300	2.39697700	-0.13103300
C	0.42813600	3.10845500	-1.64387600
C	0.62863500	3.27833300	1.53726500
O	2.60896500	-2.39645400	-0.13111200

C	0.42877700	-3.10847500	-1.64383800
C	0.62943600	-3.27819000	1.53729200
C	3.27532200	1.18493200	-0.19400500
C	3.27559100	-1.18425600	-0.19404600
C	1.29985200	4.34523300	-1.94467200
C	-1.06206500	3.50114800	-1.64154800
C	0.67299000	2.05818000	-2.75219900
C	-0.87966600	3.50702700	1.76334100
C	1.37145400	4.62901000	1.52277900
C	1.20115900	2.41442500	2.68616400
C	0.67329900	-2.05816200	-2.75219600
C	1.30081000	-4.34502500	-1.94464700
C	-1.06132200	-3.50155000	-1.64141000
C	1.20203700	-2.41424900	2.68613200
C	1.37231800	-4.62883300	1.52274400
C	-0.87882700	-3.50695800	1.76352600
C	4.66495200	1.21338900	-0.31847500
C	4.66522800	-1.21239500	-0.31851500
H	1.04820800	4.70739600	-2.94979600
H	2.36686700	4.10872800	-1.92564900
H	1.11530200	5.16668600	-1.24820600
H	-1.34865400	3.77568500	-2.66516900
H	-1.24918600	4.37513300	-1.01042400
H	-1.72228100	2.69311600	-1.31331700
H	1.71353700	1.71721100	-2.77565000
H	0.44758500	2.51392700	-3.72486000
H	0.02508600	1.18610900	-2.62950000
H	-1.27020000	4.29705600	1.11676800
H	-1.03744100	3.82708200	2.80142600
H	-1.47542800	2.60896700	1.58739700
H	2.43202900	4.51112400	1.28357700
H	1.29674600	5.08045800	2.52071500
H	0.92912600	5.33573100	0.81551500
H	1.07507500	2.95454700	3.63317600
H	2.26955400	2.21573000	2.55252700
H	0.68130000	1.45608000	2.76976500
H	0.44792200	-2.51397100	-3.72483300
H	1.71376600	-1.71695600	-2.77573300
H	0.02520500	-1.18624100	-2.62945000
H	2.36776100	-4.10822700	-1.92567900
H	1.04921500	-4.70727900	-2.94975000
H	1.11652500	-5.16651100	-1.24815000
H	-1.34790900	-3.77617000	-2.66500900
H	-1.72173100	-2.69368800	-1.31314500
H	-1.24817300	-4.37558200	-1.01026800
H	0.68212300	-1.45594000	2.76982900
H	2.27039900	-2.21547500	2.55236400
H	1.07611300	-2.95439800	3.63315000
H	2.43286400	-4.51091500	1.28342200
H	0.92993800	-5.33559400	0.81555200
H	1.29774700	-5.08026000	2.52069900
H	-1.03647100	-3.82713400	2.80159400
H	-1.26942300	-4.29691500	1.11690500
H	-1.47460900	-2.60888200	1.58775400
H	5.18278400	2.16593500	-0.36408300
C	5.35261400	0.00057600	-0.37948900
H	5.18327400	-2.16482400	-0.36415000
H	6.43467400	0.00070100	-0.47623800

H	-7.52973900	1.23609200	-0.54422500
C	-6.59097000	0.69696700	-0.44844000
C	-6.59090300	-0.69787900	-0.44852200
C	-5.39097800	1.42247600	-0.32737000
C	-5.39084100	-1.42328600	-0.32753700
H	-7.52962100	-1.23708300	-0.54437000
C	-4.21313500	0.70252400	-0.20981500
H	-5.38044800	2.50851500	-0.32520700
C	-4.21306700	-0.70323400	-0.20989600
H	-5.38020400	-2.50932500	-0.32550000
O	-2.94281100	1.17687500	-0.07888900
O	-2.94270300	-1.17747900	-0.07901700
B	-2.04736200	-0.00026900	0.01562000
H	-1.16693000	-0.00018200	-0.88061500
C	-1.87205500	-0.00022500	2.50682000
H	-2.50197800	-0.88950100	2.62659200
H	-1.10771500	-0.00048300	3.28994500
H	-2.50153200	0.88934600	2.62673500

TSC3-1

	x	y	z
Ni	-0.49390100	0.30331700	0.13132100
P	-2.10086400	-1.26321200	-0.05623800
P	0.66789800	2.19950100	0.04927200
C	-1.85488000	1.41676000	-0.64777500
O	-3.37741600	-0.41841600	-0.76733700
C	-1.89422300	-2.64650700	-1.35279100
C	-2.98652200	-1.83266700	1.52501900
O	-0.41898900	3.32377000	-0.57732100
C	2.05934100	2.32820700	-1.24410200
C	1.07893600	3.07931100	1.67970700
C	-3.11613000	0.92079700	-0.99436500
C	-1.65216800	2.77823300	-0.89979800
C	-3.21969900	-2.95374800	-2.08033100
C	-1.32964100	-3.94151000	-0.73907500
C	-0.88327300	-2.08841700	-2.38099700
C	-2.11321800	-2.78612300	2.36226700
C	-4.34806700	-2.48911200	1.22500600
C	-3.22161300	-0.53447300	2.33252900
C	1.74399900	1.25201700	-2.30835500
C	2.08198300	3.70920000	-1.93087700
C	3.43553400	2.03455700	-0.61972100
C	-0.24307500	3.05838500	2.48289900
C	1.51109300	4.54213500	1.46168500
C	2.15710700	2.32137200	2.47767200
C	-4.12539400	1.70608700	-1.55533600
C	-2.62094800	3.61384100	-1.45736900
H	-3.01936200	-3.70591400	-2.85462100
H	-3.63539700	-2.06693500	-2.56358300
H	-3.98038200	-3.36372800	-1.41099300
H	-1.07299000	-4.62774800	-1.55726700
H	-2.06825200	-4.45096500	-0.11293700
H	-0.42002900	-3.77001000	-0.15887200
H	-1.23050100	-1.14921600	-2.82633000
H	-0.76037900	-2.81663000	-3.19362900
H	0.09702000	-1.91725900	-1.92768400
H	-2.04001300	-3.78017400	1.91432900
H	-2.57904700	-2.90791100	3.34935500

H	-1.09709000	-2.41131000	2.50688800
H	-4.97184400	-1.86240500	0.58157100
H	-4.88253900	-2.64330200	2.17173200
H	-4.23397900	-3.47058600	0.75493400
H	-3.74146800	-0.78722900	3.26575800
H	-3.83913400	0.18558900	1.78699700
H	-2.27644800	-0.04705100	2.59515800
H	2.49050700	1.31346400	-3.11075400
H	0.75587900	1.39996700	-2.75757900
H	1.78407400	0.24254000	-1.88814000
H	1.13959300	3.92562500	-2.43910300
H	2.88406600	3.70809800	-2.68053000
H	2.28337900	4.52463300	-1.23127000
H	4.16741100	1.89609600	-1.42525800
H	3.43295400	1.12414600	-0.01638000
H	3.78444200	2.86598000	0.00080600
H	-0.57149000	2.03479100	2.69413100
H	-1.05110200	3.57421600	1.95577100
H	-0.08441400	3.56697700	3.44234700
H	0.78240300	5.09641100	0.86332900
H	2.48898600	4.61269400	0.97552600
H	1.59589200	5.03797500	2.43761200
H	2.19272100	2.72843500	3.49667900
H	3.15320800	2.43408100	2.04471000
H	1.94375500	1.25296200	2.54895000
H	-5.08567000	1.26481000	-1.80229200
C	-3.86093900	3.05851100	-1.78226100
H	-2.40410800	4.66316100	-1.62967300
H	-4.63147700	3.68844700	-2.21849200
O	1.11200600	-2.05756600	2.50762800
C	1.33068500	-1.26447600	3.65576100
H	2.38198800	-0.96541000	3.74576200
H	0.70473600	-0.36071600	3.63747200
H	1.05331600	-1.85897800	4.53183200
H	6.28267600	-1.87588100	-1.86227700
C	5.29384000	-2.06880300	-1.45570100
C	4.86008200	-1.34071700	-0.33369500
C	4.47805200	-3.03311700	-2.05086900
C	3.59415400	-1.61990600	0.15442500
H	5.49133100	-0.59590200	0.14065600
C	3.19729800	-3.31562200	-1.54468100
H	4.83823600	-3.58133000	-2.91687700
C	2.78028000	-2.59715300	-0.43612100
O	2.94753200	-1.05521100	1.22316600
H	2.56088200	-4.07340100	-1.99070200
O	1.60344700	-2.70200900	0.25012000
B	1.66682400	-1.71409900	1.28890000
H	0.64905000	-0.58472500	0.76938100

TSD1-1

	x	y	z
C	-5.78891100	-0.40044700	-0.86218400
C	-4.48318600	0.04113800	-0.64460100
C	-3.42553500	-0.80887600	-0.29091800
C	-3.76655200	-2.16326200	-0.15786000
C	-5.05613700	-2.65678800	-0.36079200
C	-6.06436600	-1.76050800	-0.71674500
H	-6.55965400	0.31238600	-1.13663500

H	-5.25091600	-3.71755900	-0.24135100
H	-7.07454200	-2.12501700	-0.88063600
O	-2.77981700	-3.06741200	0.18813800
O	-4.23149900	1.39410000	-0.78909100
P	-1.27957500	-2.36725200	0.46929600
P	-2.65306100	1.84086600	-0.43745300
C	-1.08268200	-2.75630000	2.32322200
C	-0.21273600	-3.45883700	-0.65722600
C	-2.94818800	2.95913500	1.07772300
C	-2.25964700	2.79855400	-2.02678900
H	1.87812500	1.46251300	-1.55506800
C	1.27926500	0.56139700	-1.71700800
O	0.41049900	0.35585600	-0.64470500
O	2.13397500	-0.56325200	-1.91196900
C	6.59798400	0.90510800	-0.76659000
C	5.47444500	0.18062200	-1.11916800
C	5.51980100	-1.19847300	-1.34102200
C	6.69596600	-1.91819000	-1.22991600
C	7.84667000	-1.19367800	-0.87885900
C	7.79824100	0.18541200	-0.65081000
H	6.54229900	1.97171700	-0.57870700
H	6.72030200	-2.98871300	-1.40474400
H	8.79209000	-1.71922600	-0.77981400
H	8.70632200	0.71358000	-0.37489300
O	4.25641400	-1.65356300	-1.66273300
O	4.18224700	0.62893300	-1.30916300
B	3.45321500	-0.51520500	-1.62557800
H	0.68785200	0.65477900	-2.63085100
Ni	-1.64205300	-0.18193700	-0.08243500
C	-0.41118900	-2.88449100	-2.07897200
H	-0.01697800	-1.87149200	-2.16284000
H	0.13386300	-3.51421600	-2.79342800
H	-1.46746200	-2.88442300	-2.37116700
C	1.27229800	-3.37607700	-0.25257900
H	1.47475500	-3.96442100	0.64826200
H	1.88702800	-3.78954400	-1.06107200
H	1.60922600	-2.35102600	-0.08435400
C	-0.67916800	-4.92979000	-0.66972300
H	-0.08248400	-5.46859600	-1.41696400
H	-0.53154900	-5.43100000	0.28873600
H	-1.73247300	-5.02033100	-0.94702300
C	-1.24503800	-4.26049700	2.61851800
H	-0.37819700	-4.83843700	2.28620100
H	-1.32730100	-4.39613400	3.70471300
H	-2.14584500	-4.67712500	2.15853400
C	0.26803700	-2.25834400	2.87158900
H	0.27206600	-2.40190800	3.96012400
H	1.11469600	-2.81594900	2.46439700
H	0.44249900	-1.20021900	2.66996300
C	-2.22429200	-1.98755600	3.02759300
H	-2.14679900	-0.90804200	2.87015100
H	-3.21207100	-2.31685400	2.69095400
H	-2.15667900	-2.17479900	4.10673200
C	-3.00889900	2.00820300	2.29497200
H	-3.78564500	1.24376700	2.18316100
H	-2.05069100	1.50822500	2.46084300
H	-3.24514600	2.59674000	3.19079500
C	-1.79827700	3.96513600	1.28014100

H	-1.91015900	4.42420100	2.27092300
H	-0.80990100	3.49804800	1.23615300
H	-1.83697500	4.77477600	0.54461400
C	-4.29349400	3.70891400	0.97946800
H	-4.44717200	4.26037800	1.91596800
H	-4.31149900	4.43679200	0.16477800
H	-5.13445900	3.02437400	0.84466700
C	-0.87297500	3.46946700	-1.95273400
H	-0.55923900	3.74777000	-2.96699700
H	-0.89475500	4.38396800	-1.35558900
H	-0.10938400	2.81986700	-1.52232000
C	-3.33339400	3.85103700	-2.36456600
H	-3.30210900	4.70295500	-1.67927400
H	-3.14145900	4.23923600	-3.37347800
H	-4.34102500	3.42621600	-2.35261800
C	-2.25803800	1.72053000	-3.13686900
H	-1.51376200	0.93969000	-2.95120600
H	-3.23565000	1.23891200	-3.23668800
H	-2.01706000	2.19762800	-4.09521200
C	2.95519400	3.55473700	1.72804100
C	2.27824400	2.39188700	1.40216900
C	2.80666400	1.12618500	1.70399400
C	4.02741400	0.99052900	2.34383200
C	4.72102000	2.16800800	2.68151600
C	4.19667300	3.42477500	2.37895800
H	2.53768800	4.52811700	1.48756300
H	4.43014300	0.00816600	2.57124700
H	5.67939100	2.09124400	3.18806000
H	4.74885000	4.32000400	2.65245400
O	1.96315900	0.14420600	1.27353200
O	1.07242600	2.26246600	0.77495200
B	0.76785500	0.81617800	0.72612600
H	-0.27700800	0.53149700	1.35421600

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	x	y	z
C	5.77163800	1.33403600	-0.76731800
C	4.57374400	0.64063000	-0.58611000
C	3.37335700	1.26258800	-0.22779600
C	3.42936200	2.64892600	-0.04902700
C	4.59676900	3.39605100	-0.21538300
C	5.76479500	2.71909800	-0.57819800
H	6.67688400	0.80390700	-1.04596700
H	4.58717600	4.47096800	-0.06512800
H	6.68551100	3.28024100	-0.71457400
O	2.26028600	3.30646600	0.31307500
O	4.56497500	-0.73732800	-0.76582100
P	0.94711100	2.26045100	0.50991500
P	3.05760300	-1.43698500	-0.45667300
C	0.55187900	2.56251300	2.34002400
C	-0.29355200	3.07749700	-0.67259800
C	3.50317600	-2.56069600	1.00606900
C	2.82557400	-2.38325200	-2.08901300
H	-2.77894100	-2.08203400	-2.42644200
C	-2.10153700	-1.24081900	-2.61218800
O	-1.01073200	-1.26773800	-1.73141100
O	-2.81251900	-0.01596600	-2.52651400
C	-7.04732600	-1.10942600	-0.45685100

C	-5.94994200	-0.47649800	-1.01127900
C	-5.88014100	0.91388100	-1.13586700
C	-6.90749000	1.73781100	-0.71268300
C	-8.02844600	1.10778500	-0.14800400
C	-8.09683800	-0.28335500	-0.02257500
H	-7.08826000	-2.18953000	-0.36423200
H	-6.84358300	2.81594600	-0.81532600
H	-8.85842900	1.71701600	0.19774900
H	-8.97865300	-0.73779700	0.41942800
O	-4.67868600	1.26267900	-1.71911300
O	-4.79327300	-1.03682700	-1.51782000
B	-4.02617900	0.05188700	-1.93490500
H	-1.68933200	-1.29986600	-3.62078200
Ni	1.74216800	0.27290500	0.00568400
C	0.02237700	2.47315200	-2.06049600
H	-0.16400100	1.39592500	-2.08137200
H	-0.62640800	2.94379400	-2.81051000
H	1.06275600	2.65365500	-2.35337200
C	-1.74353700	2.73237600	-0.28620500
H	-2.06049600	3.26234200	0.61825800
H	-2.41443500	3.03960000	-1.09735800
H	-1.89311200	1.66085300	-0.13248400
C	-0.11665800	4.60761000	-0.74925800
H	-0.81044600	4.99830600	-1.50520100
H	-0.34530100	5.10573600	0.19609400
H	0.89919000	4.88275800	-1.04255100
C	0.20233200	4.02969400	2.65128700
H	-0.75842400	4.32669700	2.22066200
H	0.12524900	4.15590000	3.73942900
H	0.97491300	4.71496100	2.28884500
C	-0.58528100	1.62674200	2.79444200
H	-0.72655400	1.73793800	3.87758700
H	-1.53831500	1.85608700	2.31136100
H	-0.34908400	0.57858900	2.59014300
C	1.83658100	2.18421800	3.11201600
H	2.11973600	1.14113100	2.93727200
H	2.68221400	2.81987700	2.83470100
H	1.65359500	2.30857800	4.18718400
C	4.07860100	-1.62527700	2.09346700
H	5.00509900	-1.14342000	1.76866500
H	3.36624400	-0.84190500	2.37207400
H	4.29745800	-2.21828900	2.99084600
C	2.22763100	-3.22874800	1.55480600
H	2.48966100	-3.81446100	2.44601400
H	1.47810800	-2.48639900	1.84228500
H	1.76319800	-3.90633800	0.83406600
C	4.56114000	-3.62419000	0.65896900
H	4.87149100	-4.13431500	1.58069400
H	4.17157400	-4.38886700	-0.01977300
H	5.45256600	-3.17670800	0.20846400
C	1.81764600	-3.53752800	-1.93350400
H	1.58457900	-3.93598500	-2.92984900
H	2.22841100	-4.36369300	-1.34394900
H	0.87806000	-3.21823500	-1.47692600
C	4.15316600	-2.91905400	-2.66318700
H	4.59078200	-3.70808900	-2.04729100
H	3.95381000	-3.34740000	-3.65443000
H	4.89331500	-2.12378600	-2.77798200

C	2.25386600	-1.33379000	-3.07150200
H	1.28117500	-0.96158600	-2.73836600
H	2.93257300	-0.48223700	-3.19275300
H	2.12609100	-1.80102000	-4.05737100
C	-1.57144000	-3.55319400	2.48940900
C	-1.57535500	-2.62696400	1.46002400
C	-2.35788800	-1.46900200	1.51653500
C	-3.17500000	-1.18893100	2.59761600
C	-3.17907100	-2.12248700	3.64692400
C	-2.39374800	-3.27807200	3.59413600
H	-0.96517800	-4.45143000	2.43513600
H	-3.78557800	-0.29237800	2.62472700
H	-3.80674200	-1.94058500	4.51445900
H	-2.41976400	-3.98100400	4.42182800
O	-2.17409400	-0.73873800	0.36410000
O	-0.89308100	-2.66259100	0.26819200
B	-1.20128900	-1.44596700	-0.37526500
H	0.41024500	-0.50595500	0.17150100

TSE1-1

	x	y	z
C	-5.91449400	-1.64962500	-0.06048100
C	-4.54374900	-1.42555800	-0.18926500
C	-3.94089800	-0.19230800	0.08247100
C	-4.79313400	0.83091100	0.51126400
C	-6.17042500	0.66378400	0.65938500
C	-6.71780100	-0.58813200	0.36577900
H	-6.33383600	-2.62550300	-0.28280000
H	-6.78975100	1.49062600	0.99160700
H	-7.78822700	-0.73995900	0.47326400
O	-4.23536500	2.07009300	0.79831100
O	-3.72768400	-2.47463500	-0.59630500
P	-2.59707700	2.16496300	0.41544500
P	-2.08943300	-2.09164100	-0.51983800
C	-2.64636100	3.43654800	-0.99307800
C	-1.91655500	2.83482600	2.05490800
C	-1.53560700	-2.68777500	-2.23137600
C	-1.51823100	-3.19915600	0.90825000
H	1.02837700	0.21097800	-1.48560900
C	0.92254000	0.84819100	-0.62261300
O	2.38904400	1.91533800	-1.70554300
O	1.57467000	0.56256400	0.52103200
C	4.70123000	-2.62527200	2.31230700
C	3.85385000	-1.90466000	1.48954500
C	3.60282800	-2.29025900	0.16893200
C	4.18718700	-3.41119400	-0.39151300
C	5.05021600	-4.15042600	0.43388900
C	5.30088700	-3.76651600	1.75493700
H	4.88902400	-2.31704600	3.33543800
H	3.99255800	-3.69425900	-1.42065000
H	5.53577600	-5.03523700	0.03294100
H	5.97627200	-4.35936500	2.36473500
O	2.71438400	-1.39987600	-0.40350100
O	3.13867300	-0.76126600	1.77952100
B	2.50693800	-0.44368200	0.58724700
H	0.52265100	1.83701100	-0.69899500
Ni	-2.05776300	0.07552000	-0.11004300
C	-1.83045400	1.59991400	2.98262800

H	-1.14000800	0.84630600	2.58944900
H	-1.45937900	1.91623600	3.96575100
H	-2.81033300	1.13270800	3.12920300
C	-0.50439700	3.42356200	1.87117400
H	-0.50388400	4.32335100	1.24825700
H	-0.11305200	3.71075500	2.85516300
H	0.20002800	2.70081100	1.44802800
C	-2.84934700	3.87485300	2.70770800
H	-2.47051700	4.09809500	3.71333900
H	-2.88233000	4.81599400	2.15498200
H	-3.86994600	3.49624200	2.80555500
C	-3.16936800	4.81375900	-0.54446500
H	-2.45551500	5.33735500	0.09852800
H	-3.32500200	5.43899300	-1.43303500
H	-4.12589200	4.73529500	-0.01882800
C	-1.25501500	3.58119000	-1.64122800
H	-1.31887400	4.31199400	-2.45693900
H	-0.48775800	3.94094800	-0.94960800
H	-0.90963200	2.64045900	-2.08063500
C	-3.61755300	2.85047100	-2.04459900
H	-3.30542300	1.85550900	-2.37993900
H	-4.63908800	2.77748100	-1.66153200
H	-3.62784900	3.51270500	-2.91935000
C	-1.89176600	-1.52839200	-3.19131000
H	-2.96043600	-1.28950100	-3.15885600
H	-1.32945200	-0.61824600	-2.95733300
H	-1.64449300	-1.82283900	-4.21901300
C	-0.01526200	-2.93372900	-2.26796400
H	0.29271000	-3.09339600	-3.30892200
H	0.56600600	-2.09132100	-1.88087100
H	0.26947800	-3.82749400	-1.70379900
C	-2.29017800	-3.95321500	-2.68791500
H	-1.99894000	-4.17812600	-3.72200400
H	-2.04814700	-4.82821500	-2.08037800
H	-3.37284600	-3.80750900	-2.66262100
C	-0.05069900	-2.88134200	1.25574600
H	0.24286200	-3.47174100	2.13279900
H	0.64084400	-3.12940300	0.44719700
H	0.08169600	-1.82416400	1.50813300
C	-1.68977900	-4.70154200	0.61857300
H	-0.99801700	-5.05749400	-0.15066000
H	-1.47534100	-5.26694000	1.53462200
H	-2.71235400	-4.94162800	0.31094600
C	-2.40355400	-2.81962200	2.11815600
H	-2.32764100	-1.75496200	2.36211500
H	-3.45713000	-3.05655900	1.94596600
H	-2.06486900	-3.39078800	2.99163200
C	7.07103600	3.00238400	-1.22435000
C	5.80275700	2.45536300	-1.11313100
C	5.53683400	1.41241800	-0.21366300
C	6.52065400	0.88178000	0.60210600
C	7.80983800	1.43346400	0.49440700
C	8.07836500	2.47203300	-0.39971800
H	7.26892900	3.80873400	-1.92365300
H	6.30287100	0.07127300	1.29057000
H	8.60805100	1.04131200	1.11889700
H	9.08385300	2.87971700	-0.46245800
O	4.21549800	1.06289700	-0.31204600

O	4.67094900	2.79203300	-1.79323700
B	3.62786100	1.93150300	-1.32093600
H	-0.47790000	0.25975900	-0.27388700

TSF1-1

	x	y	z
H	0.06184600	3.20186900	1.32806700
C	0.53243000	3.30299500	0.34312100
O	1.71657100	2.87128300	0.12672600
H	0.09978200	4.05559500	-0.32649100
C	3.20441800	-1.36811000	1.46946300
C	2.57887800	-0.40023700	0.70423000
C	2.85608900	-0.24764100	-0.66050800
C	3.76948300	-1.05547000	-1.31323500
C	4.41056900	-2.04188400	-0.54492700
C	4.13406000	-2.19463300	0.81587900
H	2.98242700	-1.47801400	2.52603200
H	3.97570100	-0.92683700	-2.37081500
H	5.13517500	-2.69599600	-1.02156000
H	4.64683500	-2.96585700	1.38374500
O	2.09517000	0.77359800	-1.17650000
O	1.63811300	0.52303000	1.08980600
B	1.39190600	1.31037900	-0.07291600
C	-4.67775000	0.27069200	0.19279400
C	-3.30679700	0.30077400	0.01733700
C	-2.55923700	-0.86082800	-0.18617700
C	-3.14481000	-2.11267600	-0.22435800
C	-4.53631400	-2.15783900	-0.04713800
C	-5.28516500	-0.99418300	0.15649700
H	-5.24824600	1.17998500	0.34937600
H	-2.55284800	-3.00762400	-0.38268000
H	-5.03999400	-3.11963200	-0.06913800
H	-6.36041900	-1.06739500	0.28955200
O	-1.22377500	-0.52631600	-0.32856900
O	-2.45774900	1.39596100	0.00728800
B	-1.19813200	0.85204300	-0.20688000
O	-0.08386100	1.63319900	-0.29937100

[NijH

	x	y	z
C	-1.22109900	-3.51585100	-0.02484800
C	-1.18958100	-2.12031600	-0.02485300
C	0.00001400	-1.38688200	-0.00026100
C	1.18962800	-2.12029200	0.02405600
C	1.22118100	-3.51582700	0.02362700
C	0.00004900	-4.19874400	-0.00070700
H	-2.16647300	-4.04903800	-0.04347300
H	2.16656800	-4.04899700	0.04206800
H	0.00006400	-5.28567900	-0.00086900
O	2.38977400	-1.40944800	0.04956600
O	-2.38974800	-1.40949600	-0.05023700
P	2.14878700	0.26828800	0.00472700
P	-2.14879100	0.26822500	-0.00470000
C	3.07979000	0.77612300	1.57732700
C	3.06319000	0.70826100	-1.59668700
C	-3.06308500	0.70756500	1.59696000
C	-3.07990900	0.77674200	-1.57697900
H	-0.00008900	2.05121300	0.00015000

Ni	-0.00001300	0.53006900	0.00003100
C	2.36253200	-0.11551200	-2.70223700
H	1.29012200	0.10054400	-2.74975900
H	2.80468300	0.14413400	-3.67280300
H	2.48679000	-1.19097400	-2.54733300
C	4.55966300	0.34815500	-1.58184600
H	4.96886900	0.47147300	-2.59335200
H	5.13560100	1.00120600	-0.91878000
H	4.72390600	-0.69076700	-1.27934400
C	2.87444900	2.20789500	-1.90690800
H	3.29480800	2.42176300	-2.89842700
H	1.81626000	2.48674200	-1.91392600
H	3.38721200	2.85231800	-1.18715500
C	4.38152900	-0.01748500	1.80429700
H	5.15145600	0.21785800	1.06584200
H	4.78396400	0.23909800	2.79320700
H	4.20086500	-1.09540700	1.77997500
C	3.36432400	2.29014800	1.56801700
H	3.71769300	2.59474700	2.56175800
H	4.14559800	2.55840800	0.84967300
H	2.46553900	2.87299600	1.33870500
C	2.10342200	0.45863000	2.73414400
H	1.17625000	1.03427500	2.64413100
H	1.84536800	-0.60502800	2.76749700
H	2.57940500	0.72068000	3.68837300
C	-2.36219500	-0.11641500	2.70220900
H	-2.48625000	-1.19185500	2.54698800
H	-1.28982600	0.09983400	2.74972700
H	-2.80433400	0.14284100	3.67288500
C	-2.87456600	2.20714600	1.90755400
H	-3.29492600	2.42070200	2.89914000
H	-1.81641900	2.48614700	1.91460600
H	-3.38744600	2.85166900	1.18797000
C	-4.55950000	0.34724200	1.58215700
H	-4.96860200	0.47009100	2.59376300
H	-5.13562700	1.00046500	0.91942400
H	-4.72360900	-0.69158600	1.27926000
C	-4.38151600	-0.01697500	-1.80435800
H	-5.15142900	0.21771800	-1.06568400
H	-4.78407800	0.24018600	-2.79306700
H	-4.20062900	-1.09487500	-1.78076400
C	-3.36472400	2.29071100	-1.56679400
H	-3.71845600	2.59576300	-2.56026600
H	-4.14582600	2.55844200	-0.84806000
H	-2.46598300	2.87361900	-1.33746400
C	-2.10351400	0.46006800	-2.73400400
H	-1.17651500	1.03596200	-2.64379600
H	-1.84513300	-0.60349500	-2.76784300
H	-2.57964400	0.72239100	-3.68808500

[Ni]OBcat

	x	y	z
Ni	-0.64724800	0.00010600	0.17764800
P	-0.91999300	2.21462800	0.07420000
P	-0.92136000	-2.21424200	0.07415000
C	-2.38952100	0.00066100	-0.57857400
O	-2.45300300	2.39934600	-0.59064900
C	-1.12121900	3.07224100	1.75024800

C	0.10896700	3.20666700	-1.17548500
O	-2.45434400	-2.39798900	-0.59103800
C	-1.12345400	-3.07162700	1.75021600
C	0.10717000	-3.20707400	-1.17523600
C	-3.07967400	1.18719200	-0.86303200
C	-3.08033400	-1.18544100	-0.86322400
C	-1.50727600	4.55812100	1.64137400
C	0.17433000	2.90378600	2.57299800
C	-2.26215600	2.30853500	2.46168800
C	1.47285100	3.60830900	-0.58261000
C	-0.63745800	4.45552700	-1.68774700
C	0.33965600	2.24424400	-2.36439100
C	-2.26367400	-2.30685500	2.46166100
C	-1.51090600	-4.55715000	1.64137800
C	0.17228000	-2.90440400	2.57292700
C	0.33844400	-2.24501700	-2.36433000
C	-0.63985800	-4.45566200	-1.68728400
C	1.47079600	-3.60928400	-0.58215300
C	-4.36557300	1.21747100	-1.40333300
C	-4.36624900	-1.21491400	-1.40352800
H	-1.74425600	4.93981400	2.64318600
H	-2.38947400	4.70593400	1.00993500
H	-0.68837800	5.16788100	1.24813100
H	-0.01512000	3.24052100	3.60061800
H	0.99781000	3.50670700	2.17979600
H	0.50417800	1.86110100	2.60436700
H	-3.20846700	2.38607900	1.91818800
H	-2.40599100	2.73929400	3.46068700
H	-2.02233300	1.24721600	2.58505700
H	1.37689900	4.36597400	0.20103200
H	2.09175000	4.03874000	-1.38020400
H	2.01704400	2.75087200	-0.17582200
H	-1.61340600	4.19706000	-2.10634800
H	-0.03699200	4.91739900	-2.48225800
H	-0.78752500	5.20792200	-0.90988900
H	0.86958300	2.78434400	-3.16003200
H	-0.60496100	1.87895300	-2.78196200
H	0.95066900	1.38497300	-2.07351200
H	-2.40787400	-2.73745800	3.46067500
H	-3.21006800	-2.38355800	1.91818800
H	-2.02289700	-1.24574800	2.58499600
H	-2.39322700	-4.70415300	1.00992000
H	-1.74828700	-4.93857900	2.64319600
H	-0.69257600	-5.16771100	1.24819400
H	-0.01740900	-3.24110800	3.60051400
H	0.50306700	-1.86202000	2.60439400
H	0.99520500	-3.50799900	2.17959000
H	0.94983300	-1.38597100	-2.07357700
H	-0.60595900	-1.87938000	-2.78208500
H	0.86820300	-2.78554500	-3.15979200
H	-1.61570400	-4.19680500	-2.10588100
H	-0.79022700	-5.20788100	-0.90931400
H	-0.03964100	-4.91792600	-2.48175600
H	2.08947700	-4.04037000	-1.37956300
H	1.37436500	-4.36659600	0.20177100
H	2.01546400	-2.75201100	-0.17565900
H	-4.85054100	2.16747900	-1.60338100
C	-4.99893700	0.00147600	-1.67112800

H	-4.85174800	-2.16461900	-1.60372600
H	-6.00068700	0.00178800	-2.09200500
H	7.09334600	-0.00158100	-2.14613100
C	6.35096700	-0.00138400	-1.35293600
C	6.76614700	-0.00123700	-0.01878500
C	4.98639500	-0.00128200	-1.69066600
C	5.83651000	-0.00098000	1.03516400
H	7.82782800	-0.00132200	0.21194800
C	4.07975400	-0.00103100	-0.64521600
H	4.65232300	-0.00139600	-2.72367300
C	4.49483100	-0.00087900	0.69300300
H	6.14845400	-0.00086500	2.07476600
O	2.70714400	-0.00089100	-0.69526300
O	3.40183400	-0.00063600	1.51680000
B	2.25990600	-0.00064700	0.66676200
O	1.01900800	-0.00045700	1.07993000

[Ni]OCH₂OBcat

	x	y	z
C	5.34691900	0.43088400	-0.49227900
C	4.05660300	-0.07071300	-0.31958200
C	2.92299800	0.74100600	-0.17488600
C	3.16180500	2.12113600	-0.19784700
C	4.42966400	2.67958600	-0.36826100
C	5.51834400	1.81715500	-0.51640800
H	6.18670300	-0.24831800	-0.59837000
H	4.55259100	3.75783200	-0.38116600
H	6.51437600	2.23072100	-0.64919100
O	2.08268500	2.97935300	-0.04282700
O	3.88991800	-1.45350200	-0.28334500
P	0.59385000	2.19006000	0.02358500
P	2.30168800	-1.90599400	0.02712400
C	-0.12167400	2.96335700	1.60479800
C	-0.18267800	2.86267400	-1.57414500
C	2.48161700	-2.83180000	1.66993000
C	1.98195000	-3.03270000	-1.46479600
H	-1.98852100	-2.05695500	0.34741700
C	-1.54364000	-1.10508000	0.01217900
O	-0.42473600	-0.81512200	0.68432600
O	-2.58741500	-0.07197500	0.24999000
C	-6.83587500	-2.27485600	-0.45152500
C	-5.81831900	-1.37541000	-0.18877300
C	-6.07679000	-0.04350100	0.15120200
C	-7.36715700	0.44771000	0.24363900
C	-8.40942600	-0.45598500	-0.02084200
C	-8.15014800	-1.78713100	-0.36068900
H	-6.62195300	-3.30577500	-0.71395200
H	-7.55691600	1.48260600	0.50881500
H	-9.43731300	-0.11030100	0.04115100
H	-8.97917900	-2.46032000	-0.55900800
O	-4.88749100	0.61807800	0.35582900
O	-4.45575400	-1.58494100	-0.20785200
B	-3.89194300	-0.34538500	0.13629800
H	-1.43005800	-1.13290200	-1.08659200
Ni	1.18234100	0.01930500	0.10942800
C	0.77633300	2.44156000	-2.71206900
H	0.90673000	1.35476000	-2.75381900
H	0.34913800	2.76651700	-3.66951300

H	1.76353800	2.90010100	-2.60845300
C	-1.55661800	2.21549400	-1.83196000
H	-2.29618800	2.46004400	-1.06725800
H	-1.93773100	2.57573200	-2.79680200
H	-1.48628600	1.12560400	-1.88531700
C	-0.30548700	4.39790800	-1.57223500
H	-0.61595300	4.73213500	-2.57104100
H	-1.05985400	4.75031100	-0.86270000
H	0.64886000	4.88025500	-1.33949600
C	0.37008000	4.40816100	1.82555500
H	-0.00584100	5.10008900	1.06778600
H	0.00150000	4.75417000	2.80018600
H	1.46110300	4.46932900	1.83163200
C	-1.66108600	2.91722000	1.60448200
H	-2.02001100	3.20918700	2.60017200
H	-2.09255800	3.62262200	0.88669700
H	-2.04613200	1.91785700	1.38691100
C	0.40670900	2.07449000	2.75578100
H	0.03088500	1.05011700	2.67337900
H	1.50242800	2.04535600	2.77696000
H	0.06663200	2.49162300	3.71281800
C	3.01653600	-1.77323000	2.66375400
H	3.99700100	-1.38909500	2.36629100
H	2.32914200	-0.92662900	2.76263700
H	3.12085100	-2.23993700	3.65157500
C	1.09941200	-3.31326700	2.16003800
H	1.19403600	-3.65386700	3.19945500
H	0.35750100	-2.51024700	2.11792100
H	0.72509100	-4.15793400	1.57447500
C	3.47651700	-4.00461300	1.60390400
H	3.65211100	-4.38109200	2.62025600
H	3.08912200	-4.84001800	1.01252100
H	4.44198900	-3.69882300	1.18818800
C	0.75770500	-3.93639900	-1.22595800
H	0.47914700	-4.41847100	-2.17187200
H	0.97099600	-4.73141000	-0.50503300
H	-0.11086400	-3.37413900	-0.86996100
C	3.20903700	-3.88816900	-1.84012300
H	3.43925700	-4.64359200	-1.08509600
H	2.99630300	-4.41525600	-2.77949700
H	4.09856600	-3.27089900	-1.98985900
C	1.68042600	-2.06804000	-2.63581400
H	0.77799700	-1.47550800	-2.45136700
H	2.51048800	-1.37716700	-2.81799200
H	1.52217600	-2.65272600	-3.55138100

[Ni]OCH₃

	x	y	z
Ni	-0.03901800	-0.38592800	-0.01218200
P	-2.21980800	-0.07520900	0.00997000
P	2.19347600	-0.09551900	-0.02744200
C	-0.02454000	1.52151600	0.11514200
O	-2.42357100	1.58474300	0.20111500
C	-3.12971100	-0.38485600	-1.62335500
C	-3.13143600	-0.72520400	1.53679700
O	2.36703700	1.57943500	0.02024800
C	3.01643000	-0.50057000	-1.68364300
C	3.28011600	-0.53809200	1.47657200

C	-1.20831500	2.26859400	0.20110500
C	1.16004400	2.26612500	0.10697100
C	-4.60142200	0.06576000	-1.59199100
C	-3.01845800	-1.87298900	-2.01873300
C	-2.36835700	0.46269600	-2.66956800
C	-3.44308800	-2.22570300	1.37464300
C	-4.41367600	0.06786600	1.85755100
C	-2.13425000	-0.54299500	2.70493600
C	2.23046000	0.30812300	-2.74157700
C	4.50265800	-0.11007800	-1.76321800
C	2.82755500	-2.00450900	-1.97593800
C	2.34651800	-0.37182800	2.69773500
C	4.47592600	0.42317800	1.63865800
C	3.78785000	-1.99046900	1.42239500
C	-1.23459400	3.66125200	0.28146500
C	1.19645400	3.65922100	0.18345400
H	-5.01284500	0.01738400	-2.60899400
H	-4.70504600	1.09616500	-1.23688100
H	-5.21682900	-0.58494000	-0.96335000
H	-3.32428600	-1.98232500	-3.06777000
H	-3.67841300	-2.50607700	-1.41905100
H	-1.99619500	-2.24567200	-1.90166400
H	-2.38731300	1.52999500	-2.42936000
H	-2.84588700	0.32601300	-3.64822100
H	-1.32362000	0.14800100	-2.75795600
H	-4.26978300	-2.39848900	0.67830800
H	-3.74441400	-2.63607300	2.34737200
H	-2.56869200	-2.78054400	1.02138100
H	-4.20913700	1.13682700	1.96344700
H	-4.82437900	-0.29685400	2.80831500
H	-5.18655200	-0.05860100	1.09572100
H	-2.61475600	-0.86217300	3.63916600
H	-1.83048600	0.50253100	2.82332600
H	-1.23362600	-1.14794900	2.55997800
H	2.63443000	0.07626600	-3.73550100
H	2.31988100	1.38635700	-2.58033300
H	1.16702100	0.04725000	-2.74171300
H	4.65914900	0.94335800	-1.50971200
H	4.85945300	-0.26446200	-2.79010200
H	5.12775700	-0.72327100	-1.10703500
H	3.15715500	-2.21208400	-3.00237800
H	1.77677100	-2.30037700	-1.88546300
H	3.42213500	-2.63549800	-1.30864800
H	1.50900500	-1.07633000	2.66639000
H	1.93612500	0.64175900	2.75867600
H	2.91614800	-0.55960700	3.61734800
H	4.15251400	1.46543000	1.68358200
H	5.20452600	0.32762300	0.82985200
H	4.99221600	0.18344700	2.57778900
H	4.28731200	-2.22621300	2.37117100
H	4.51994500	-2.14381900	0.62334900
H	2.97614300	-2.71116200	1.29020200
H	-2.18194100	4.18704900	0.34564100
C	-0.01670000	4.34662100	0.27232400
H	2.14698600	4.18321800	0.17281300
H	-0.01327600	5.43157600	0.33371500
H	0.27681200	-3.08044900	1.55036500
H	-0.20959900	-4.20139300	0.26803900

C	0.30108300	-3.23929400	0.45388500
H	1.36291300	-3.39643300	0.18033100
O	-0.31135500	-2.22651700	-0.27669200

[Ni]OCHO

	x	y	z
C	-1.21712500	3.76320900	-0.29664300
C	-1.18749300	2.37225900	-0.19366800
C	-0.00018000	1.62903700	-0.14219500
C	1.18705200	2.37241300	-0.19326300
C	1.21650700	3.76337500	-0.29623700
C	-0.00034300	4.44794000	-0.34827100
H	-2.16643200	4.28783400	-0.33217100
H	2.16575600	4.28812800	-0.33145000
H	-0.00040300	5.53155400	-0.42791700
O	2.39882500	1.68966100	-0.13638200
O	-2.39919600	1.68930700	-0.13721000
P	2.21038200	0.02560200	0.01739400
P	-2.21049600	0.02536400	0.01724100
C	3.18747400	-0.56438200	-1.49781200
C	3.07059700	-0.31422300	1.66847900
C	-3.18750200	-0.56538900	-1.49767400
C	-3.07061800	-0.31400500	1.66851200
H	0.00080300	-2.82373700	-1.52588100
Ni	-0.00010400	-0.26274600	0.02562700
C	2.29499800	0.52786800	2.70840800
H	1.23942900	0.24050000	2.75530700
H	2.73375500	0.35435800	3.69904200
H	2.35136800	1.59953300	2.49532100
C	4.55091300	0.10698900	1.68734500
H	4.93121300	0.02715100	2.71404300
H	5.17064300	-0.54227400	1.06186000
H	4.68608400	1.14290900	1.36008400
C	2.92380000	-1.80805800	2.03230400
H	3.26021400	-1.95039900	3.06750100
H	1.88780800	-2.15161500	1.95449900
H	3.54007500	-2.45223400	1.39925800
C	4.46119500	0.27064000	-1.74193800
H	5.21085200	0.13046500	-0.95993800
H	4.91070700	-0.04769700	-2.69149400
H	4.23518100	1.33774600	-1.81337800
C	3.54564600	-2.05902500	-1.38094600
H	3.93520500	-2.40573400	-2.34667700
H	4.32566900	-2.23611900	-0.63422800
H	2.68294800	-2.68441800	-1.13058000
C	2.23167000	-0.35960300	-2.69625500
H	1.33442200	-0.98119500	-2.61214300
H	1.91649300	0.68483000	-2.79154200
H	2.75139900	-0.64022000	-3.62129400
C	-2.23183500	-0.36072100	-2.69625100
H	-1.91697700	0.68377800	-2.79188600
H	-1.33439500	-0.98202000	-2.61201200
H	-2.75154600	-0.64178300	-3.62116400
C	-3.54516100	-2.06010800	-1.38025200
H	-3.93453200	-2.40734400	-2.34586800
H	-2.68222600	-2.68505500	-1.12959600
H	-4.32515400	-2.23718500	-0.63350400
C	-4.46147700	0.26917200	-1.74204400

H	-4.91096800	-0.04968300	-2.69143400
H	-5.21105000	0.12916200	-0.95993400
H	-4.23573700	1.33630900	-1.81394000
C	-4.55102900	0.10687400	1.68723700
H	-4.93129000	0.02733400	2.71397400
H	-4.68642200	1.14265000	1.35960600
H	-5.17063700	-0.54274500	1.06200600
C	-2.92347800	-1.80766800	2.03290100
H	-3.25974500	-1.94967900	3.06819200
H	-3.53968500	-2.45222500	1.40017500
H	-1.88743200	-2.15105900	1.95508200
C	-2.29522600	0.52867300	2.70810600
H	-1.23957400	0.24162700	2.75511500
H	-2.35188300	1.60024300	2.49462000
H	-2.73392700	0.35542300	3.69881200
O	-0.00000400	-2.12758200	0.39142300
C	0.00082100	-3.12517700	-0.44965900
O	0.00154700	-4.30829500	-0.15216200

9-BBN reductant

9-BBN

	x	y	z
C	-0.00188900	1.30492100	0.70871200
C	1.32332700	1.29539700	-0.10488400
C	1.60678400	-0.00004200	-0.89416700
C	1.32326600	-1.29545300	-0.10484900
C	-0.00195800	-1.30489200	0.70873400
H	1.34629600	2.15296200	-0.79363900
H	-0.02297600	2.22890800	1.30126600
H	1.02706300	-0.00004200	-1.82177600
H	2.65898500	-0.00006900	-1.20925000
H	1.34618900	-2.15303200	-0.79358600
H	2.14814900	-1.46177200	0.60384400
H	-0.02308100	-2.22884700	1.30134100
H	2.14821900	1.46169400	0.60380600
C	-1.30036500	-1.29547000	-0.16616100
H	-1.28638300	-2.15654200	-0.85035400
H	-2.15824800	-1.45998700	0.50263100
C	-1.30032600	1.29549900	-0.16616000
H	-1.28635600	2.15657500	-0.85035100
C	-1.54403800	0.00002000	-0.97034000
H	-2.15819000	1.46002700	0.50265600
H	-0.92036700	0.00001900	-1.86876900
H	-2.58014600	0.00004000	-1.33494400
B	-0.10484200	0.00002900	1.57750900
H	-0.34375300	0.00003800	2.75427000

BBNOBBN

	x	y	z
O	0.00008400	0.00440900	-0.00622400
C	-2.22400700	-0.91843900	-0.93946700
C	-3.06198800	-1.84643400	-0.01078500
C	-3.85562800	-1.12513500	1.10159500
C	-3.06350800	-0.02698600	1.84552700
C	-2.22341600	0.91808100	0.93662000
H	-3.75497800	-2.45473700	-0.61092800
H	-1.61673900	-1.55823300	-1.59463800
H	-4.77018900	-0.69621800	0.68181300
H	-4.19476300	-1.87129200	1.83274400

H	-3.75764600	0.56154100	2.46385900
H	-2.37170400	-0.51146500	2.55045400
H	-1.61640400	1.55911700	1.59077800
H	-2.36889500	-2.55993600	0.45928000
C	-3.06627400	1.84421400	0.01079300
H	-3.75908900	2.45008400	0.61353100
H	-2.37674100	2.55978000	-0.46124200
C	-3.06830000	0.02470800	-1.84615300
H	-3.76263200	-0.56487900	-2.46327100
C	-3.86131000	1.12098000	-1.09969200
H	-2.37909800	0.51120900	-2.55228700
H	-4.77339300	0.68953900	-0.67725900
H	-4.20442700	1.86659500	-1.82951800
B	-1.34635300	0.00229000	-0.00375600
C	2.22051700	-0.93044600	0.92401200
C	3.07027400	-1.84539000	-0.00547000
C	3.86683600	-1.11017100	-1.10671700
C	3.07462000	-0.00721400	-1.84383700
C	2.22704400	0.92744100	-0.93093600
H	3.76315000	-2.45508200	0.59342700
H	1.61057100	-1.57923300	1.56782200
H	4.77768200	-0.68376300	-0.67667900
H	4.21229800	-1.84769400	-1.84364200
H	3.77033600	0.58945100	-2.45242100
H	2.38852800	-0.48617900	-2.55818400
H	1.62244900	1.57459000	-1.58122200
H	2.38421300	-2.55788000	-0.48707500
C	3.06198400	1.84676900	0.00864100
H	3.75836800	2.45909000	-0.58346300
H	2.36704100	2.55639900	0.48161500
C	3.05384700	0.00758100	1.84705400
H	3.74349100	-0.58623000	2.46548400
C	3.84929200	1.11450200	1.11882100
H	2.35591400	0.48405400	2.55118300
H	4.76586800	0.69059700	0.69872800
H	4.18471600	1.85314800	1.85931000
B	1.34665200	-0.00069200	-0.00593000

BBNOCH₂OBBN

	x	y	z
H	-0.60790800	-2.65647000	0.65882600
C	-0.00004900	-2.03065200	-0.00033200
O	0.81300200	-1.23422900	0.83423200
O	-0.81285600	-1.23367300	-0.83447700
H	0.60770800	-2.65638900	-0.65965700
C	-2.51818300	-0.60373000	1.09329400
C	-2.38545800	0.85746500	1.62513800
C	-2.96653400	1.95632300	0.70728800
C	-2.61976700	1.79029900	-0.78903900
C	-2.75409800	0.34016600	-1.34263900
H	-2.85055700	0.93397500	2.61900900
H	-1.97095800	-1.24573500	1.79606700
H	-4.05266900	2.00011100	0.82944800
H	-2.59704500	2.93218300	1.05034200
H	-3.23748800	2.48029600	-1.38290200
H	-1.57876300	2.11053000	-0.94592600
H	-2.35023100	0.33376700	-2.36394300
H	-1.31441400	1.05333200	1.77883800

C	-4.21193300	-0.19931800	-1.40108100
H	-4.84210600	0.47595500	-1.99880700
H	-4.19139600	-1.15247900	-1.95027800
C	-3.98012600	-1.13338000	1.01189300
H	-4.45678000	-1.07026800	2.00130100
C	-4.88276300	-0.43586900	-0.02976800
H	-3.93360700	-2.20649800	0.77176100
H	-5.23929300	0.51612800	0.37430900
H	-5.78554300	-1.04392300	-0.17721600
B	-1.93001300	-0.58581000	-0.37153500
C	2.51712100	-0.60213700	-1.09388600
C	2.38547300	0.85971100	-1.62421400
C	2.96759700	1.95724300	-0.70541600
C	2.62131000	1.78994400	0.79089300
C	2.75454000	0.33913700	1.34292200
H	2.85043400	0.93685700	-2.61809800
H	1.96909500	-1.24296300	-1.79710000
H	4.05371100	2.00049200	-0.82796900
H	2.59858100	2.93368300	-1.04735600
H	3.23991600	2.47875300	1.38520300
H	1.58066500	2.11094100	0.94855400
H	2.35106700	0.33197600	2.36437800
H	1.31455800	1.05658900	-1.77747900
C	4.21197500	-0.20169600	1.40030200
H	4.84290100	0.47236300	1.99860500
H	4.19077700	-1.15545900	1.94842500
C	3.97867200	-1.13304700	-1.01353600
H	4.45503800	-1.06930200	-2.00304000
C	4.88217100	-0.43728100	0.02853300
H	3.93144100	-2.20637600	-0.77446200
H	5.23927400	0.51487200	-0.37465500
H	5.78455600	-1.04614700	0.17505400
B	1.92965100	-0.58552200	0.37126000

CH₃OBBN

	x	y	z
H	-3.84689500	0.93826200	-0.03885800
H	-3.96142100	-0.82613800	-0.22430000
C	-3.30692800	-0.00635700	0.08996700
H	-3.05590800	-0.13363200	1.14762900
O	-2.15822300	-0.00105700	-0.74674900
C	0.30056900	0.00248100	-1.37741300
C	1.11234100	1.31382200	-1.17104900
C	1.57279900	1.57937900	0.27948400
C	0.49474700	1.30933900	1.35240200
C	-0.32055100	-0.00656600	1.16984900
H	1.98957900	1.32793500	-1.83532800
H	-0.08184200	0.00356400	-2.40693400
H	2.46354100	0.98298500	0.49789400
H	1.89758200	2.62545300	0.36336400
H	0.96497500	1.32336300	2.34701100
H	-0.21988600	2.14617000	1.34814900
H	-1.09612600	-0.01090100	1.94824800
H	0.47765400	2.15165100	-1.49602000
C	0.50903300	-1.31355000	1.34842100
H	0.98243700	-1.32428200	2.34159200
H	-0.19698400	-2.15763800	1.34495600
C	1.12027500	-1.30467400	-1.17657900

H	1.99576500	-1.31209000	-1.84324500
C	1.58653200	-1.57105400	0.27189600
H	0.48962700	-2.14545600	-1.50189600
H	2.47286800	-0.96785700	0.48963900
H	1.92037400	-2.61460400	0.35152600
B	-0.86849100	-0.00304900	-0.31626000

***cis*-HCOBBN**

	x	y	z
C	0.18350700	0.15963100	1.09604500
C	-0.22694400	1.64329300	0.82976600
C	-1.29731000	1.84678100	-0.26638800
C	-1.07652600	1.00335000	-1.54248400
C	-0.67768900	-0.48802800	-1.29675100
H	-0.57445000	2.10256200	1.76646200
H	1.02312400	0.17782100	1.79900500
H	-2.28948300	1.63819400	0.14399500
H	-1.31630600	2.90847500	-0.54649800
H	-1.97926000	1.04584700	-2.16907600
H	-0.27670800	1.46824500	-2.13750900
H	-0.41808500	-0.92681600	-2.26917800
H	0.68551700	2.18573000	0.54651500
C	-1.79441600	-1.35951400	-0.65508200
H	-2.70174900	-1.32404600	-1.27561500
H	-1.45517200	-2.40564100	-0.68095300
C	-0.94026000	-0.72605900	1.71184400
H	-1.28665000	-0.27958700	2.65523600
C	-2.15745200	-0.99368200	0.80050300
H	-0.48961900	-1.69137400	1.98751400
H	-2.81961300	-0.12313800	0.80678700
H	-2.74937400	-1.81128500	1.23328700
B	0.54286700	-0.42492000	-0.31479500
H	3.74135200	-1.28690300	-0.44247700
O	3.22374100	0.48526300	0.41645500
C	2.99004800	-0.51958200	-0.20106200
O	1.79805900	-0.85409100	-0.75418900

***trans*-HCOBBN**

	x	y	z
C	-0.04520300	0.00034000	1.20630300
C	-0.87880100	1.31359800	1.33908700
C	-1.89660400	1.57621400	0.20779700
C	-1.35302400	1.31098600	-1.21292600
C	-0.52648100	-0.00019900	-1.37092200
H	-1.40154400	1.31917700	2.30627600
H	0.67982700	0.00059400	2.03052900
H	-2.79544800	0.97669200	0.37703600
H	-2.22844900	2.62097800	0.27119700
H	-2.18824900	1.31505000	-1.92811100
H	-0.70509900	2.15038600	-1.50494900
H	-0.08457400	-0.00030900	-2.37553200
H	-0.17057100	2.15461400	1.37740800
C	-1.35260900	-1.31160000	-1.21246800
H	-2.18783400	-1.31618400	-1.92764600
H	-0.70442000	-2.15090200	-1.50419000
C	-0.87835700	-1.31317500	1.33953100
H	-1.40106800	-1.31861700	2.30673900
C	-1.89609900	-1.57649500	0.20835300

H	-0.16984100	-2.15394000	1.37810500
H	-2.79512000	-0.97718600	0.37738900
H	-2.22762400	-2.62133900	0.27212300
B	0.56858500	0.00011800	-0.24706100
H	2.66726000	0.00068400	1.30614200
O	4.09883800	0.00001300	-0.13495300
C	2.96309900	0.00024600	0.24565000
O	1.90795000	0.00001500	-0.61875200

IMA1-2

	x	y	z
C	-4.69778400	0.99610800	0.83128700
C	-4.51273900	1.89223400	-0.41700300
C	-4.79838300	1.20744500	-1.77191800
C	-4.21570300	-0.21738400	-1.89744700
C	-4.40929200	-1.12160700	-0.65553000
H	-5.12906000	2.80378100	-0.34434100
H	-4.36002100	1.58746900	1.70145500
H	-5.87862000	1.17754300	-1.94703800
H	-4.39409700	1.83307400	-2.58213900
H	-4.63684900	-0.69119800	-2.79954800
H	-3.13449200	-0.13111200	-2.08468800
H	-3.87242400	-2.06294200	-0.86010200
H	-3.46913300	2.23797100	-0.42506800
C	-5.88546100	-1.51381800	-0.37995900
H	-6.33674600	-1.98965500	-1.26605800
H	-5.87879200	-2.28139100	0.40728500
C	-6.17092300	0.60150700	1.11537600
H	-6.80845900	1.49646500	1.20285400
C	-6.80434900	-0.35663800	0.07869800
H	-6.19635300	0.11196500	2.09958100
H	-7.13338200	0.21731300	-0.79421000
H	-7.72491900	-0.78189700	0.50442000
B	-3.88586000	-0.39485100	0.68826900
C	4.23124700	1.08515800	-2.27625700
C	3.14515500	1.09673300	-1.40153200
C	2.52520000	-0.06665300	-0.92316600
C	3.08107600	-1.27429400	-1.36828400
C	4.16627100	-1.34424300	-2.24207300
C	4.73194300	-0.15006500	-2.69306400
H	4.66680000	2.01975500	-2.61411100
H	4.55036900	-2.30990900	-2.55401300
H	5.57674900	-0.18231600	-3.37529900
O	2.52932100	-2.46518900	-0.91726700
O	2.65801400	2.32830000	-0.98076700
P	1.23316700	-2.25355600	0.12692300
P	1.39243200	2.20255700	0.11129300
C	-0.09581500	-3.24717400	-0.79065900
C	1.87773500	-3.09498900	1.69895800
C	0.08487000	3.26126300	-0.75836400
C	2.13792000	3.00930400	1.65509700
H	-2.10579000	-0.09474200	2.54672800
Ni	1.05114400	-0.00922400	0.27042100
C	3.18585300	-2.35532000	2.05993700
H	3.01624900	-1.28597900	2.22511100
H	3.58621900	-2.77834100	2.98995100
H	3.94639000	-2.46593000	1.28163900
C	2.18899100	-4.59041500	1.50399500

H	2.68982500	-4.96922000	2.40445500
H	1.28236100	-5.18561500	1.36185000
H	2.85709100	-4.76066700	0.65390600
C	0.86576400	-2.90251200	2.84853900
H	1.30226100	-3.30450100	3.77184600
H	0.63437500	-1.84653800	3.01548000
H	-0.07410300	-3.43301300	2.67331200
C	0.48228200	-4.51052700	-1.46223600
H	0.79503800	-5.26784500	-0.73965100
H	-0.30360200	-4.95574300	-2.08545600
H	1.33305900	-4.27523900	-2.10633300
C	-1.25910200	-3.63144700	0.14308600
H	-2.05778900	-4.08021300	-0.45989700
H	-0.95956600	-4.37245100	0.89095500
H	-1.69685700	-2.76773500	0.65069600
C	-0.61516400	-2.29383600	-1.89247200
H	-1.10268300	-1.41195700	-1.46848400
H	0.18968000	-1.96803200	-2.56097300
H	-1.35859300	-2.82573900	-2.49894900
C	-0.55491100	2.32545800	-1.81045000
H	0.19324400	1.92543000	-2.50394000
H	-1.08441200	1.48816500	-1.34687200
H	-1.28374400	2.89668100	-2.39892900
C	-0.99207700	3.73310900	0.23667800
H	-1.81431700	4.19433900	-0.32294500
H	-1.42040500	2.90709900	0.81251900
H	-0.60685900	4.48384900	0.93357400
C	0.70532900	4.47222800	-1.48531400
H	-0.08962400	4.98314700	-2.04322600
H	1.14532300	5.19935200	-0.79873000
H	1.47497000	4.16362800	-2.19727500
C	2.53371800	4.48179000	1.44063500
H	3.08348300	4.83439600	2.32301400
H	3.18534500	4.60579900	0.56993000
H	1.66185000	5.13140900	1.32093300
C	1.15649600	2.87958000	2.83943800
H	1.65756300	3.22953200	3.75108600
H	0.25772900	3.48753100	2.70668600
H	0.84457500	1.84329400	2.99904100
C	3.41128800	2.19288200	1.97627700
H	3.18436100	1.13559300	2.14910100
H	4.15283400	2.25705500	1.17471300
H	3.86429700	2.59321100	2.89188200
O	-0.31807800	0.06027600	1.63880300
C	-1.57649900	-0.04136600	1.58556700
O	-2.26982800	-0.09899600	0.52964800
H	-3.94011600	-1.09759400	1.68752800

IMA2-2

	x	y	z
Ni	0.65374500	-0.00281700	0.19383400
P	0.97745000	2.27077400	-0.02173400
P	0.95870300	-2.27804400	-0.02084600
O	-1.32639600	0.00408100	0.71189300
C	2.54539100	-0.01088800	-0.06611300
O	2.64824900	2.38459900	-0.07928600
C	0.54807200	3.05346100	-1.71522200
C	0.66874700	3.44275700	1.43994200

O	2.62861200	-2.40717200	-0.07102400
C	0.52971000	-3.05254700	-1.71771100
C	0.63229300	-3.44858500	1.43810600
C	-1.44110400	0.00666000	2.02719100
C	3.30319500	1.16792500	-0.12147900
C	3.29367200	-1.19602600	-0.11719500
C	1.60304500	4.09546300	-2.14352600
C	-0.85001600	3.69557800	-1.72297700
C	0.56652200	1.89178100	-2.73242500
C	-0.83277400	3.54417000	1.77120200
C	1.24403200	4.85071600	1.18930300
C	1.40898900	2.80637500	2.64031700
C	0.58008900	-1.89115900	-2.73433000
C	1.56736800	-4.11495500	-2.13792000
C	-0.88103000	-3.66591100	-1.73668900
C	1.37390300	-2.82051700	2.64205000
C	1.19400200	-4.86225100	1.18894300
C	-0.87151800	-3.53568500	1.76295100
O	-0.48352100	0.00516600	2.78550400
H	-2.47476900	0.01016000	2.38984700
C	4.69520000	1.19176100	-0.21908200
C	4.68541000	-1.23155300	-0.21466200
H	1.34146900	4.45088300	-3.14864900
H	2.60643700	3.66584700	-2.18535500
H	1.63262700	4.96536000	-1.48391300
H	-1.08770100	4.00334900	-2.74935500
H	-0.90066900	4.59134700	-1.09645300
H	-1.62858500	2.99855800	-1.40375400
H	1.52928400	1.37004000	-2.74158000
H	0.39566000	2.29717000	-3.73835400
H	-0.22225900	1.16397100	-2.52259500
H	-1.41778200	3.99321000	0.96496400
H	-0.95126000	4.17951800	2.65815100
H	-1.26630200	2.57127100	2.00780100
H	2.29581500	4.81476900	0.89100000
H	1.18007300	5.42429000	2.12303200
H	0.68041400	5.40235800	0.43093400
H	1.23565800	3.43184500	3.52552500
H	2.48835700	2.75945600	2.46854200
H	1.03995900	1.80116500	2.86122700
H	0.40910400	-2.29300200	-3.74164300
H	1.55324900	-1.38901800	-2.73559500
H	-0.19534500	-1.14752600	-2.53079400
H	2.58003200	-3.70640100	-2.16614800
H	1.31041200	-4.46080200	-3.14756000
H	1.57057400	-4.98800100	-1.48189800
H	-1.11727000	-3.96847000	-2.76495000
H	-1.64731500	-2.95308000	-1.42270300
H	-0.95449500	-4.56066700	-1.11096900
H	1.01459800	-1.81155700	2.86198400
H	2.45441900	-2.78479400	2.47492900
H	1.19017300	-3.44456600	3.52615700
H	2.24662100	-4.83730900	0.89249600
H	0.62588600	-5.40827700	0.42985300
H	1.12245900	-5.43479800	2.12274900
H	-0.99974400	-4.16952600	2.64962100
H	-1.45700800	-3.97976600	0.95428000
H	-1.29758300	-2.55887100	1.99687400

H	5.21600500	2.14299100	-0.25502000
C	5.37973100	-0.02276100	-0.26316600
H	5.19848000	-2.18709500	-0.24732600
H	6.46356700	-0.02726800	-0.33740200
C	-3.58795600	-1.28747700	-0.21322300
C	-4.47197000	-1.28672400	1.05979000
C	-5.24840200	0.02237300	1.33422500
C	-4.45956200	1.32291300	1.05444600
C	-3.57579200	1.31030300	-0.21869200
H	-5.19567100	-2.11652200	1.02062700
H	-3.03596500	-2.23955800	-0.19616800
H	-6.16363100	0.02550000	0.73448100
H	-5.59153500	0.02617000	2.37879200
H	-5.17534800	2.15940800	1.01217300
H	-3.82015700	1.54805300	1.92147800
H	-3.01449400	2.25701700	-0.20499400
H	-3.83489200	-1.51454900	1.92784300
C	-4.41071400	1.31686500	-1.53083300
H	-5.11685900	2.16266700	-1.53579000
H	-3.71836500	1.49119200	-2.36648600
C	-4.42304100	-1.29104400	-1.52539300
H	-5.13715200	-2.13013100	-1.52694100
C	-5.19947400	0.01602600	-1.81141400
H	-3.73248900	-1.47532000	-2.36040900
H	-6.12601400	0.02162600	-1.22802200
H	-5.52268900	0.01533500	-2.86213000
B	-2.61712400	0.00669500	-0.35030200
H	-1.97119900	0.00116400	-1.38474500

IMA3-2

	x	y	z
C	-4.27078300	-1.22194900	0.21325200
C	-5.42122800	-0.82078900	1.17083800
C	-6.15910900	0.48679000	0.80727800
C	-5.22964500	1.64289000	0.37823700
C	-4.08250000	1.24546600	-0.58403700
H	-6.16194700	-1.63309500	1.25302400
H	-3.79451100	-2.10890400	0.66395400
H	-6.88516800	0.28833300	0.01203000
H	-6.75947900	0.81049000	1.67032900
H	-5.84522700	2.44750100	-0.05682000
H	-4.77074800	2.06968500	1.28207800
H	-3.46896400	2.14935200	-0.72685800
H	-4.98946800	-0.70393900	2.17518300
C	-4.55392100	0.81958900	-1.99876200
H	-5.16688300	1.61042600	-2.46156100
H	-3.65853000	0.72236000	-2.63139200
C	-4.73991900	-1.64648200	-1.20144200
H	-5.47412300	-2.46679100	-1.14142600
C	-5.33771500	-0.51103900	-2.06258900
H	-3.86798400	-2.05847200	-1.73200900
H	-6.37665200	-0.33703500	-1.76391400
H	-5.39102900	-0.84500500	-3.10928700
B	-3.22396400	0.00675500	0.01812400
C	4.25476300	1.10585100	-2.15999900
C	3.11297700	1.10924800	-1.35905500
C	2.50005700	-0.05700300	-0.87757600
C	3.13126600	-1.25792400	-1.23470600

C	4.27470400	-1.31869100	-2.03184400
C	4.82655600	-0.12300800	-2.49425800
H	4.67855900	2.04419600	-2.50239600
H	4.71199200	-2.28088600	-2.27744700
H	5.71561200	-0.14871800	-3.11801300
O	2.59919800	-2.45179800	-0.77271600
O	2.56668500	2.33768000	-1.01391600
P	1.19959000	-2.25643400	0.13147100
P	1.27527000	2.21614200	0.04649500
C	-0.00401000	-3.27735900	-0.91323100
C	1.71219600	-3.07076700	1.76652600
C	0.00041100	3.27406900	-0.86971500
C	1.98713200	3.04203600	1.60085600
H	-1.60505700	0.55325800	3.11821600
Ni	0.95600400	-0.01013400	0.22519300
C	2.94514700	-2.27425200	2.25145400
H	2.71477300	-1.21229600	2.38800500
H	3.26577200	-2.67496300	3.22143900
H	3.78525700	-2.35724400	1.55579800
C	2.10482700	-4.55225800	1.61494300
H	2.55701500	-4.89637100	2.55424800
H	1.23759800	-5.18975200	1.42047600
H	2.83775500	-4.70280200	0.81635900
C	0.58477400	-2.92123900	2.80910800
H	0.94025600	-3.31574000	3.76972300
H	0.30520600	-1.87429400	2.95358400
H	-0.31455500	-3.48071200	2.53777800
C	0.62743600	-4.58220000	-1.44020500
H	0.81810200	-5.31131200	-0.64976900
H	-0.07625400	-5.04063100	-2.14649300
H	1.56436500	-4.39335800	-1.97092300
C	-1.28631600	-3.58058400	-0.11908200
H	-2.02948900	-4.01597400	-0.79812000
H	-1.11307800	-4.30657300	0.68216500
H	-1.73312900	-2.67761800	0.30508100
C	-0.34697700	-2.37555900	-2.12258500
H	-0.85928700	-1.46031800	-1.81313800
H	0.54656100	-2.10859800	-2.69742700
H	-1.02123200	-2.92690200	-2.79009400
C	-0.58343700	2.34047700	-1.95569100
H	0.19820800	1.97040100	-2.62892900
H	-1.11213200	1.48445500	-1.52644800
H	-1.30280500	2.90714600	-2.55988800
C	-1.11995300	3.73525800	0.08113300
H	-1.90727900	4.21803500	-0.50991200
H	-1.58975800	2.90351900	0.61396800
H	-0.76208200	4.46853900	0.81101900
C	0.64238300	4.49369800	-1.56411800
H	-0.12614200	4.98042700	-2.17784900
H	1.01716800	5.23732200	-0.85725500
H	1.46325300	4.19766500	-2.22195400
C	2.35165200	4.52320700	1.38963000
H	2.88858400	4.88599300	2.27584300
H	3.00601200	4.66240100	0.52348100
H	1.46689900	5.15427600	1.26549100
C	0.99660500	2.89647300	2.77486900
H	1.45798700	3.31309400	3.67941100
H	0.06067400	3.43627500	2.60593300

H	0.75724700	1.84743600	2.96954300
C	3.27504500	2.25820800	1.94235700
H	3.07534300	1.19372700	2.10339000
H	4.02961000	2.34880700	1.15587400
H	3.69930100	2.66475000	2.86911800
O	-0.44356500	0.05061200	1.56884800
C	-1.57652600	0.33528000	2.03773200
O	-2.70554900	0.41193800	1.47998900
H	-2.23682600	-0.27926600	-0.64229500

IMA4-2

	x	y	z
Ni	0.52219800	0.01168400	-0.15620600
P	0.81515800	2.29334500	-0.10449200
P	0.91637700	-2.25468200	-0.10483400
O	-1.68512200	-0.03443000	1.54177100
C	2.44197500	0.05445500	-0.03476600
O	2.48520900	2.44449600	-0.06009500
C	0.49242000	3.29080100	-1.70558300
C	0.43685800	3.26122300	1.49462600
O	2.59151500	-2.33127100	-0.06036400
C	0.63843000	-3.26418700	-1.70664700
C	0.58211500	-3.24014600	1.49344000
C	-2.20032500	-0.05058200	2.75650500
C	3.17213500	1.24997000	-0.01282400
C	3.22461700	-1.10736500	-0.01290100
C	1.59537700	4.34142200	-1.95847300
C	-0.87661300	3.99442500	-1.69803100
C	0.54216500	2.25420500	-2.85119300
C	-1.06885300	3.43707500	1.75376600
C	1.12576200	4.64086200	1.48328500
C	1.03177600	2.40177000	2.63598000
C	0.64255700	-2.22543800	-2.85136400
C	1.78688100	-4.26469600	-1.96019400
C	-0.69816700	-4.02759100	-1.69956100
C	1.13784600	-2.35555900	2.63536300
C	1.33281600	-4.58723800	1.48084200
C	-0.91391100	-3.48473200	1.75311700
O	-1.51885300	-0.03529500	3.76395700
H	-3.30161900	-0.07887400	2.80369900
C	4.56543500	1.31283400	0.04676200
C	4.61933500	-1.10816800	0.04671400
H	1.37959800	4.83835000	-2.91333600
H	2.58544800	3.88639300	-2.02640900
H	1.62836300	5.11199900	-1.18492000
H	-1.06231700	4.41339400	-2.69537200
H	-0.90283200	4.82554800	-0.98669700
H	-1.70160300	3.31735100	-1.46988800
H	1.50743100	1.73666200	-2.88441700
H	0.40660000	2.77042600	-3.81051400
H	-0.24449200	1.49978900	-2.75735300
H	-1.55780100	4.06847800	1.00716200
H	-1.19569700	3.92343600	2.72939100
H	-1.58350300	2.47729200	1.79299500
H	2.19263100	4.56614400	1.25693700
H	1.02245800	5.08767800	2.48045200
H	0.66072800	5.32967200	0.77085800
H	0.89838400	2.94487900	3.58030000

H	2.10319800	2.22396200	2.50385700
H	0.51677700	1.44203300	2.73706800
H	0.53034000	-2.74631800	-3.81118100
H	1.58396700	-1.66563100	-2.88368000
H	-0.17675200	-1.50666800	-2.75713700
H	2.75580300	-3.76613400	-2.02771800
H	1.59341400	-4.77005700	-2.91541400
H	1.85400900	-5.03354800	-1.18716300
H	-0.86585100	-4.45288400	-2.69740700
H	-1.55208600	-3.38797300	-1.46976800
H	-0.68706400	-4.86002300	-0.98939100
H	0.57986400	-1.42026400	2.73759600
H	2.19998100	-2.12905500	2.50279300
H	1.02981600	-2.90498500	3.57926700
H	2.39489500	-4.46433900	1.25308000
H	0.89847200	-5.29638800	0.76896400
H	1.25117100	-5.03837600	2.47807200
H	-1.01764600	-3.97897300	2.72751600
H	-1.37442800	-4.13567400	1.00521800
H	-1.47190100	-2.54959600	1.79557600
H	5.06022300	2.27832900	0.06586100
C	5.28345300	0.11771800	0.07880500
H	5.15660100	-2.05068800	0.06575900
H	6.36857100	0.14187800	0.12583600
C	-3.12180100	-1.36410200	-0.28766200
C	-4.44316000	-1.40646100	0.52938300
C	-5.30018900	-0.11800100	0.48895700
C	-4.50130600	1.20719400	0.52994000
C	-3.18022400	1.22462900	-0.28869500
H	-5.06500600	-2.25093700	0.19353300
H	-2.59780900	-2.29896800	-0.05386400
H	-5.92575900	-0.13169500	-0.40853100
H	-6.00794600	-0.13390900	1.32958400
H	-5.16049700	2.02357800	0.19587500
H	-4.25801900	1.44650400	1.57428100
H	-2.69903300	2.18237300	-0.05551100
H	-4.19082200	-1.63603300	1.57373200
C	-3.41881100	1.20854300	-1.82004800
H	-4.05079100	2.06000300	-2.11835100
H	-2.45116400	1.36284600	-2.31847000
C	-3.35961700	-1.35934100	-1.81930000
H	-3.95123300	-2.23923800	-2.11786300
C	-4.03008600	-0.09034700	-2.37753700
H	-2.38551000	-1.46869600	-2.31699100
H	-5.10479000	-0.11512200	-2.17446900
H	-3.94175600	-0.08865100	-3.47322800
B	-2.27310200	-0.04972600	0.14492100
H	-1.11741800	-0.02481000	-0.55954800

IMA5-2

	x	y	z
C	3.33208100	-1.30150900	0.10134800
C	4.67567100	-1.31260900	-0.68208400
C	5.50541100	-0.00776500	-0.60751200
C	4.67942100	1.29943600	-0.68216300
C	3.33585500	1.29225900	0.10136400
H	5.30519200	-2.15004100	-0.34191000
H	2.83213400	-2.24717200	-0.15261200

H	6.10366900	-0.00857700	0.30930700
H	6.23881100	-0.00884100	-1.42609700
H	5.31136600	2.13508900	-0.34210400
H	4.44529200	1.50370200	-1.73447700
H	2.83866300	2.23937800	-0.15255400
H	4.44101900	-1.51629000	-1.73439600
C	3.52131900	1.27702500	1.63776000
H	4.11594900	2.14580300	1.96242800
H	2.53397300	1.39819600	2.10523300
C	3.51746200	-1.28676000	1.63776400
H	4.10940900	-2.15732800	1.96254600
C	4.14775500	-0.00581300	2.21330500
H	2.52971200	-1.40485500	2.10518700
H	5.22783300	-0.00744700	2.04263200
H	4.02654900	-0.00563600	3.30617000
B	2.49063600	-0.00340200	-0.39110000
C	-4.59877400	1.21611100	0.13946300
C	-3.20422300	1.18278800	0.08189800
C	-2.44801900	0.00346600	0.03293200
C	-3.20762900	-1.17365600	0.08201100
C	-4.60226700	-1.20294000	0.13960000
C	-5.29365000	0.00758700	0.16223700
H	-5.11171100	2.17198800	0.16745900
H	-5.11796400	-2.15732700	0.16770800
H	-6.37919500	0.00915400	0.20561700
O	-2.55284200	-2.38887000	0.08531300
O	-2.54592300	2.39610300	0.08510400
P	-0.88132000	-2.28328200	0.04934500
P	-0.87471100	2.28568100	0.04929400
C	-0.48962000	-3.12590400	1.72377900
C	-0.59987500	-3.45420600	-1.42789700
C	-0.48070900	3.12710900	1.72383600
C	-0.58983800	3.45585300	-1.42787100
H	1.68495600	-0.00233000	-3.76560700
Ni	-0.52202600	0.00069500	-0.12602500
C	-1.37219500	-2.82843900	-2.61376800
H	-1.02981700	-1.81658400	-2.84004000
H	-1.20605200	-3.45366800	-3.50094700
H	-2.44832700	-2.80134600	-2.42059400
C	-1.17115400	-4.86389000	-1.17414400
H	-1.10766700	-5.43568000	-2.10917400
H	-0.60810300	-5.41790300	-0.41780000
H	-2.22301100	-4.82914600	-0.87633400
C	0.89342800	-3.55631900	-1.78883200
H	0.99257500	-4.14454000	-2.71036700
H	1.34420600	-2.57848300	-1.96803700
H	1.47847200	-4.06143000	-1.01557700
C	-1.59872000	-4.11503800	2.14309600
H	-1.69030100	-4.96368700	1.46185100
H	-1.34450500	-4.51166700	3.13485900
H	-2.57420800	-3.62853800	2.21108800
C	0.86455300	-3.85855800	1.70107700
H	1.12274200	-4.15840400	2.72482200
H	0.82673400	-4.76940100	1.09651700
H	1.67797700	-3.23295100	1.33006400
C	-0.44712800	-1.98714600	2.76654300
H	0.34371300	-1.26395500	2.55037900
H	-1.39837900	-1.44595100	2.81189900

H	-0.25669500	-2.41506200	3.75945400
C	-0.44133000	1.98812800	2.76646700
H	-1.39407300	1.44955700	2.81177300
H	0.34750300	1.26276500	2.55024400
H	-0.24973000	2.41541800	3.75942300
C	0.87541000	3.85615000	1.70126500
H	1.13432400	4.15520700	2.72505800
H	1.68720200	3.22844100	1.33023800
H	0.84006200	4.76716500	1.09679900
C	-1.58716500	4.11918000	2.14324300
H	-1.33194000	4.51493700	3.13509700
H	-1.67641500	4.96821500	1.46215900
H	-2.56397500	3.63532400	2.21109200
C	-1.15713500	4.86712300	-1.17398400
H	-1.09202900	5.43882200	-2.10896000
H	-2.20908800	4.83530900	-0.87618200
H	-0.59253300	5.41945500	-0.41757600
C	0.90377400	3.55373900	-1.78867100
H	1.00469000	4.14193000	-2.71003200
H	1.49023000	4.05692200	-1.01522700
H	1.35173000	2.57464500	-1.96811400
C	-1.36385800	2.83240500	-2.61383200
H	-1.02426200	1.81964300	-2.84022700
H	-2.44006200	2.80826100	-2.42067300
H	-1.19596400	3.45729700	-3.50092400
O	0.20143000	-0.00032200	-2.38733200
C	1.39462700	-0.00191600	-2.70163900
O	2.42026400	-0.00323000	-1.91923100
H	1.23902800	-0.00161300	0.06368000

IMB1-2

	x	y	z
Ni	0.76783000	0.07421100	-0.05595300
P	1.53667000	-2.12656000	-0.51171000
P	0.99086300	2.36069000	0.53236100
C	2.68868800	0.31458000	-0.10965500
O	2.98887400	-1.74846600	-1.26731300
C	2.18573300	-3.17970900	0.98094200
C	0.87259300	-3.22811600	-1.90259700
O	2.56425800	2.35438400	1.12509500
C	0.17239600	3.08011200	2.08396200
C	1.17926200	3.67838800	-0.86430800
C	3.54356700	-0.59506700	-0.74619700
C	3.33822500	1.40298200	0.49005600
C	3.59369300	-3.73688500	0.67424000
C	1.25800500	-4.36092400	1.33617000
C	2.29728400	-2.24594000	2.20660800
C	-0.51841700	-3.78012600	-1.53608900
C	1.82188500	-4.39210100	-2.25451800
C	0.78509500	-2.29869900	-3.13703000
C	0.42662100	2.02803400	3.18741300
C	0.79976000	4.41406100	2.53560000
C	-1.34249800	3.25657700	1.87010300
C	1.51009900	2.93271500	-2.17703900
C	2.34834800	4.63987500	-0.55696300
C	-0.11116400	4.49689100	-1.05510700
C	4.92837600	-0.43670900	-0.83318500
C	4.72060200	1.60116200	0.45554700

H	3.92313200	-4.32195600	1.54298200
H	4.32398200	-2.94107800	0.51242400
H	3.60976200	-4.39682000	-0.19581100
H	1.63671000	-4.83005300	2.25335900
H	1.24953900	-5.13096600	0.56048200
H	0.22728200	-4.05691300	1.53118700
H	2.99696900	-1.42485400	2.03127800
H	2.66467200	-2.82731900	3.06265700
H	1.33323300	-1.81465000	2.48575100
H	-0.46495500	-4.54938700	-0.76147800
H	-0.96661800	-4.23901200	-2.42602800
H	-1.19669100	-2.99589100	-1.19521500
H	2.83393000	-4.03929200	-2.47126500
H	1.43899300	-4.88611400	-3.15709100
H	1.87353800	-5.15045300	-1.46854600
H	0.26030700	-2.82743900	-3.94239700
H	1.78279700	-2.03165400	-3.49576600
H	0.23649600	-1.37741000	-2.93193400
H	-0.08061900	2.34450100	4.10744200
H	1.49359000	1.92461800	3.40406900
H	0.03677600	1.04356500	2.91382200
H	1.88500800	4.33777800	2.64654700
H	0.37898000	4.68299700	3.51346000
H	0.57258000	5.23462900	1.84959900
H	-1.81340900	3.48806300	2.83369700
H	-1.81228000	2.35450300	1.47340100
H	-1.57038000	4.07961800	1.18945500
H	0.71662000	2.24056600	-2.46564500
H	2.44445500	2.36887600	-2.10037100
H	1.63094300	3.67446800	-2.97762200
H	3.30541500	4.11638900	-0.50009900
H	2.21126900	5.20143500	0.36943100
H	2.41078600	5.36479400	-1.37910600
H	-0.00507600	5.10934700	-1.95952400
H	-0.29103900	5.18161900	-0.22086900
H	-0.99320400	3.86895200	-1.18948000
H	5.52270500	-1.18607800	-1.34576700
C	5.51157600	0.67411400	-0.22310000
H	5.14859500	2.47470300	0.93645600
H	6.58768600	0.81439700	-0.27125900
O	-1.34601800	-0.10332800	0.06130900
C	-1.57045700	-1.88355900	1.93308700
C	-1.33974800	-1.64339400	3.44681100
C	-2.47298700	-0.88592200	4.16939900
C	-3.04768600	0.29029100	3.35676000
C	-3.35009900	-0.00140100	1.85479300
H	-1.15496500	-2.59877200	3.96256300
H	-0.64066700	-2.28304000	1.51275700
H	-3.27594300	-1.58004300	4.43229300
H	-2.09339300	-0.50606800	5.12817100
H	-3.96879000	0.64349300	3.84455800
H	-2.34387200	1.12931700	3.41467400
H	-3.70587000	0.94025200	1.42598600
H	-0.41310400	-1.06292700	3.56118100
C	-4.49022000	-1.04968200	1.68583700
H	-5.36301200	-0.74338900	2.28242600
H	-4.82073900	-1.02694600	0.64183400
C	-2.69236800	-2.92674400	1.63133500

H	-2.44662300	-3.88798900	2.10982500
C	-4.11538000	-2.50450600	2.05633700
H	-2.69494900	-3.12307600	0.55007800
H	-4.23124200	-2.65656800	3.13325200
H	-4.83838600	-3.18675300	1.58906900
B	-2.02079000	-0.56513600	1.16104000
C	-2.35060400	-0.59973200	-2.42879700
C	-3.79951800	-1.00438100	-2.08222600
C	-4.80421400	0.16265500	-2.02053900
C	-4.28062400	1.42220400	-1.29049000
C	-2.78364500	1.77592100	-1.50757000
H	-4.17658300	-1.75345600	-2.79793100
H	-1.77189800	-1.52968000	-2.42379600
H	-5.10718900	0.42283700	-3.03952400
H	-5.72734700	-0.17670800	-1.52791300
H	-4.91023900	2.27899000	-1.58155800
H	-4.45711900	1.29125400	-0.21916600
H	-2.56108200	2.58453900	-0.79290200
H	-3.78321200	-1.51719000	-1.10927100
C	-2.55922600	2.36976600	-2.92929100
H	-3.20171200	3.25277800	-3.07971700
H	-1.52529900	2.73049200	-3.00324400
C	-2.20039400	-0.02292400	-3.86384700
H	-2.63062700	-0.71536800	-4.60603700
C	-2.80544000	1.38098900	-4.08862500
H	-1.12569200	0.03176900	-4.08982400
H	-3.88138700	1.29551900	-4.26998800
H	-2.39144500	1.80492600	-5.01503100
B	-1.74689300	0.51317900	-1.40323000
H	-0.61352300	0.84375700	-1.76680900

IMC1-2

	x	y	z
Ni	0.61416100	-0.06153200	0.24765000
P	1.22580700	2.15737900	0.01678500
P	0.65324000	-2.34695100	0.03103600
C	2.50368100	-0.29498200	0.02433200
O	2.90224500	2.07006800	0.01487600
C	0.93241300	2.90224400	-1.71076100
C	1.03916300	3.41204400	1.43684700
O	2.29605700	-2.68530600	0.01852900
C	0.16252200	-3.05925400	-1.67322900
C	0.15281000	-3.46015800	1.48483900
C	3.40300600	0.78088000	-0.01830200
C	3.10442100	-1.56284000	-0.01606800
C	1.65587700	4.24453800	-1.92908700
C	-0.57370700	3.05882700	-1.98004100
C	1.50991400	1.86985100	-2.70637900
C	-0.39264600	3.97588500	1.49230900
C	2.05589600	4.57025000	1.35477300
C	1.34952300	2.61146900	2.72398300
C	0.38826700	-1.91474400	-2.68615900
C	1.05757500	-4.25112300	-2.07292200
C	-1.31715000	-3.47591000	-1.72142900
C	0.92992300	-2.90688000	2.70251800
C	0.56079800	-4.93135100	1.27220500
C	-1.35962600	-3.36802900	1.76169000
C	4.78901100	0.63452200	-0.09418400

C	4.48280400	-1.76924100	-0.09023700
H	1.61868700	4.48880100	-2.99860200
H	2.70814600	4.20142200	-1.63248900
H	1.17019400	5.06670100	-1.39637400
H	-0.71431200	3.37125700	-3.02310000
H	-1.03408400	3.82245500	-1.34687800
H	-1.11426500	2.12063200	-1.83226300
H	2.58828500	1.73425200	-2.58121000
H	1.33140700	2.23549700	-3.72550000
H	1.02448300	0.89544200	-2.61163400
H	-0.58730900	4.67344300	0.67139000
H	-0.52341200	4.53165300	2.42963900
H	-1.15733300	3.19520700	1.45705200
H	3.07879700	4.20457600	1.23557700
H	2.00613900	5.13816200	2.29292500
H	1.83720500	5.26487400	0.54254900
H	1.27814400	3.28622100	3.58657100
H	2.36458400	2.20105300	2.70433500
H	0.64969100	1.78933800	2.88534900
H	0.17373800	-2.28855000	-3.69598400
H	1.42353000	-1.55753500	-2.67635900
H	-0.28040700	-1.07098500	-2.48888300
H	2.11644000	-3.98240100	-2.08011900
H	0.77684900	-4.56194800	-3.08753600
H	0.93004500	-5.11570900	-1.41755100
H	-1.57054400	-3.74270800	-2.75543500
H	-1.98449800	-2.66668900	-1.41753900
H	-1.52088600	-4.35410000	-1.10118500
H	0.68123400	-1.86120400	2.90931300
H	2.01199200	-2.97973800	2.56123700
H	0.66170800	-3.49497300	3.58919200
H	1.61888300	-5.02957400	1.01221900
H	-0.03946700	-5.41770900	0.49785800
H	0.39175700	-5.48167200	2.20706200
H	-1.57685500	-3.87605600	2.71016000
H	-1.95441300	-3.85510900	0.98548000
H	-1.70280400	-2.33560600	1.84172000
H	5.42287800	1.51475300	-0.12450400
C	5.32076600	-0.65462400	-0.12733300
H	4.87558200	-2.78043200	-0.11640400
H	6.39699000	-0.79171400	-0.18460200
H	-1.56354800	1.35674200	2.44391200
H	-2.38170200	-0.21028300	2.54008200
C	-1.47622900	0.29312500	2.19000500
H	-0.62322900	-0.11987100	2.74310300
O	-1.28984500	0.08996900	0.79994400
C	-3.34012600	1.65268200	-0.14008400
C	-4.13563300	1.75399400	-1.47180400
C	-5.05851100	0.55195600	-1.78077700
C	-4.45009800	-0.83400000	-1.46580300
C	-3.67186400	-0.91973300	-0.12333400
H	-4.74344900	2.67391000	-1.49339300
H	-2.67599900	2.53138100	-0.11796800
H	-5.99863200	0.66562000	-1.23119400
H	-5.34315200	0.58435100	-2.84266000
H	-5.25846000	-1.58361100	-1.49662300
H	-3.75585200	-1.09988800	-2.27571800
H	-3.25179200	-1.93632700	-0.07832900

H	-3.41003700	1.85027500	-2.29144200
C	-4.61275200	-0.80397600	1.10478500
H	-5.43964200	-1.52885300	1.02046900
H	-4.05914900	-1.11409200	2.00343200
C	-4.26018500	1.78023600	1.10359900
H	-4.86223200	2.70193300	1.03873100
C	-5.22161500	0.59553500	1.35118500
H	-3.63199000	1.91223200	1.99533400
H	-6.10651900	0.71512200	0.71817400
H	-5.60056700	0.64832900	2.38251700
B	-2.51699500	0.24040300	-0.21821900
H	-1.90510300	0.14112100	-1.28193200

IMD1-2

	x	y	z
C	-4.21873300	-3.03774800	-0.72516500
C	-3.17713000	-2.27923400	-0.18803100
C	-2.56459500	-1.20603000	-0.84850100
C	-3.08732100	-0.93394500	-2.12218600
C	-4.12214800	-1.66051500	-2.71378100
C	-4.68518200	-2.71815500	-2.00015700
H	-4.63734500	-3.85862800	-0.15212700
H	-4.47363500	-1.38664000	-3.70318100
H	-5.49382300	-3.29568300	-2.43927100
O	-2.56494800	0.12659700	-2.83581400
O	-2.72509800	-2.62939000	1.07094500
P	-1.56582500	1.11392400	-1.91723000
P	-1.29388500	-1.88800800	1.52811300
C	-0.22253900	1.40914500	-3.22245300
C	-2.73771700	2.60658900	-1.67280900
C	-0.15373200	-3.42203900	1.44954600
C	-1.78456800	-1.42685900	3.30858000
H	1.73533000	-0.33448300	1.63259800
C	1.68030800	0.28851700	0.72923800
O	0.43654900	0.89690000	0.61251300
O	1.90615800	-0.56814700	-0.39723800
H	2.46109500	1.04590300	0.76716800
Ni	-1.10914900	-0.20169500	-0.08664700
C	-3.59006000	2.28089400	-0.42464400
H	-2.97094600	2.18061800	0.47100600
H	-4.29890000	3.10298100	-0.25874600
H	-4.17027700	1.36148200	-0.55520500
C	-1.95226700	3.90512200	-1.42573900
H	-1.41064600	4.23747000	-2.31719500
H	-2.66201100	4.69961300	-1.16125200
H	-1.24619300	3.80591600	-0.60047400
C	-3.68907800	2.78995300	-2.87419500
H	-4.37634100	3.61247300	-2.63743400
H	-3.16568900	3.05400000	-3.79554700
H	-4.28522400	1.89446400	-3.06444900
C	-0.76992600	2.06999400	-4.50180600
H	-1.06358400	3.11032400	-4.33631300
H	0.02347000	2.07194700	-5.26070600
H	-1.62355400	1.52243500	-4.91204000
C	0.92848600	2.25244100	-2.64350400
H	1.74140000	2.29010500	-3.38050800
H	0.62622700	3.28179900	-2.43519200
H	1.32197400	1.82359200	-1.72011000

C	0.30575900	0.00039800	-3.57738800
H	0.68958500	-0.52251000	-2.69739100
H	-0.46869900	-0.61627500	-4.04209200
H	1.13075200	0.10606500	-4.29349800
C	-0.11575100	-3.82756200	-0.04279200
H	-1.10412000	-4.10695400	-0.41880500
H	0.28119300	-3.02520300	-0.67260700
H	0.54230100	-4.69954200	-0.15222700
C	1.28571600	-3.12795000	1.91015200
H	1.87135500	-4.05261200	1.82439200
H	1.76459500	-2.38030100	1.27659300
H	1.34497200	-2.80065300	2.95091800
C	-0.72363700	-4.59575800	2.27119000
H	-0.15075400	-5.50147100	2.03280700
H	-0.63044300	-4.42844200	3.34845900
H	-1.77324000	-4.78973100	2.03475900
C	-0.55006900	-1.33185300	4.22428000
H	-0.83955700	-0.84717600	5.16497800
H	-0.15545500	-2.32175000	4.47462300
H	0.25534300	-0.73353800	3.79038800
C	-2.79756600	-2.41865600	3.91978100
H	-2.38546100	-3.42104900	4.05422600
H	-3.08291100	-2.04256200	4.91083200
H	-3.70199800	-2.49918600	3.31312200
C	-2.47474200	-0.04880200	3.19006700
H	-1.80702300	0.72280700	2.80081400
H	-3.35439000	-0.10348100	2.53832400
H	-2.81714400	0.26521000	4.18456800
C	4.54566400	-0.48842500	-0.17707100
C	5.22315000	-1.78382700	0.36792200
C	5.32840900	-2.95344800	-0.63550400
C	4.04821100	-3.20261100	-1.46297200
C	3.35738400	-1.92198300	-2.02040900
H	6.22625500	-1.54463700	0.75031100
H	4.46396100	0.20606000	0.66949900
H	6.17283700	-2.78270000	-1.30909600
H	5.57837100	-3.86988100	-0.08382300
H	4.27942300	-3.89371000	-2.28721500
H	3.31711200	-3.72729400	-0.83009300
H	2.40339600	-2.23173500	-2.46834600
H	4.64473400	-2.12096000	1.24134500
C	4.17610100	-1.17930800	-3.11591900
H	4.40348300	-1.86424000	-3.94627000
H	3.53054500	-0.39669800	-3.54059800
C	5.35392800	0.24222500	-1.29119100
H	6.35770100	0.49412400	-0.91875600
C	5.48565200	-0.52221800	-2.62679200
H	4.85744000	1.20485900	-1.48451500
H	6.26735900	-1.28214600	-2.53827600
H	5.84291200	0.17369600	-3.39779600
B	3.16214100	-0.92894900	-0.80818900
C	0.95457400	3.60183100	0.91581200
C	0.25221100	4.80473900	1.61117600
C	0.23538800	4.76248900	3.15571100
C	-0.08869300	3.37566600	3.75132000
C	0.63082900	2.18343200	3.06135900
H	0.71078200	5.75469000	1.29079500
H	0.80655400	3.74877700	-0.16445500

H	1.19957700	5.10884300	3.54253700
H	-0.49958300	5.49264700	3.52448800
H	0.13991700	3.39466500	4.82959400
H	-1.17172900	3.20635500	3.67042400
H	0.24847100	1.28298400	3.56257200
H	-0.78919400	4.83792600	1.26316100
C	2.16264100	2.19918800	3.31287000
H	2.36809700	2.28875300	4.39222200
H	2.57864100	1.22171500	3.02982700
C	2.48869400	3.62314300	1.13891000
H	2.90100900	4.60485900	0.85311900
C	2.95618900	3.30899600	2.58047000
H	2.95770300	2.91276800	0.44137700
H	2.90766100	4.22810600	3.17227900
H	4.02214900	3.03822500	2.56425900
B	0.20057800	2.26474200	1.48531000
H	-1.01193200	2.35768400	1.36901000

TSA1

	x	y	z
C	1.10341100	3.73677000	-0.33295600
C	1.10758700	2.34579900	-0.22457200
C	-0.06391600	1.58168400	-0.13787300
C	-1.26807300	2.29924800	-0.14884300
C	-1.32617600	3.68892100	-0.25487300
C	-0.12656800	4.39792900	-0.34880500
H	2.04177500	4.27773300	-0.39859400
H	-2.28738400	4.19247300	-0.26228000
H	-0.15064300	5.48080900	-0.43245000
O	-2.46011500	1.59510100	-0.04948000
O	2.33028100	1.69178400	-0.19528200
P	-2.24141200	-0.06792200	0.04760500
P	2.20068700	0.02986300	0.01569300
C	-3.11257700	-0.44386200	1.69020100
C	-3.19410900	-0.62364500	-1.49595000
C	3.08918300	-0.18772900	1.67820700
C	3.17827000	-0.58749600	-1.48759100
H	-0.08144000	-1.86525800	0.83196600
Ni	-0.02055700	-0.30262200	0.02071200
C	-2.25808100	-0.29841700	-2.68426300
H	-1.32985900	-0.87057900	-2.62428100
H	-2.77184100	-0.56828800	-3.61600500
H	-2.01872200	0.76941100	-2.73413600
C	-4.51415500	0.15206800	-1.68226200
H	-4.93151300	-0.11287400	-2.66214000
H	-5.26372800	-0.10059000	-0.92915500
H	-4.35564800	1.23376300	-1.66435600
C	-3.45818500	-2.14143600	-1.46386100
H	-3.87758300	-2.44244900	-2.43253500
H	-2.53543900	-2.70778800	-1.31093800
H	-4.18890500	-2.41808000	-0.69685500
C	-4.59803700	-0.03601000	1.69533200
H	-5.21015000	-0.70374800	1.08243100
H	-4.97886000	-0.09804200	2.72294400
H	-4.74202200	0.99138300	1.34727600
C	-2.97273500	-1.93827100	2.04562600
H	-3.41791100	-2.10690700	3.03448700
H	-3.49004800	-2.59085500	1.33742000

H	-1.92667700	-2.25542200	2.09671400
C	-2.35959700	0.39237200	2.75064000
H	-1.29469500	0.13948000	2.78517200
H	-2.45073400	1.46627300	2.56379000
H	-2.78866200	0.18058800	3.73808300
C	2.21344400	0.57084100	2.70270800
H	2.12563000	1.63509700	2.46348700
H	1.20541900	0.14788700	2.76392300
H	2.67636200	0.48346200	3.69370300
C	3.15464200	-1.67549600	2.08075300
H	3.47010000	-1.73832300	3.13030200
H	2.19611000	-2.19374800	1.98420300
H	3.88528800	-2.23095700	1.48747300
C	4.50120000	0.42822800	1.67657500
H	4.88391700	0.44150300	2.70536200
H	5.20280000	-0.15947100	1.07785300
H	4.49800800	1.45733900	1.30469900
C	4.41912600	0.28439600	-1.77102200
H	4.87098400	-0.05737000	-2.71095000
H	4.15697900	1.33961700	-1.88452100
H	5.18024300	0.20076100	-0.99159200
C	3.59462800	-2.06340600	-1.31822700
H	3.96005700	-2.43226500	-2.28505800
H	4.41276900	-2.17474000	-0.59970100
H	2.76956100	-2.71143600	-1.00858300
C	2.20126000	-0.46468600	-2.68100500
H	1.34113100	-1.12822900	-2.56042500
H	1.84424700	0.56324100	-2.81059000
H	2.73210000	-0.74993700	-3.59848200
O	-0.12045600	-2.38667000	-1.16362400
C	0.23087800	-2.69252700	0.00219000
O	0.82240800	-3.63656700	0.50740500

TSA2-2

	x	y	z
C	-4.26180900	-1.30099700	0.38686000
C	-5.17433600	-0.70654000	1.48713800
C	-6.00105300	0.52823900	1.06448500
C	-5.21804800	1.56599600	0.22980700
C	-4.31201500	0.97422400	-0.87850200
H	-5.85936000	-1.47273500	1.88535300
H	-3.66997300	-2.10029600	0.86660200
H	-6.88402900	0.20121200	0.50583800
H	-6.39705400	1.01807000	1.96624200
H	-5.93339000	2.29006600	-0.19312800
H	-4.57431900	2.14055400	0.91174400
H	-3.75526500	1.81680500	-1.31956300
H	-4.53164100	-0.41483600	2.33182000
C	-5.08516600	0.30455500	-2.04714600
H	-5.80484600	1.00932600	-2.49399100
H	-4.35486400	0.07521800	-2.83706400
C	-5.02661500	-1.97000100	-0.78669300
H	-5.70573600	-2.75412300	-0.41429000
C	-5.83131300	-1.00039100	-1.68306200
H	-4.28438700	-2.48503800	-1.41487900
H	-6.77996700	-0.75566900	-1.19404200
H	-6.11159500	-1.52192200	-2.60983100
B	-3.33681300	-0.15921600	-0.28431400

C	4.32024100	1.36869700	-1.98334900
C	3.15268200	1.28626600	-1.22411400
C	2.58573900	0.07431900	-0.80513700
C	3.28701400	-1.08008700	-1.18414300
C	4.45796900	-1.05581000	-1.94200200
C	4.96446200	0.18274000	-2.33996200
H	4.70650200	2.33843000	-2.27967000
H	4.95164200	-1.98519200	-2.20637700
H	5.87429100	0.22438300	-2.93216600
O	2.79884200	-2.31562300	-0.78220900
O	2.52932500	2.47054200	-0.86220500
P	1.38529000	-2.21358300	0.11420500
P	1.14931800	2.25301000	0.06672200
C	0.23471200	-3.25167100	-0.97387300
C	1.93137800	-3.04435200	1.73081900
C	-0.11991000	3.17070100	-1.00701600
C	1.63988200	3.18650600	1.64197400
H	-1.94920200	0.01039300	2.82029300
Ni	1.01624100	0.00682200	0.26335000
C	3.07221600	-2.15186100	2.27317100
H	2.73505600	-1.12562300	2.45347800
H	3.41878000	-2.56388300	3.22940300
H	3.92578100	-2.11849800	1.58974700
C	2.47047600	-4.47326300	1.53117800
H	2.94101800	-4.80715400	2.46513400
H	1.67341500	-5.18502000	1.29884500
H	3.22559900	-4.52015300	0.74046200
C	0.77479400	-3.04545000	2.75093000
H	1.15576900	-3.41001600	3.71362400
H	0.36888400	-2.04180100	2.90292900
H	-0.04392800	-3.70611600	2.45242700
C	0.90734200	-4.54172200	-1.48546700
H	1.07187500	-5.27521900	-0.69313700
H	0.24373300	-5.00400200	-2.22719000
H	1.86457600	-4.33455500	-1.97175000
C	-1.07109800	-3.58479800	-0.22999600
H	-1.77614100	-4.03601500	-0.93883500
H	-0.91312000	-4.30746300	0.57697700
H	-1.55749700	-2.69438400	0.17758600
C	-0.08198200	-2.34811700	-2.18922700
H	-0.62807900	-1.44699800	-1.89673400
H	0.82625100	-2.05670300	-2.72733900
H	-0.71875800	-2.90898400	-2.88488800
C	-0.57348300	2.13735600	-2.06462600
H	0.27186600	1.76128600	-2.65222200
H	-1.09603100	1.28907300	-1.61308800
H	-1.26942400	2.62518000	-2.75866100
C	-1.33737400	3.62893700	-0.18251100
H	-2.09682900	4.01929900	-0.87108900
H	-1.80112700	2.80741400	0.36967100
H	-1.08451300	4.43679300	0.51222300
C	0.50957300	4.37805100	-1.73369300
H	-0.24596500	4.80056600	-2.40828500
H	0.81820500	5.17139600	-1.04885200
H	1.37473100	4.08565300	-2.33333800
C	1.93262000	4.67708200	1.38710700
H	2.35508600	5.11783100	2.29947100
H	2.65962000	4.81579600	0.58107500

H	1.02761600	5.24065800	1.14297800
C	0.54523800	3.02996800	2.71797500
H	0.88029100	3.53066500	3.63540400
H	-0.40438100	3.48519600	2.42411900
H	0.36367300	1.97856600	2.95838200
C	2.93142500	2.50411200	2.14882200
H	2.77770900	1.43804100	2.34786500
H	3.75395400	2.60460600	1.43482400
H	3.23666400	2.98045200	3.08904600
O	-0.36723900	-0.10766900	1.61472200
C	-1.59452600	0.14046600	1.78233600
O	-2.42919100	0.55307200	0.93919700
H	-2.48909000	-0.56837400	-1.05784000

TSA3-2

	x	y	z
Ni	0.51682500	0.04729200	0.04555200
P	0.64009100	2.35236300	-0.06732700
P	1.07570100	-2.19054700	-0.06810000
O	-1.37999500	-0.13104500	1.27770500
C	2.42029100	0.22992200	-0.06559400
O	2.29298100	2.62092400	-0.07379200
C	0.19898400	3.19578100	-1.73240900
C	0.21917200	3.41394800	1.45317000
O	2.74943800	-2.14163300	-0.08041800
C	0.79696500	-3.10308900	-1.73124500
C	0.86563800	-3.30986900	1.45444000
C	-1.68951000	-0.16273500	2.56013100
C	3.06219100	1.47653800	-0.08610500
C	3.28745700	-0.87188800	-0.08931500
C	1.23077100	4.28529200	-2.09835800
C	-1.20924000	3.81687000	-1.73182400
C	0.26800500	2.08346200	-2.80228500
C	-1.29124700	3.43900800	1.74787500
C	0.74535400	4.85534800	1.30142700
C	0.95108300	2.73271200	2.63440100
C	0.65781700	-1.99869000	-2.80258500
C	2.01204000	-3.98323900	-2.09767700
C	-0.47228500	-3.97352300	-1.72692600
C	1.45931800	-2.50166200	2.63326800
C	1.65199400	-4.62760900	1.30371900
C	-0.61300300	-3.61641400	1.75209800
O	-0.86897400	-0.08578900	3.45633500
H	-2.76618700	-0.26589300	2.76614500
C	4.44804400	1.63963600	-0.11897600
C	4.67902400	-0.76864300	-0.12223100
H	0.95389700	4.69958300	-3.07654500
H	2.24261900	3.88190500	-2.17353400
H	1.24699700	5.11029700	-1.38244700
H	-1.43713400	4.16688000	-2.74685500
H	-1.27710500	4.68369300	-1.06745800
H	-1.98534500	3.10227200	-1.45198900
H	1.25417700	1.60704300	-2.82873300
H	0.08324400	2.52536800	-3.79015100
H	-0.48124400	1.30593300	-2.62986700
H	-1.86312000	3.96491500	0.97885800
H	-1.45175800	3.96681400	2.69649600
H	-1.70243500	2.43452400	1.85340200

H	1.80923100	4.87719100	1.04944700
H	0.61620500	5.37497500	2.25961800
H	0.19217800	5.42375700	0.54743800
H	0.75383200	3.31558000	3.54337200
H	2.03418500	2.71071900	2.48141800
H	0.59485200	1.71391000	2.81281400
H	0.55813900	-2.46869200	-3.78973800
H	1.53846100	-1.34759300	-2.83027100
H	-0.22276800	-1.37361200	-2.63098000
H	2.93154300	-3.39943500	-2.17466900
H	1.81544300	-4.44283100	-3.07504900
H	2.18154300	-4.79009500	-1.38101100
H	-0.63527200	-4.35912500	-2.74153900
H	-1.36605200	-3.41484300	-1.44333800
H	-0.37613200	-4.83808200	-1.06323300
H	0.91813300	-1.56796000	2.81231900
H	2.51857000	-2.27650100	2.47735800
H	1.37760300	-3.11032400	3.54306100
H	2.70092800	-4.45071500	1.05004500
H	1.21380000	-5.29081500	0.55155400
H	1.62364200	-5.16056900	2.26287700
H	-0.67108600	-4.15973100	2.70373700
H	-1.07651100	-4.24440700	0.98670500
H	-1.20513300	-2.70624500	1.85284900
H	4.86924500	2.63956600	-0.12888200
C	5.25336600	0.50168700	-0.13538300
H	5.28258300	-1.67027000	-0.13463400
H	6.33443400	0.60541700	-0.15986900
C	-3.09936300	-1.59602000	-0.22503000
C	-4.26153100	-1.70844200	0.79680700
C	-5.20394200	-0.48485000	0.87669400
C	-4.49780300	0.88826500	0.79167700
C	-3.33654300	0.98293600	-0.23248400
H	-4.86833100	-2.60315100	0.58518100
H	-2.47937500	-2.48936000	-0.06955900
H	-5.95038500	-0.55410100	0.07954700
H	-5.77951800	-0.53546700	1.81179400
H	-5.25622700	1.65835100	0.57901900
H	-4.10134600	1.14707700	1.78437300
H	-2.88871400	1.97469800	-0.08336800
H	-3.82753000	-1.88913500	1.79104000
C	-3.81958700	0.93305700	-1.70670800
H	-4.56481400	1.72202600	-1.89640000
H	-2.96109900	1.16699400	-2.35346700
C	-3.58033900	-1.64292000	-1.70010800
H	-4.16684900	-2.55670400	-1.88666900
C	-4.40319100	-0.42147000	-2.16087000
H	-2.69235800	-1.71719500	-2.34505300
H	-5.43339800	-0.51646800	-1.80406900
H	-4.47580400	-0.43100500	-3.25770900
B	-2.26433500	-0.21798200	-0.02685000
H	-1.29593700	-0.13071900	-0.84938300

TSA4-2

	x	y	z
C	-3.51250900	-1.28917200	-0.13339200
C	-4.84535800	-1.29015200	0.66373700
C	-5.67080800	0.01448700	0.58208300

C	-4.83613800	1.31277900	0.67058300
C	-3.50363100	1.30625000	-0.12695800
H	-5.48221700	-2.13097700	0.34490500
H	-3.01339600	-2.23769500	0.12243800
H	-6.25708700	0.01904000	-0.34255300
H	-6.41459100	0.01497300	1.39180600
H	-5.46703600	2.15981200	0.35636700
H	-4.58825600	1.49391600	1.72472200
H	-2.99757100	2.24997200	0.13310100
H	-4.59903100	-1.47865800	1.71694200
C	-3.70051000	1.30398900	-1.66279300
H	-4.31083700	2.16563600	-1.97851700
H	-2.71732900	1.44508600	-2.13463700
C	-3.70863400	-1.27830300	-1.66922900
H	-4.32415100	-2.13456500	-1.98947000
C	-4.31915100	0.01619800	-2.24457900
H	-2.72606800	-1.42313800	-2.14134500
H	-5.40100500	0.01913800	-2.08239200
H	-4.19041500	0.01856100	-3.33674900
B	-2.63141300	0.00444400	0.30721900
C	4.66159000	1.19679400	-0.41989800
C	3.27723800	1.17133200	-0.24324900
C	2.52249200	-0.00728400	-0.15559600
C	3.27045300	-1.19045100	-0.24025200
C	4.65462600	-1.22436800	-0.41680800
C	5.34487100	-0.01587200	-0.50705400
H	5.17748400	2.14964000	-0.47879900
H	5.16500900	-2.18031800	-0.47337300
H	6.42256300	-0.01914100	-0.64384800
O	2.61342300	-2.40123600	-0.13601500
O	2.62733000	2.38618200	-0.14195500
P	0.94814300	-2.27154300	0.00286400
P	0.96174800	2.26689500	0.00250400
C	0.43433800	-3.08921500	-1.65021600
C	0.70735800	-3.42195600	1.49403200
C	0.44832500	3.09018000	-1.64779100
C	0.73258200	3.41673700	1.49601700
H	-1.66797000	-0.00043000	3.65675300
Ni	0.64710100	-0.00152500	0.24696700
C	1.48292300	-2.75509500	2.65553200
H	1.10155200	-1.75573600	2.87887100
H	1.36595300	-3.37642100	3.55303400
H	2.55229500	-2.68290400	2.43579200
C	1.29686300	-4.82580100	1.25256100
H	1.25654100	-5.38871100	2.19425000
H	0.73045700	-5.39591300	0.51041000
H	2.34295500	-4.77794700	0.93634200
C	-0.78181400	-3.53606900	1.87485800
H	-0.85969700	-4.06541100	2.83327100
H	-1.25763800	-2.56080300	1.99465900
H	-1.35920500	-4.10330500	1.14101900
C	1.50700500	-4.08430300	-2.14284500
H	1.64948300	-4.92558000	-1.46073900
H	1.17603900	-4.49082000	-3.10743700
H	2.47506500	-3.60104300	-2.29149800
C	-0.92196700	-3.80995000	-1.54970600
H	-1.24086700	-4.10164900	-2.55846800
H	-0.85682500	-4.72501500	-0.95351900

H	-1.70676800	-3.17701200	-1.13128100
C	0.33127100	-1.94050600	-2.67704500
H	-0.44966700	-1.22449700	-2.40795900
H	1.27648700	-1.39556500	-2.77165000
H	0.08528000	-2.36053000	-3.66102700
C	0.33580100	1.94344300	-2.67584100
H	1.27782300	1.39359400	-2.77403600
H	-0.44810300	1.23122600	-2.40536800
H	0.08911400	2.36606400	-3.65853400
C	-0.90328100	3.81902300	-1.54237000
H	-1.22342000	4.11393200	-2.54980000
H	-1.69072200	3.19045900	-1.12232800
H	-0.83066500	4.73289300	-0.94521800
C	1.52552000	4.07951300	-2.14218100
H	1.19415000	4.48935300	-3.10522900
H	1.67506400	4.91897600	-1.45936200
H	2.49019300	3.59062600	-2.29434100
C	1.32931500	4.81747700	1.25445100
H	1.29510400	5.37947000	2.19692700
H	2.37414900	4.76399500	0.93497300
H	0.76395700	5.39174100	0.51471300
C	-0.75468000	3.53855900	1.88183600
H	-0.82662100	4.06812900	2.84059000
H	-1.33173600	4.10877000	1.15004100
H	-1.23451600	2.56546500	2.00322400
C	1.50795600	2.74391600	2.65419400
H	1.12072900	1.74693900	2.87807000
H	2.57608400	2.66505000	2.43070700
H	1.39811700	3.36525100	3.55259600
O	-0.27579300	0.00334800	2.19617400
C	-1.46080500	0.00106700	2.57442400
O	-2.51981600	-0.00017100	1.85941700
H	-1.43696500	0.00179400	-0.15873300

TSA5-2

	x	y	z
C	-3.44476000	-1.42635900	0.12036600
C	-4.93711400	-1.30921800	0.57991900
C	-5.72827800	-0.12426800	-0.02172700
C	-4.94595800	1.20841200	-0.08182000
C	-3.45699600	1.09494800	-0.55401200
H	-5.46432400	-2.24712800	0.35061100
H	-3.00681900	-2.23507100	0.70911900
H	-6.07660000	-0.38982900	-1.02415000
H	-6.64102600	0.02924400	0.57030200
H	-5.48608900	1.91427000	-0.73045700
H	-4.93869500	1.65860300	0.91984100
H	-3.02277500	2.09155900	-0.40976300
H	-4.94349900	-1.22489000	1.67532700
C	-3.29691100	0.70435600	-2.03888800
H	-3.82467100	1.42252200	-2.68505500
H	-2.23106100	0.78965000	-2.29298000
C	-3.27619500	-1.78304100	-1.37502200
H	-3.76861700	-2.74270600	-1.59510000
C	-3.75678400	-0.72502600	-2.38746300
H	-2.20467600	-1.93878100	-1.54576600
H	-4.84678300	-0.75636300	-2.47565400
H	-3.37770800	-0.98984900	-3.38454300

B	-2.84613000	0.00895800	0.43142100
C	4.59235800	1.60469700	0.31433000
C	3.20865200	1.45204900	0.20600600
C	2.56020400	0.21452400	0.13235600
C	3.41042200	-0.89626800	0.16628900
C	4.80051200	-0.81221900	0.27256800
C	5.38216000	0.45428200	0.34799200
H	5.02742000	2.59740900	0.36978800
H	5.39906700	-1.71717300	0.29585200
H	6.46172300	0.54582700	0.43176900
O	2.84488700	-2.15234900	0.09285400
O	2.43441600	2.59640400	0.16929500
P	1.16732800	-2.15837100	-0.06962400
P	0.78498800	2.31289500	-0.01993800
C	1.03093000	-3.00686200	-1.79068900
C	0.82938000	-3.36223300	1.36348300
C	0.54363800	3.16990300	-1.71772400
C	0.21321300	3.38190400	1.45048700
H	-2.46860100	0.53371500	3.75424200
Ni	0.62834200	0.04971100	0.02577200
C	1.22337100	-2.57753600	2.63702400
H	0.58812100	-1.69762100	2.77622300
H	1.08081500	-3.22827800	3.50906700
H	2.27085500	-2.26225200	2.61756800
C	1.71018000	-4.62450700	1.25624900
H	1.57690700	-5.21892300	2.16941700
H	1.42497700	-5.26071400	0.41247300
H	2.77108300	-4.37766600	1.16479400
C	-0.65188200	-3.75969100	1.47565200
H	-0.77031800	-4.39906300	2.36043400
H	-1.29184600	-2.89013900	1.62653900
H	-1.00714900	-4.32967400	0.61418300
C	2.34447100	-3.73024700	-2.15589400
H	2.59531400	-4.52477600	-1.44881400
H	2.22030400	-4.18797900	-3.14626700
H	3.19147000	-3.04230500	-2.20184200
C	-0.13089900	-4.01439100	-1.87859800
H	-0.23292600	-4.33965900	-2.92212500
H	0.05399100	-4.90752100	-1.27569800
H	-1.08902400	-3.58709100	-1.57607200
C	0.79649500	-1.87320100	-2.81291600
H	-0.14252700	-1.34361400	-2.62517600
H	1.60902400	-1.13930600	-2.79437300
H	0.75188600	-2.29972400	-3.82396600
C	0.81046000	2.07296700	-2.77285300
H	1.81596300	1.65078400	-2.67300600
H	0.08859400	1.25423100	-2.69936800
H	0.72820800	2.51119800	-3.77630500
C	-0.88161800	3.71797400	-1.90556200
H	-1.00480300	4.03000000	-2.95082600
H	-1.65116500	2.97233300	-1.69480800
H	-1.06793400	4.59686300	-1.28125800
C	1.55932200	4.31001700	-1.93832800
H	1.41035400	4.71188100	-2.94929500
H	1.42629400	5.13316000	-1.23288200
H	2.59017500	3.95904600	-1.85850000
C	0.86621100	4.77894700	1.43713100
H	0.66378500	5.26908600	2.39861100

H	1.94959500	4.72721700	1.30467400
H	0.44512200	5.41887100	0.65533000
C	-1.31515400	3.53389600	1.52905400
H	-1.56115200	4.07631500	2.45203700
H	-1.71951600	4.11629400	0.69720900
H	-1.82780700	2.57207800	1.56446300
C	0.70470900	2.60757200	2.69632000
H	0.26912000	1.60395700	2.74714400
H	1.79411300	2.50833900	2.71214400
H	0.40147700	3.15481400	3.59823100
O	-2.18617400	-1.33510800	3.01899300
C	-2.42843900	-0.15678000	2.89470900
O	-2.67204800	0.51684200	1.77043500
H	-0.96815900	-0.07963400	-0.02188200

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	x	y	z
C	0.10431200	-0.07468000	1.13041600
C	-0.50985600	1.34712300	1.32032200
C	-1.59601200	1.74093700	0.29414800
C	-1.25473300	1.38493100	-1.17027800
C	-0.64560900	-0.03399800	-1.38524700
H	-0.91970300	1.44061100	2.33636300
H	0.93209900	-0.16954900	1.84793500
H	-2.54840500	1.28087300	0.57277100
H	-1.76594000	2.82356300	0.36297600
H	-2.15481300	1.50337600	-1.79089000
H	-0.52899700	2.11828000	-1.55067900
H	-0.32438000	-0.10690400	-2.43244600
H	0.31281400	2.07417100	1.25985600
C	-1.62529000	-1.21114700	-1.10011000
H	-2.52654600	-1.10770000	-1.72166200
H	-1.13736100	-2.13900900	-1.43380100
C	-0.88554300	-1.24988300	1.39179500
H	-1.29986700	-1.16871200	2.40709000
C	-2.04444700	-1.37723100	0.37771400
H	-0.30537500	-2.18493500	1.38049100
H	-2.82563600	-0.65193300	0.62185600
H	-2.51382900	-2.36202200	0.50323800
B	0.54756600	-0.16703200	-0.37640400
H	3.06268400	-1.49609700	0.33089100
O	3.75922800	0.40267500	0.12313500
C	2.95688100	-0.46803300	-0.05354200
O	1.84167500	-0.32354600	-0.82854500

TSB1-2

	x	y	z
C	-5.21487500	-0.17372200	-0.39716600
C	-3.86099800	-0.47602600	-0.25003500
C	-2.85511900	0.49891600	-0.21002800
C	-3.29152400	1.82825700	-0.28284100
C	-4.63259300	2.18518800	-0.43072300
C	-5.58770600	1.16865900	-0.49224200
H	-5.94836600	-0.97280800	-0.42948700
H	-4.91081500	3.23255100	-0.48743900
H	-6.63690000	1.42599100	-0.60763600
O	-2.35136400	2.84054500	-0.19028000
O	-3.49755300	-1.80991700	-0.12724000

P	-0.77966800	2.29313500	0.05757500
P	-1.84508600	-2.03653100	0.06080100
C	0.07576400	3.11204000	-1.42840300
C	-0.39351800	3.09767400	1.72952300
C	-1.50906500	-3.11991000	-1.46242700
C	-1.80010800	-2.96109600	1.71604600
H	1.51306300	-1.67538500	0.29082300
C	1.33862700	-0.66635500	-0.13511300
O	1.04887500	-0.56081500	-1.36947300
O	2.43626400	0.18150800	0.36293200
H	0.47485400	-0.24859900	0.68858200
Ni	-1.03093000	0.05918100	0.07364600
C	4.92705900	0.69905500	0.65270400
C	5.72391100	-0.09629900	1.72619000
C	6.15876400	-1.51733300	1.30377700
C	5.06090100	-2.33497400	0.58570900
C	4.24018900	-1.56036800	-0.48568200
H	6.61233700	0.47245600	2.04081000
H	4.57759600	1.63063400	1.11971300
H	7.04458400	-1.45333200	0.66503800
H	6.48438800	-2.06920700	2.19643300
H	5.51675500	-3.23129200	0.13795900
H	4.35321600	-2.70676600	1.34277500
H	3.43689400	-2.22278300	-0.83166400
H	5.08794300	-0.17604300	2.62098800
C	5.05065100	-1.14517100	-1.74975500
H	5.48972500	-2.03706800	-2.22218200
H	4.33246900	-0.74018200	-2.47683300
C	5.74782200	1.08333600	-0.61245800
H	6.64566400	1.65227100	-0.32611700
C	6.16422900	-0.10144200	-1.51317700
H	5.13256500	1.77397500	-1.20828400
H	7.04463500	-0.59344400	-1.08876900
H	6.49229700	0.29158800	-2.48534300
B	3.72685800	-0.21716400	0.17945000
C	-0.26249700	2.20314000	-2.63385800
H	0.16485000	1.20553400	-2.50259400
H	-1.34445800	2.11574800	-2.78618100
H	0.16406300	2.65455500	-3.53933700
C	1.60402500	3.15285000	-1.24245000
H	2.01400100	2.17230800	-0.98838000
H	2.05910300	3.47379300	-2.18852500
H	1.90693900	3.87446100	-0.47625200
C	-0.46787000	4.52932800	-1.70244500
H	-0.19324300	5.24782700	-0.92635900
H	-0.03238700	4.88374000	-2.64568500
H	-1.55549300	4.53422300	-1.80955500
C	-0.09860700	-3.73696500	-1.41388500
H	0.06311300	-4.30396400	-2.33985800
H	0.66800800	-2.95915800	-1.36794600
H	0.02721600	-4.43844900	-0.58182600
C	-1.58556800	-2.14664100	-2.66344400
H	-2.56973300	-1.67241700	-2.74184400
H	-0.81407100	-1.37648600	-2.59076600
H	-1.41856700	-2.72053400	-3.58443800
C	-2.57458200	-4.22026800	-1.64705700
H	-2.43153300	-4.66990700	-2.63793900
H	-2.48864300	-5.02209800	-0.91050000

H	-3.58939200	-3.81547000	-1.60508500
C	-0.33627700	-3.12958400	2.17218300
H	-0.32469300	-3.60053000	3.16345900
H	0.24431500	-3.76774700	1.49954300
H	0.17448600	-2.16511700	2.25666800
C	-2.50445600	-4.33012100	1.69321700
H	-1.94210700	-5.07126200	1.11818900
H	-2.58181900	-4.70611300	2.72178800
H	-3.51771200	-4.26494000	1.28510500
C	-2.52905200	-2.04039500	2.72176400
H	-2.07233600	-1.04589900	2.76810300
H	-3.58624900	-1.91967400	2.46911100
H	-2.46509900	-2.48772500	3.72179900
C	-1.42686600	2.50554300	2.71561800
H	-1.34976200	1.41452400	2.77497000
H	-1.23329500	2.91245200	3.71622100
H	-2.45340700	2.76251100	2.43785600
C	1.02196800	2.70669700	2.19906500
H	1.80466000	3.15982700	1.58597100
H	1.15971000	3.06092100	3.22908000
H	1.18212000	1.62507700	2.18582000
C	-0.54350300	4.63031500	1.70963000
H	-0.48254300	5.00694000	2.73900000
H	0.25662000	5.11191500	1.14033300
H	-1.50703700	4.94173600	1.29477500

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	x	y	z
Ni	0.61429500	-0.00101500	0.10245800
P	0.98000600	-2.26723600	0.05023000
P	0.99092500	2.26304300	0.04874400
C	2.29453600	-0.00521600	-0.82337000
O	2.38197500	-2.40378200	-0.86034900
C	1.56306200	-3.10780900	1.65686300
C	-0.14622400	-3.36491800	-1.01308200
O	2.38631900	2.39296800	-0.87290400
C	1.59098600	3.09879500	1.65189300
C	-0.13722100	3.36698200	-1.00571600
C	2.94748300	-1.18795700	-1.20411800
C	2.94944900	1.17432300	-1.21074500
C	2.13339100	-4.51801400	1.41126600
C	0.43544400	-3.16473200	2.70511600
C	2.68997700	-2.19805900	2.19853000
C	-1.42580500	-3.73997100	-0.24316000
C	0.54754400	-4.64074500	-1.53311100
C	-0.49644900	-2.48568500	-2.23528000
C	2.71229200	2.17835700	2.18726300
C	2.17372700	4.50332500	1.40252600
C	0.47046600	3.16700800	2.70706500
C	-0.49408900	2.49266000	-2.22945400
C	0.55689600	4.64328800	-1.52399800
C	-1.41256400	3.74262700	-0.22918700
C	4.14692000	-1.22051100	-1.91735200
C	4.14885200	1.20095000	-1.92426300
H	2.65337200	-4.84441000	2.32134000
H	2.85470400	-4.53764300	0.58890100
H	1.34803200	-5.25243400	1.21030900
H	0.83467300	-3.62520600	3.61872700

H	-0.41449200	-3.77291900	2.38196300
H	0.09856100	-2.15632300	2.95195600
H	3.53121300	-2.12707500	1.50227200
H	3.06531000	-2.63018100	3.13545400
H	2.31485100	-1.19547400	2.41516900
H	-1.22838400	-4.48388500	0.53462900
H	-2.15000200	-4.18218500	-0.93899400
H	-1.90073000	-2.87170800	0.22358800
H	1.50135500	-4.41295100	-2.01583700
H	-0.10689000	-5.10977400	-2.27957200
H	0.72452500	-5.37672800	-0.74667900
H	-1.16321900	-3.04589300	-2.90329600
H	0.40084300	-2.21942600	-2.80405100
H	-1.00230700	-1.56273200	-1.94456200
H	3.09912100	2.60858100	3.12037800
H	3.54771300	2.09688100	1.48514500
H	2.32828400	1.18020400	2.40869200
H	2.88750900	4.51665600	0.57354000
H	2.70549200	4.82322600	2.30806700
H	1.39424600	5.24607800	1.20970400
H	0.88162400	3.61778500	3.62021600
H	0.12068800	2.16251700	2.95208700
H	-0.37245700	3.78871900	2.39139700
H	-1.00048900	1.56971300	-1.93983300
H	0.40041800	2.22690100	-2.80278400
H	-1.16255200	3.05635700	-2.89282600
H	1.50742600	4.41524100	-2.01305600
H	0.74002200	5.37535400	-0.73530600
H	-0.10051400	5.11730500	-2.26467300
H	-2.13635200	4.19409300	-0.91950100
H	-1.20885100	4.47996900	0.55323700
H	-1.89127800	2.87433900	0.23364600
H	4.59204000	-2.17563900	-2.17664000
C	4.74202100	-0.01127500	-2.27627800
H	4.59564600	2.15388300	-2.18868600
H	5.67566400	-0.01361500	-2.83186900
H	-1.72694900	0.92822000	2.61047100
O	-1.48504900	0.00504700	0.60581700
C	-1.15931200	0.00730900	2.38344800
H	-1.73412700	-0.90802300	2.61460100
O	0.09785100	0.00258600	2.50031800
C	-4.04281800	0.00888600	1.14880200
C	-4.84562200	1.31622800	0.88994500
C	-5.23036500	1.57971100	-0.58139000
C	-4.09717100	1.30469500	-1.59438200
C	-3.27354100	0.00752300	-1.34573900
H	-5.75786000	1.32757900	1.50614300
H	-3.78115000	0.00890200	2.21376800
H	-6.11001900	0.98377900	-0.84194200
H	-5.55073200	2.62591000	-0.68365100
H	-4.52225300	1.28486100	-2.60976500
H	-3.40450600	2.15552600	-1.57939500
H	-2.45224300	0.00664600	-2.07595400
H	-4.23547200	2.15897700	1.24968100
C	-4.10091600	-1.28720600	-1.59454500
H	-4.52673400	-1.26571400	-2.60958800
H	-3.41055600	-2.13989400	-1.58056700
C	-4.84790700	-1.29720500	0.89038600

H	-5.75977000	-1.30715400	1.50715800
C	-5.23411200	-1.55957900	-0.58077500
H	-4.23889500	-2.14103700	1.24955300
H	-6.11243900	-0.96136200	-0.84056900
H	-5.55720500	-2.60494100	-0.68302500
B	-2.77009500	0.00683400	0.17428100

TSB3-2

	x	y	z
Ni	-0.85039400	0.03625100	0.14098600
P	-1.34806000	-2.24774400	0.48135600
P	-1.27046500	2.22489500	-0.57584900
C	-2.76947400	0.00643700	-0.03621500
O	-2.90127900	-2.08290700	1.10509500
C	-1.70289400	-3.30183800	-1.10843900
C	-0.67833900	-3.32712600	1.88591400
O	-2.78551200	2.04018400	-1.28142300
C	-0.39895600	2.95202500	-2.09332000
C	-1.69727800	3.55724700	0.74696900
C	-3.55204800	-1.00549300	0.53591500
C	-3.49239100	1.00760500	-0.69933000
C	-3.08302500	-3.98622200	-0.99532100
C	-0.63904800	-4.39023400	-1.36339500
C	-1.73092700	-2.34544000	-2.32067700
C	0.78260200	-3.73811300	1.60844600
C	-1.54137600	-4.58180900	2.13491700
C	-0.76282300	-2.43474400	3.14569200
C	-0.44773700	1.82873100	-3.15406000
C	-1.12483200	4.19080400	-2.65507400
C	1.06793800	3.29498700	-1.77784400
C	-2.04419800	2.80709700	2.05329100
C	-2.93579900	4.37704400	0.32311900
C	-0.52289900	4.52108200	1.00084100
C	-4.94823600	-1.01695200	0.50655300
C	-4.88648500	1.03469400	-0.77800100
H	-3.24140300	-4.58212200	-1.90378500
H	-3.89830600	-3.26263900	-0.92616700
H	-3.15232500	-4.66053400	-0.13851100
H	-0.84789100	-4.84997100	-2.33783500
H	-0.67235500	-5.18782100	-0.61717400
H	0.37876000	-3.99704800	-1.40402500
H	-2.51756100	-1.59268600	-2.22861300
H	-1.92460900	-2.93047500	-3.22948800
H	-0.77881700	-1.82625000	-2.45492400
H	0.84883900	-4.54213300	0.87197500
H	1.23235900	-4.10610000	2.53870000
H	1.39227800	-2.90199200	1.25866100
H	-2.59075400	-4.32492500	2.30361500
H	-1.16828300	-5.08149200	3.03844500
H	-1.48433000	-5.30624200	1.31819000
H	-0.28434100	-2.95706600	3.98353300
H	-1.80329300	-2.23512100	3.41719500
H	-0.25239900	-1.48007000	3.01235000
H	0.08129600	2.16600200	-4.05412300
H	-1.47575200	1.58316200	-3.43523200
H	0.04081400	0.91527300	-2.80233700
H	-2.18326400	3.99297100	-2.84608000
H	-0.65559000	4.46631100	-3.60859500

H	-1.04254700	5.05659300	-1.99195600
H	1.57573600	3.56656700	-2.71173200
H	1.60020000	2.44949900	-1.33788900
H	1.15987900	4.14417500	-1.09699400
H	-1.21447400	2.19191300	2.40775600
H	-2.91743100	2.15967700	1.92846100
H	-2.28225000	3.54550500	2.83014900
H	-3.82504200	3.75210900	0.21490800
H	-2.78743300	4.92338200	-0.61096900
H	-3.13661100	5.11416500	1.11148400
H	-0.76864400	5.14890300	1.86671000
H	-0.35327400	5.19177100	0.15300500
H	0.40988400	4.00361900	1.22865900
H	-5.48678100	-1.83589600	0.97217100
C	-5.61039600	0.01631400	-0.15712000
H	-5.37805100	1.84943700	-1.29959500
H	-6.69583700	0.02363900	-0.19777600
O	1.52672400	-0.03207200	-0.02667800
C	2.13419900	-1.73092600	-1.86369300
C	1.97707000	-1.52745900	-3.39159700
C	3.03772600	-0.61530400	-4.04154800
C	3.36685000	0.64003600	-3.21067500
C	3.59707000	0.40615500	-1.68769600
H	1.96649100	-2.49881700	-3.91095100
H	1.24505100	-2.26038100	-1.50193200
H	3.95325900	-1.18379000	-4.22786900
H	2.68271800	-0.30456300	-5.03418500
H	4.25419400	1.12898400	-3.64105800
H	2.54629400	1.36010100	-3.32954000
H	3.77625800	1.39357800	-1.24966400
H	0.98722400	-1.08433400	-3.57526600
C	4.86038700	-0.46135700	-1.40217900
H	5.73114500	-0.03092400	-1.92033200
H	5.08451500	-0.38730600	-0.33142500
C	3.37078600	-2.59569600	-1.46811100
H	3.31511600	-3.58061000	-1.95830000
C	4.74267800	-1.95773500	-1.78064700
H	3.31381000	-2.79499600	-0.38789400
H	4.96833600	-2.09012200	-2.84283300
H	5.52226900	-2.51936200	-1.24806000
B	2.32791800	-0.35792200	-1.07508000
C	2.21473700	-0.37957600	2.53985300
C	3.73810800	-0.53310300	2.32958600
C	4.53387900	0.78692300	2.34582700
C	3.86981400	1.94379000	1.56202700
C	2.32084800	2.03929200	1.64746300
H	4.16851000	-1.21301300	3.08299600
H	1.80438400	-1.39440500	2.48843200
H	4.70179600	1.08877000	3.38429800
H	5.53897700	0.61036200	1.93542700
H	4.31965200	2.89366200	1.89466700
H	4.15140700	1.84618300	0.50993700
H	2.03265200	2.80460300	0.91017000
H	3.89501300	-1.03377200	1.36299200
C	1.87346800	2.57200600	3.03690500
H	2.32986900	3.55580400	3.23480500
H	0.78911800	2.74082600	3.02048800
C	1.83852400	0.15689900	3.94728000

H	2.29480400	-0.46709900	4.73316900
C	2.18849400	1.63497200	4.21938200
H	0.75136700	0.04611900	4.07035800
H	3.24523600	1.72645800	4.48796400
H	1.63547300	1.97673200	5.10642300
B	1.56644500	0.60445400	1.40996800
H	0.31620400	0.71057000	1.62417900

TSC1

	x	y	z
Ni	-0.00000400	-0.38367100	0.16923600
P	-2.21625900	-0.10378100	0.10621600
P	2.21625700	-0.10378800	0.10622600
C	0.00000600	1.43299200	-0.39982000
O	-2.39268600	1.51488300	-0.32049500
C	-3.17993900	-0.90971000	-1.32018000
C	-3.12077600	-0.09875600	1.77502500
O	2.39269900	1.51487100	-0.32049700
C	3.17995700	-0.90969400	-1.32017100
C	3.12072400	-0.09876200	1.77506200
C	-1.18599800	2.16211900	-0.55069800
C	1.18601400	2.16211400	-0.55069500
C	-4.60104100	-0.33465100	-1.47543900
C	-3.23327900	-2.44334600	-1.17284700
C	-2.35972300	-0.57374200	-2.58945500
C	-3.28003500	-1.53866200	2.30083800
C	-4.48695700	0.61372100	1.74328300
C	-2.18584500	0.68123500	2.72878800
C	2.35956300	-0.57400600	-2.58940600
C	4.60093500	-0.33437600	-1.47563000
C	3.23360000	-2.44330000	-1.17266700
C	2.18609200	0.68186200	2.72860000
C	4.48722900	0.61308600	1.74322800
C	3.27932100	-1.53862300	2.30120600
C	-1.21578100	3.51309600	-0.89919200
C	1.21580200	3.51309200	-0.89918600
H	-5.00254600	-0.66171700	-2.44325000
H	-4.60962000	0.75930100	-1.46266400
H	-5.28335400	-0.70181800	-0.70375100
H	-3.78276900	-2.85112200	-2.03179300
H	-3.76339200	-2.76524900	-0.27108800
H	-2.22573200	-2.86839900	-1.19060100
H	-2.29761700	0.50467000	-2.76551100
H	-2.86298400	-1.02642900	-3.45361500
H	-1.35160600	-0.99129500	-2.52824200
H	-4.01650400	-2.10959200	1.72762000
H	-3.62978200	-1.50368800	3.34067900
H	-2.33171200	-2.08768200	2.28819800
H	-4.41671500	1.60508600	1.28649700
H	-4.84214100	0.74244800	2.77414500
H	-5.24513800	0.03782500	1.20814500
H	-2.64520200	0.72070600	3.72496100
H	-2.02596900	1.70993500	2.39054500
H	-1.20902900	0.19640500	2.82256600
H	2.86285800	-1.02664600	-3.45357100
H	2.29721700	0.50438100	-2.76554000
H	1.35154400	-0.99177700	-2.52807100
H	4.60929300	0.75957800	-1.46295000

H	5.00239500	-0.66144700	-2.44345700
H	5.28340500	-0.70133200	-0.70398400
H	3.78305300	-2.85108200	-2.03163300
H	2.22613200	-2.86854300	-1.19024500
H	3.76388900	-2.76499700	-0.27093600
H	1.20899600	0.19758500	2.82232500
H	2.02683000	1.71059900	2.39018800
H	2.64534500	0.72121300	3.72482500
H	4.41751100	1.60431100	1.28605400
H	5.24521800	0.03662600	1.20842100
H	4.84233900	0.74205000	2.77408600
H	3.62911000	-1.50357000	3.34103100
H	4.01551000	-2.11003100	1.72810600
H	2.33074900	-2.08721300	2.28870700
H	-2.16603400	4.02475100	-1.01325400
C	0.00001200	4.17688300	-1.07944700
H	2.16605700	4.02474400	-1.01324700
H	0.00001400	5.22883500	-1.35151100
H	-0.00001600	-1.79339200	0.92893600
H	-0.91002100	-3.34371600	0.58531300
C	0.00004100	-2.91658000	0.10999500
H	0.91006000	-3.34368600	0.58541600
O	0.00010800	-2.70178700	-1.15153900

TSC2-2

	x	y	z
Ni	-0.16270900	0.46399600	-0.14266200
P	1.85908300	1.56092600	0.01048700
P	-2.42666000	0.01751500	0.01540400
C	-0.80883400	2.26703000	0.00604800
O	1.40698300	3.17526900	-0.01129600
C	2.79066200	1.53385100	1.68562600
C	3.02049600	1.61011100	-1.49424900
O	-3.09431800	1.55547200	0.04220600
C	-3.11368100	-0.63586500	1.68319000
C	-3.39892200	-0.62549600	-1.48945900
C	0.04297500	3.38198800	0.02059800
C	-2.17435500	2.58354100	0.04988400
C	-0.39991300	4.70500200	0.06537500
C	-2.67546300	3.88579700	0.09684900
H	0.32488000	5.51261700	0.07080100
C	-1.77240100	4.94807400	0.10253500
H	-3.74829500	4.04635700	0.12594900
H	-2.13971800	5.96985100	0.13819700
H	1.49876400	-2.10513200	-2.97563100
H	-0.25695200	-2.34293300	-2.91864600
C	0.54924700	-1.63208500	-2.68992700
H	0.40784600	-0.75201100	-3.33037500
O	0.54694400	-1.21973500	-1.34460000
C	2.32092000	-2.59748600	0.16570900
C	2.42883500	-3.06265300	1.64120900
C	1.42876000	-4.16164500	2.05606000
C	-0.00638000	-3.92856800	1.53903700
C	-0.11498800	-3.45641600	0.06420600
H	3.45023200	-3.41059100	1.86830600
H	3.04490800	-1.78017200	0.04536800
H	1.79088100	-5.13628800	1.71392200
H	1.40686900	-4.23307500	3.15330000

H	-0.59144600	-4.84984800	1.69653200
H	-0.47226100	-3.16342100	2.17665700
H	-1.18362300	-3.27536400	-0.12221000
H	2.25767600	-2.18820100	2.28688700
C	0.30601700	-4.55919000	-0.94541500
H	-0.26148700	-5.48541900	-0.75643000
H	0.00909700	-4.23907800	-1.95318400
C	2.75942100	-3.69284300	-0.84312900
H	3.76690200	-4.06370400	-0.59126400
C	1.81176300	-4.90677400	-0.96598600
H	2.86451500	-3.22568200	-1.83275600
H	2.02910400	-5.61625200	-0.16121900
H	2.04154400	-5.45030200	-1.89396100
B	0.78620400	-2.10426000	-0.10727000
H	0.44531500	-1.22499600	0.76981100
C	-4.40275700	0.11180700	2.08738400
H	-5.22272400	-0.04640200	1.38291900
H	-4.72580700	-0.27150500	3.06414700
H	-4.23981500	1.18751800	2.18080600
C	-3.39644100	-2.14887700	1.65488700
H	-2.53715400	-2.73421600	1.32239500
H	-3.64268800	-2.47744100	2.67278000
H	-4.25332400	-2.39349000	1.01981200
C	-2.02722800	-0.33500000	2.73926000
H	-1.09804200	-0.87189000	2.53171600
H	-1.79812800	0.73512500	2.79099900
H	-2.39320700	-0.64662500	3.72637500
C	3.65698000	0.23733400	-1.77250300
H	2.90106600	-0.54576700	-1.84236500
H	4.19598600	0.28701800	-2.72775200
H	4.37949700	-0.05185500	-1.00477700
C	1.74065200	1.14216600	2.74864000
H	0.89675400	1.84060700	2.76202300
H	1.34800900	0.13599800	2.57941500
H	2.21132800	1.16632900	3.74021600
C	3.94372200	0.51458700	1.71012800
H	4.76415800	0.80263500	1.04545900
H	4.35066300	0.47242900	2.72867000
H	3.61865800	-0.49307500	1.44605600
C	3.34258700	2.93205200	2.03974200
H	3.81922100	2.86848300	3.02659200
H	4.09644900	3.28131700	1.33033400
H	2.55188800	3.68349000	2.09084900
C	4.11619000	2.68381300	-1.34933300
H	4.85185700	2.42107700	-0.58362200
H	4.65447800	2.76616300	-2.30272200
H	3.69852100	3.66673600	-1.11343000
C	2.10578400	1.98778000	-2.68326800
H	1.30159200	1.25910400	-2.82120600
H	1.65771500	2.97726200	-2.55522400
H	2.70800100	2.00395300	-3.60065000
C	-3.11114500	-2.10591300	-1.79303100
H	-3.51211800	-2.77642700	-1.02945900
H	-3.59120600	-2.36795000	-2.74496600
H	-2.04320500	-2.30361300	-1.88936100
C	-2.89705600	0.23585400	-2.67232100
H	-3.11670800	1.29737600	-2.52507600
H	-1.81939100	0.12401100	-2.82538100

H	-3.40484300	-0.09096800	-3.58881000
C	-4.91766400	-0.41487000	-1.32797000
H	-5.40661900	-0.64398300	-2.28390800
H	-5.34878000	-1.08293800	-0.57621000
H	-5.16188800	0.61727500	-1.06331200

TSD1-2

	x	y	z
C	-2.65938500	-0.07425700	-4.29151600
C	-2.16711900	-0.38650900	-3.02291900
C	-1.87375900	0.56853500	-2.03703900
C	-2.12924600	1.89300500	-2.42177500
C	-2.62152000	2.26349100	-3.67442200
C	-2.88345300	1.26414200	-4.61040700
H	-2.85662700	-0.87254300	-4.99954900
H	-2.78766900	3.31286300	-3.89520100
H	-3.26598200	1.52946400	-5.59196900
O	-1.88156800	2.90818300	-1.52093500
O	-1.96354000	-1.72014600	-2.73983100
P	-1.32219200	2.39950400	-0.02673700
P	-1.46262700	-2.02637200	-1.17018000
C	0.20677000	3.52904300	0.04987500
C	-2.76436300	3.03143400	1.06750200
C	-0.00067000	-3.16257700	-1.59390700
C	-3.00282500	-2.98777800	-0.54860100
H	2.43052700	-1.11083800	1.60040400
C	1.95851700	-0.25634800	1.09708900
O	0.58786700	-0.41234500	1.02278300
O	2.46786000	-0.17556500	-0.23864000
H	2.24397900	0.66265500	1.62637500
Ni	-1.11218200	0.10875700	-0.33484300
C	-3.76403400	1.86003400	1.18349100
H	-3.32276600	0.99784400	1.68958800
H	-4.63596600	2.19208300	1.76230000
H	-4.12116500	1.53365800	0.20057300
C	-2.29327200	3.44518600	2.47342600
H	-1.69797900	4.36278900	2.45084200
H	-3.17595400	3.64460100	3.09443600
H	-1.71342000	2.66575900	2.97156900
C	-3.49129000	4.22117100	0.40385100
H	-4.32225000	4.51835500	1.05695100
H	-2.84680600	5.09312300	0.27150500
H	-3.90394100	3.95453500	-0.57148200
C	-0.15105900	5.00956100	-0.18416100
H	-0.70849600	5.43880700	0.65358300
H	0.78021300	5.58276400	-0.28213400
H	-0.72884000	5.14997900	-1.10174600
C	0.96773300	3.38009500	1.37816800
H	1.93020000	3.90187300	1.29585100
H	0.42979800	3.81824000	2.22229900
H	1.17105200	2.33518800	1.61517500
C	1.10918300	3.04448300	-1.10920000
H	1.40722100	1.99879300	-0.99064700
H	0.61661800	3.15687300	-2.07948900
H	2.01985000	3.65774200	-1.12287200
C	0.94739200	-2.29127500	-2.45006700
H	0.47426700	-1.97688600	-3.38473600
H	1.28969700	-1.40739000	-1.90672800

H	1.83139900	-2.89057100	-2.70551900
C	0.74111700	-3.61214700	-0.32299500
H	1.65821900	-4.13844600	-0.61807600
H	1.01728900	-2.75674100	0.29524300
H	0.14930900	-4.30031200	0.28676900
C	-0.43264900	-4.38630900	-2.42477400
H	0.46954200	-4.91529100	-2.75874000
H	-1.02892000	-5.09674000	-1.84496200
H	-0.99782600	-4.09477000	-3.31481400
C	-2.65649300	-4.04120100	0.51909200
H	-3.59202200	-4.46379000	0.90814900
H	-2.07276400	-4.87063000	0.10876200
H	-2.11212900	-3.61873800	1.36500400
C	-3.74174600	-3.67554100	-1.71775300
H	-3.13645000	-4.43885000	-2.21191800
H	-4.63258300	-4.17096800	-1.31006600
H	-4.06725600	-2.95818000	-2.47392800
C	-3.94738300	-1.93216000	0.06697300
H	-3.49823800	-1.44375200	0.93583600
H	-4.21874500	-1.15787900	-0.65893400
H	-4.87280400	-2.42656900	0.39064100
C	4.97200200	0.11553900	0.55500800
C	5.93034100	-1.09211600	0.32785000
C	6.40030100	-1.30167800	-1.12870700
C	5.28400700	-1.16399200	-2.18752800
C	4.32357800	0.04540500	-1.98552800
H	6.81046300	-0.99903600	0.98127000
H	4.64653500	0.07685900	1.60351500
H	7.20967400	-0.60218800	-1.35641700
H	6.84852100	-2.30095300	-1.21360100
H	5.73977700	-1.12195000	-3.18807300
H	4.67325500	-2.07934300	-2.17499000
H	3.51167000	-0.04640400	-2.71955300
H	5.40615400	-2.00040900	0.66121000
C	4.98948600	1.43749100	-2.18807900
H	5.44792300	1.49671100	-3.18659000
H	4.18885300	2.19205200	-2.18197300
C	5.62743600	1.51160700	0.33013000
H	6.50311300	1.62330900	0.98663200
C	6.04123300	1.82665200	-1.12476500
H	4.90713800	2.27478200	0.66217700
H	6.99151900	1.33388200	-1.35015900
H	6.24715300	2.90263900	-1.20693600
B	3.79818900	-0.01905100	-0.49898800
C	-0.14680600	0.38532000	3.52928600
C	-1.41588500	0.27320600	4.41699600
C	-1.76715800	-1.15411000	4.88688400
C	-1.64518100	-2.22563700	3.78315800
C	-0.37970600	-2.11107800	2.89316600
H	-1.32821200	0.92412100	5.30243400
H	-0.06683000	1.44348000	3.23716600
H	-1.13322300	-1.42780000	5.73592500
H	-2.79364300	-1.15864700	5.28118600
H	-1.70630900	-3.22233300	4.25039800
H	-2.52752300	-2.14339700	3.13114600
H	-0.46916300	-2.88634000	2.12028200
H	-2.27039100	0.65841000	3.84260200
C	0.92629500	-2.44197100	3.66215200

H	0.84573600	-3.42836700	4.14790400
H	1.73850500	-2.54993900	2.92858500
C	1.15381800	0.06909000	4.31868700
H	1.20522500	0.69150100	5.22693900
C	1.35155200	-1.40839100	4.72941100
H	2.01560900	0.37995000	3.71240200
H	0.80060000	-1.60239700	5.65469200
H	2.40798200	-1.57023000	4.98776100
B	-0.34834400	-0.61110000	2.24909600
H	-1.44702800	-0.36497900	1.64921200

TSF1-2

	x	y	z
H	0.44865200	2.54995500	1.28903600
C	0.65805100	2.70061200	0.22645000
O	-0.09545800	0.87745500	-0.06805000
O	1.70133900	2.24456900	-0.32347500
H	0.09863200	3.50085300	-0.27464700
C	2.07881200	0.10054700	1.27011600
C	1.75323800	-1.41290600	1.38075600
C	2.16169800	-2.26670500	0.15750500
C	1.84461000	-1.63334500	-1.21861100
C	2.12818100	-0.11250500	-1.33373700
H	2.22261300	-1.83710500	2.28109800
H	1.64290000	0.58472700	2.16017800
H	3.23070900	-2.49240800	0.21641200
H	1.65857300	-3.24143500	0.22386700
H	2.40116700	-2.17883100	-1.99569700
H	0.78403400	-1.79713400	-1.44865100
H	1.71728200	0.22866300	-2.29593400
H	0.67012300	-1.51445700	1.53649400
C	3.64006300	0.24395600	-1.32558900
H	4.16017200	-0.29515400	-2.13160000
H	3.73219000	1.31159000	-1.56552500
C	3.59682400	0.42833100	1.26855300
H	4.08044400	0.00052500	2.15967500
C	4.36916800	-0.02853200	0.00954300
H	3.69987000	1.51854400	1.36114400
H	4.60142100	-1.09506100	0.08916100
H	5.34400700	0.47800900	-0.00897000
B	1.46080700	0.64322400	-0.09927200
C	-2.61192400	1.28792200	0.11769800
C	-3.46059200	1.13361600	-1.17740700
C	-3.80623100	-0.32080600	-1.56483200
C	-2.62773600	-1.31129400	-1.44230000
C	-1.76645600	-1.17480800	-0.15059300
H	-4.39028800	1.71611900	-1.09293600
H	-2.33340000	2.34999300	0.20205300
H	-4.64593100	-0.67242400	-0.95845600
H	-4.17181100	-0.33290800	-2.60043400
H	-3.01189100	-2.33872400	-1.52574300
H	-1.95861200	-1.17184800	-2.30431500
H	-0.92120400	-1.86428200	-0.24797300
H	-2.89441000	1.59059400	-2.00282500
C	-2.51230400	-1.54804600	1.16563900
H	-2.89062100	-2.57878600	1.09789100
H	-1.77041600	-1.55592300	1.97810000
C	-3.34879700	0.89259400	1.42815300

H	-4.27733100	1.47373600	1.53172400
C	-3.67106800	-0.61068200	1.56806500
H	-2.71175800	1.19335800	2.27380100
H	-4.56054700	-0.85188200	0.97923800
H	-3.94811800	-0.81788700	2.61048300
B	-1.34215100	0.34791500	-0.03691200

[Ni]OBBN

	x	y	z
Ni	0.58143800	0.03515000	0.05155000
P	1.09138200	-2.15219300	0.03502100
P	0.70640700	2.27670300	0.00568300
C	2.47650800	0.19993200	-0.14355100
O	2.77192600	-2.17220100	0.00831500
C	0.76216000	-3.10168200	1.63941000
C	0.74941800	-3.16078900	-1.54216500
O	2.33107400	2.58903800	-0.28515000
C	0.46435900	3.13686600	1.67822300
C	-0.06441900	3.22227600	-1.44867300
C	3.33325800	-0.90936300	-0.12761800
C	3.11427300	1.44117100	-0.27998400
C	1.35014400	-4.52414700	1.64417300
C	-0.75334200	-3.13840000	1.92263300
C	1.44915500	-2.26873800	2.74680100
C	-0.67302600	-3.74410800	-1.53609600
C	1.78196500	-4.28548500	-1.75979100
C	0.87564600	-2.14665700	-2.70303600
C	1.44992000	2.43651900	2.64296800
C	0.79070900	4.64092600	1.64045000
C	-0.97144200	2.90029300	2.18931200
C	-0.02106800	2.23647500	-2.63918900
C	0.73958600	4.48398000	-1.82404200
C	-1.52755400	3.59827900	-1.15304800
C	4.72087900	-0.81953800	-0.24480200
C	4.49576700	1.59325100	-0.40323000
H	1.25376300	-4.94616600	2.65317400
H	2.41222200	-4.52760200	1.37969400
H	0.81657600	-5.19250800	0.96158300
H	-0.91606500	-3.56655800	2.92034400
H	-1.29785000	-3.76173500	1.20747600
H	-1.18673800	-2.13482700	1.90334800
H	2.53202400	-2.21120600	2.60247200
H	1.25878400	-2.74575900	3.71664600
H	1.05031700	-1.24962100	2.79036700
H	-0.78723400	-4.54799400	-0.80195600
H	-0.88893900	-4.17133400	-2.52395600
H	-1.42838600	-2.98012200	-1.33705300
H	2.80470000	-3.90111400	-1.75846100
H	1.59118100	-4.74750000	-2.73732800
H	1.71138100	-5.07265000	-1.00548800
H	0.72022900	-2.67147600	-3.65472100
H	1.86750600	-1.68344400	-2.73346600
H	0.12899300	-1.34965600	-2.62804000
H	1.33296900	2.87418100	3.64258500
H	2.49140900	2.56857200	2.33536500
H	1.24746400	1.36327700	2.71988500
H	1.78726600	4.83066300	1.22908400
H	0.76946500	5.03640300	2.66450300

H	0.05793800	5.20880400	1.05918600
H	-1.03647600	3.24287900	3.23042100
H	-1.24136200	1.84099800	2.15407400
H	-1.71587800	3.45942300	1.61587900
H	-0.63078300	1.34728800	-2.45069900
H	1.00200300	1.91097600	-2.85785700
H	-0.41252300	2.73631000	-3.53479300
H	1.78192400	4.24562900	-2.04872000
H	0.72512400	5.24127000	-1.03644400
H	0.28874800	4.92987700	-2.72036400
H	-1.99710100	3.96033400	-2.07669300
H	-1.60443000	4.40006200	-0.41232600
H	-2.11057100	2.74386000	-0.79916500
H	5.32728400	-1.71941400	-0.22676000
C	5.29252000	0.44660500	-0.38492100
H	4.92623800	2.58433900	-0.50430100
H	6.37087900	0.54105100	-0.47878500
O	-1.25590100	-0.04802000	0.46266900
C	-3.23723500	-0.67086600	-1.18110400
C	-4.08163800	-1.94891900	-0.90680700
C	-5.09093700	-1.84876300	0.25823800
C	-4.52732000	-1.17162800	1.52551400
C	-3.70407300	0.11829100	1.26853600
H	-4.61852300	-2.25532800	-1.81894800
H	-2.49786100	-0.92357100	-1.95835100
H	-5.98756800	-1.31745700	-0.07462700
H	-5.43500700	-2.86072600	0.51527000
H	-5.35783300	-0.97058200	2.22125100
H	-3.87324500	-1.88998100	2.04359000
H	-3.28227400	0.43560800	2.23378200
H	-3.39074500	-2.77375100	-0.67979600
C	-4.54474400	1.30491800	0.71809600
H	-5.39171900	1.52327700	1.38835800
H	-3.90961000	2.20325800	0.74595100
C	-4.08285300	0.51489000	-1.72558900
H	-4.63259500	0.21066000	-2.63079300
C	-5.08554500	1.13059000	-0.72095300
H	-3.38755400	1.30051900	-2.05516600
H	-5.99352800	0.52078600	-0.69646700
H	-5.40964100	2.11050500	-1.09968900
B	-2.54893000	-0.19964000	0.19355000

[Ni]OCH₂OBBN

	x	y	z
C	-5.26815800	0.21217300	-0.40014100
C	-3.94455700	-0.20418600	-0.25355800
C	-2.86470300	0.67953700	-0.12664900
C	-3.19153200	2.04229700	-0.16111800
C	-4.49607200	2.51665300	-0.30481200
C	-5.52970100	1.58432400	-0.42265200
H	-6.06375900	-0.52004700	-0.49375000
H	-4.68867500	3.58451700	-0.32577100
H	-6.55305600	1.93185000	-0.53548800
O	-2.16373300	2.97175000	-0.05029700
O	-3.68597300	-1.57229500	-0.23126500
P	-0.63905400	2.26419400	0.05209100
P	-2.05808300	-1.93291800	-0.01186200
C	0.19150400	2.94898300	-1.50407900

C	-0.01437300	3.05561500	1.66095100
C	-1.69504300	-2.98112100	-1.54470600
C	-2.16888100	-2.94240000	1.59594700
H	1.79013500	-2.01734500	0.85802500
C	1.48076900	-0.96362500	0.99273000
O	0.73953800	-0.51263300	-0.04652300
O	2.70343100	-0.18778000	1.16431900
H	0.98570300	-0.87432500	1.97438700
Ni	-1.06386700	0.07438600	0.02996900
C	5.14861300	0.41768800	0.76552100
C	6.22870700	-0.51240700	1.39054200
C	6.51451300	-1.81175300	0.60496300
C	5.25125400	-2.54565400	0.10016400
C	4.15264600	-1.63559200	-0.52346200
H	7.17214500	0.03763000	1.52941300
H	4.95441300	1.22786200	1.48220800
H	7.17192000	-1.59159800	-0.24153800
H	7.08777700	-2.49541600	1.24635200
H	5.55188800	-3.32263300	-0.61925300
H	4.79752600	-3.08205300	0.94742200
H	3.28407100	-2.27110800	-0.73932400
H	5.88864800	-0.78283600	2.40160600
C	4.56146100	-0.96050900	-1.86692900
H	4.84555100	-1.72955100	-2.60153000
H	3.66469500	-0.47195500	-2.27540800
C	5.55883600	1.06711800	-0.58572800
H	6.50023700	1.62655500	-0.47215000
C	5.69398300	0.08627400	-1.77150400
H	4.79423100	1.81672300	-0.83902800
H	6.66067700	-0.42326400	-1.71793800
H	5.72225200	0.66178200	-2.70724500
B	3.86118300	-0.46872900	0.51064700
C	-0.68674900	2.46404200	-2.68118500
H	-0.75316600	1.37144800	-2.71286500
H	-1.70169300	2.86934700	-2.63063700
H	-0.23221800	2.80060800	-3.62168500
C	1.59886600	2.33301500	-1.65349000
H	1.57518600	1.24366700	-1.55573100
H	1.99214100	2.59206600	-2.64535600
H	2.30087200	2.71945600	-0.90981000
C	0.26208400	4.48656000	-1.53628300
H	0.96380900	4.88263900	-0.79609000
H	0.61753500	4.80657200	-2.52461100
H	-0.71896600	4.94288300	-1.36931800
C	-0.19686700	-3.35391900	-1.56743200
H	0.04490300	-3.78643300	-2.54714100
H	0.43485300	-2.47369700	-1.40926800
H	0.05664200	-4.10303800	-0.81141700
C	-1.98760400	-2.04880700	-2.74394100
H	-3.03644900	-1.73907700	-2.77639400
H	-1.36212400	-1.15022000	-2.71874500
H	-1.76297000	-2.58830000	-3.67279300
C	-2.57586700	-4.23758900	-1.66261700
H	-2.41702400	-4.69516000	-2.64804300
H	-2.32196900	-4.99281000	-0.91221900
H	-3.64025100	-3.99801600	-1.57272900
C	-0.91675800	-3.81482200	1.80250300
H	-0.93954500	-4.23609700	2.81587200

H	-0.88051000	-4.65448600	1.10173000
H	0.01214400	-3.24453900	1.70415600
C	-3.43689400	-3.81793000	1.65665400
H	-3.42555100	-4.62356300	0.91903500
H	-3.49623400	-4.28064300	2.65057700
H	-4.34184000	-3.22531100	1.50200600
C	-2.24598200	-1.88983200	2.72653800
H	-1.34060300	-1.27623400	2.77493500
H	-3.10309900	-1.21989300	2.60170700
H	-2.35860600	-2.40469100	3.68960000
C	-0.60655300	2.18502100	2.79343900
H	-0.21822500	1.16195300	2.76056400
H	-0.33008600	2.62045800	3.76244500
H	-1.70001000	2.13970200	2.74561700
C	1.52323900	3.01802900	1.74613600
H	1.98551400	3.72075800	1.04556500
H	1.82526600	3.32371900	2.75660300
H	1.93315900	2.01986800	1.56384600
C	-0.52355100	4.50098000	1.83767400
H	-0.21044800	4.86106500	2.82652900
H	-0.10962300	5.18508100	1.09309500
H	-1.61364900	4.55649900	1.78344000

HBPin

	x	y	z
C	0.78911700	-0.19154400	-0.04499700
C	-0.78913500	-0.19142900	0.04501600
C	1.47980600	-0.48365300	1.29346800
H	1.36050400	-1.53119800	1.58923700
H	2.54904800	-0.27291300	1.19421600
H	1.08469100	0.15045700	2.09324200
C	1.37939500	-1.07386800	-1.14339500
H	2.46908900	-0.97024400	-1.14898000
H	1.14040300	-2.12907500	-0.96788400
H	1.00991600	-0.79232000	-2.13201800
C	-1.37962800	-1.07377500	1.14331600
H	-2.46934000	-0.97034500	1.14864600
H	-1.14041500	-2.12894400	0.96789400
H	-1.01046300	-0.79216800	2.13204000
O	1.08616000	1.20092800	-0.36715800
O	-1.08599400	1.20106900	0.36725100
B	0.00014400	1.94493200	0.00002000
H	0.00033100	3.13488400	-0.00002900
C	-1.47981300	-0.48340000	-1.29348700
H	-1.36078500	-1.53099800	-1.58920700
H	-2.54899000	-0.27232700	-1.19426200
H	-1.08449000	0.15056500	-2.09327400

cis-HCOOBPin

	x	y	z
H	-4.19173200	-0.41568800	-0.75124600
O	-3.33141500	0.53913400	0.83045700
C	-3.30583300	-0.14123600	-0.15929800
O	-2.20942400	-0.72139300	-0.70024500
C	1.27821400	-0.69887500	0.15195100
C	0.98410300	0.83927800	-0.07843900
C	2.48573800	-1.24965000	-0.60234000
H	3.40809900	-0.76010200	-0.26980900
H	2.58209500	-2.32229800	-0.40664100

H	2.38643500	-1.11160200	-1.68123600
C	1.35108100	-1.09058000	1.63279100
H	1.34894600	-2.18205500	1.71100100
H	2.26380300	-0.71283700	2.10507200
H	0.48898000	-0.70979900	2.18939000
C	1.42566400	1.34517700	-1.45715300
H	1.01183500	2.34545400	-1.61691800
H	2.51618000	1.40692000	-1.53388400
H	1.05851900	0.69581700	-2.25844400
O	0.07536800	-1.33004300	-0.38421900
O	-0.47570600	0.88267600	-0.06838300
B	-0.90255000	-0.37838200	-0.35914700
C	1.49661300	1.77064500	1.01703800
H	2.58987600	1.73015700	1.08207200
H	1.20833900	2.80084400	0.78570100
H	1.07731300	1.51554900	1.99249500

trans-HCOOBPin

	x	y	z
O	2.20343900	-0.67104100	-0.16366400
C	3.17138200	0.25930900	0.07533500
O	4.33786500	-0.01136600	0.04368600
H	2.76733000	1.26055200	0.29251600
C	-1.06175500	0.84297000	0.03038900
C	-1.37491300	-0.70712100	-0.01076200
C	-1.24431000	1.53818700	-1.32391600
H	-2.30240800	1.63023800	-1.58927200
H	-0.81568500	2.54355700	-1.26872400
H	-0.73311400	0.99522300	-2.12535000
C	-1.77746500	1.62380100	1.12895200
H	-1.46520500	2.67249200	1.09760700
H	-2.86310400	1.58990300	0.98394600
H	-1.54538000	1.23203800	2.12157800
C	-2.43228100	-1.12816700	-1.02790500
H	-2.54977700	-2.21602600	-1.00382900
H	-3.40226600	-0.67691800	-0.79008800
H	-2.15304800	-0.84259900	-2.04442600
O	0.37319800	0.85840800	0.31681700
O	-0.09344200	-1.27404400	-0.42101900
B	0.85867900	-0.35768900	-0.08789900
C	-1.69459700	-1.30057100	1.36664900
H	-2.67839900	-0.98094800	1.72555100
H	-1.69292300	-2.39198300	1.29083500
H	-0.94426300	-1.01318400	2.11014800

IMA1-3

	x	y	z
C	3.44247000	1.47422300	-2.76453600
C	2.52633900	1.37061700	-1.71685900
C	2.08714900	0.14814900	-1.18728600
C	2.68590400	-0.99065000	-1.74627200
C	3.60406500	-0.94587000	-2.79594200
C	3.96969400	0.30087400	-3.30533200
H	3.73137400	2.45273700	-3.13405700
H	4.02166900	-1.86746500	-3.18807900
H	4.68225600	0.35902600	-4.12340100
O	2.37674700	-2.23552900	-1.21800200
O	2.04505700	2.54849500	-1.16739000

P	1.33645500	-2.17727300	0.09490500
P	0.96323000	2.32267000	0.09458500
C	0.06430400	-3.46890000	-0.46964100
C	2.47672100	-2.80816400	1.48937800
C	-0.46409900	3.38401000	-0.57565500
C	1.90536100	3.13072300	1.53854000
H	-1.31162600	-0.27539000	3.53161400
Ni	0.85079100	0.04067500	0.25811800
C	3.29929800	-1.58182800	1.94570900
H	2.65849600	-0.80840400	2.37878600
H	4.01527500	-1.89939100	2.71515800
H	3.86876900	-1.13983700	1.12162600
C	3.45981100	-3.89473700	1.00847000
H	4.16855000	-4.10785200	1.81942800
H	2.96271700	-4.83268400	0.75335400
H	4.03095300	-3.56281700	0.13757200
C	1.65551900	-3.32076400	2.68791100
H	2.33053000	-3.48053300	3.53869900
H	0.89314900	-2.60048700	3.00285000
H	1.16780000	-4.27589400	2.47544800
C	0.72636600	-4.82601500	-0.78269100
H	1.03705400	-5.35352200	0.12417100
H	-0.01155800	-5.46146200	-1.28890700
H	1.59006600	-4.72192200	-1.44604700
C	-1.05568100	-3.66420300	0.57138100
H	-1.78799200	-4.36737800	0.15546600
H	-0.68815200	-4.09362300	1.50722900
H	-1.60245100	-2.74471300	0.78221300
C	-0.54693300	-2.89893700	-1.77122500
H	-1.06602400	-1.95402700	-1.59698400
H	0.21049800	-2.75974400	-2.54874300
H	-1.28823000	-3.61597000	-2.14538200
C	-1.04187200	2.58629400	-1.76789500
H	-0.28501700	2.42316900	-2.54279600
H	-1.46015800	1.62840000	-1.46068600
H	-1.85554000	3.17305300	-2.21221100
C	-1.54702700	3.59266000	0.49887800
H	-2.38207000	4.14426400	0.04919100
H	-1.96224800	2.65027100	0.86442600
H	-1.17936500	4.18982300	1.34068900
C	0.01925400	4.74765400	-1.11678700
H	-0.81163500	5.20274600	-1.67078200
H	0.30264400	5.44565200	-0.32743200
H	0.86033500	4.63776000	-1.80680000
C	2.16623500	4.63819400	1.36288000
H	2.86712300	4.96545500	2.14207800
H	2.61553900	4.86969500	0.39244200
H	1.25445400	5.23027100	1.47868600
C	1.14053300	2.88409200	2.85604500
H	1.73303300	3.28552100	3.68865600
H	0.16967600	3.38942900	2.87338800
H	0.97447300	1.81893500	3.03677700
C	3.26963500	2.40761700	1.60361000
H	3.15810700	1.32740400	1.73034600
H	3.86458200	2.58650100	0.70316900
H	3.83127600	2.79164400	2.46483200
O	-0.04006700	-0.09365000	1.99936400
C	-1.21489600	-0.22301600	2.43483800

O	-2.30934600	-0.30538800	1.80973700
C	-4.75586400	0.48789300	-0.12228500
C	-4.61439300	-0.99376900	-0.64891000
C	-5.51397600	1.43678700	-1.05468800
H	-6.54688900	1.10185200	-1.20922300
H	-5.54826100	2.43838400	-0.61124200
H	-5.02341900	1.51805100	-2.02772300
C	-5.36589500	0.56873400	1.28939700
H	-5.23910300	1.58877600	1.66847100
H	-6.43748700	0.33727000	1.28392600
H	-4.86176500	-0.11174900	1.97990000
C	-4.52216100	-1.07171100	-2.18351800
H	-4.21651400	-2.08489900	-2.46551200
H	-5.47984700	-0.85334900	-2.67035900
H	-3.76998900	-0.37390200	-2.56494500
O	-3.38543900	0.91759600	-0.06205300
O	-3.34694700	-1.40339200	-0.11600600
B	-2.57462100	-0.23466000	0.18133300
H	-1.45457200	-0.17811000	-0.29904800
C	-5.69164200	-1.96201000	-0.15156200
H	-6.68934300	-1.66007800	-0.49330800
H	-5.49142200	-2.96557100	-0.54340600
H	-5.69939000	-2.02461600	0.93927200

IMA2-3

	x	y	z
Ni	-0.73873500	0.12266100	0.10816900
P	-1.71771000	-1.94939400	-0.03329600
P	-0.34458100	2.37365200	0.03626800
O	1.11274900	-0.47923100	0.58429300
C	-2.49678900	0.68596300	-0.35374700
O	-3.26267900	-1.57555000	-0.57327000
C	-1.17068300	-3.09015700	-1.45091100
C	-2.17312300	-2.85133400	1.58283400
O	-1.89114900	2.99631800	-0.16068600
C	0.49806700	3.09111400	-1.52263900
C	0.13315400	3.27520900	1.63339700
C	1.33224800	-0.73840400	1.86310800
C	-3.53107100	-0.21888900	-0.63096200
C	-2.85644200	2.03982700	-0.41754800
C	-2.23909400	-4.14369400	-1.80645200
C	0.16890300	-3.78682300	-1.14045300
C	-0.98986000	-2.14596300	-2.66303500
C	-0.96232000	-3.56526300	2.21235800
C	-3.32510000	-3.85820000	1.38427900
C	-2.65306800	-1.73270100	2.53868600
C	0.26512600	2.05171600	-2.64314100
C	-0.15544400	4.42304100	-1.94897700
C	2.01305200	3.29076100	-1.32817200
C	-0.87362500	2.78553300	2.70047500
C	0.01165200	4.80507400	1.48836000
C	1.55715700	2.89689200	2.08851800
O	0.53920300	-0.48605000	2.75534700
H	2.29733600	-1.22722700	2.03994200
C	-4.83155200	0.16947100	-0.95644200
C	-4.14125400	2.48422500	-0.73348100
H	-1.95316200	-4.62087400	-2.75268400
H	-3.22847000	-3.69743900	-1.93951200

H	-2.30922800	-4.93371300	-1.05465200
H	0.51114400	-4.29616300	-2.05093100
H	0.06164000	-4.55327300	-0.36690700
H	0.96254300	-3.09815600	-0.83933300
H	-1.92069500	-1.62790900	-2.91727500
H	-0.69038900	-2.74502300	-3.53278000
H	-0.20862200	-1.40192600	-2.48415500
H	-0.60264100	-4.39889700	1.60301900
H	-1.27129200	-3.97959600	3.18079400
H	-0.13407700	-2.88062800	2.40513400
H	-4.16675800	-3.41733000	0.84365600
H	-3.68436900	-4.17000900	2.37347000
H	-3.00447700	-4.76034900	0.85727600
H	-2.94831300	-2.19131600	3.49151400
H	-3.52496000	-1.20322500	2.14036300
H	-1.85968500	-1.00909300	2.74345600
H	0.67396600	2.44770000	-3.58202600
H	-0.80019100	1.85147900	-2.80213700
H	0.77004600	1.10559300	-2.42866900
H	-1.22463900	4.31123800	-2.14321400
H	0.32775100	4.75616200	-2.87669900
H	-0.02590700	5.21449100	-1.20731200
H	2.44749900	3.57243000	-2.29676900
H	2.52151100	2.38177600	-0.99300200
H	2.23038100	4.10625900	-0.63059900
H	-0.80533700	1.70392500	2.84944700
H	-1.90331500	3.04642700	2.43832000
H	-0.63449900	3.27122900	3.65543200
H	-0.96882600	5.10240300	1.10495500
H	0.78543600	5.22336800	0.83758400
H	0.13744900	5.26145300	2.47874300
H	1.78650000	3.45571600	3.00502000
H	2.32291700	3.14210100	1.34969000
H	1.63330900	1.83538200	2.32750400
H	-5.58547700	-0.58448300	-1.15806000
C	-5.12550500	1.53268900	-1.00361100
H	-4.35131800	3.54827000	-0.76625800
H	-6.13214000	1.85668000	-1.25286200
C	4.41754100	-1.71472400	-0.33630300
C	4.57580400	-0.15389700	-0.11470700
C	4.76401300	-2.15395900	-1.77091000
H	5.83728400	-2.08425600	-1.98035900
H	4.45586800	-3.19658300	-1.90011600
H	4.22579700	-1.55130700	-2.50899000
C	5.18377500	-2.58899500	0.65967300
H	4.98187000	-3.64503400	0.45070300
H	6.26550700	-2.42938300	0.57742500
H	4.88266100	-2.38906500	1.69154000
C	5.63008200	0.51177300	-1.00813800
H	5.66690800	1.58625200	-0.79621700
H	6.62903500	0.09874400	-0.82242800
H	5.39155400	0.38842500	-2.06697300
O	3.01078000	-1.92293300	-0.14405800
O	3.28420500	0.35017500	-0.49336900
B	2.33373800	-0.72142900	-0.54369600
H	1.64720800	-0.74634000	-1.54299400
C	4.85831600	0.24078000	1.34569700
H	5.87563400	-0.02842900	1.65236400

H	4.75063300	1.32631100	1.44316500
H	4.16103600	-0.22625200	2.04597000

IMA4-3

	x	y	z
Ni	-0.65457100	0.10190800	-0.09666900
P	-1.41979300	-2.01849700	-0.12398100
P	-0.48081600	2.35600200	-0.07252400
O	1.49135100	-0.31767100	1.75346500
C	-2.52301400	0.49803600	-0.09713200
O	-3.08897800	-1.82606300	-0.15509900
C	-1.16557700	-2.98773300	-1.73582400
C	-1.25996200	-3.06431100	1.45116200
O	-2.08972100	2.84981600	-0.11739700
C	0.15642400	3.17596100	-1.66779700
C	0.04399800	3.24239000	1.52688600
C	2.07641600	-0.85357500	2.82440400
C	-3.50122100	-0.50346700	-0.13597500
C	-3.00410200	1.81283300	-0.11728700
C	-2.29589800	-3.99862300	-2.00976400
C	0.20020100	-3.70172400	-1.73223100
C	-1.18053800	-1.91882300	-2.85313000
C	0.16146400	-3.63826000	1.62079800
C	-2.29145000	-4.20991900	1.49667800
C	-1.56108100	-2.07655900	2.60453900
C	-0.13744100	2.16003000	-2.79550700
C	-0.58606700	4.48972200	-1.98551100
C	1.67448800	3.42985200	-1.60242400
C	-0.68625700	2.47627200	2.65645400
C	-0.41532200	4.71480800	1.52881300
C	1.56175300	3.17500100	1.78602200
O	1.63028600	-0.74314400	3.94408900
H	2.99160600	-1.42637700	2.59805200
C	-4.87153000	-0.24136900	-0.16550700
C	-4.36229200	2.13410400	-0.14617600
H	-2.13652400	-4.44187100	-3.00146500
H	-3.27845000	-3.51982800	-2.00427300
H	-2.30852100	-4.81540000	-1.28404000
H	0.45552500	-3.98704800	-2.76112800
H	0.17438000	-4.61994600	-1.13820900
H	1.00575300	-3.06976600	-1.34675900
H	-2.11925900	-1.35456900	-2.86786600
H	-1.07335100	-2.41687400	-3.82554500
H	-0.35626900	-1.20697900	-2.74384700
H	0.31958600	-4.52064300	0.99467900
H	0.29116700	-3.94896600	2.66486700
H	0.94699400	-2.91755700	1.38645000
H	-3.30877000	-3.85334200	1.31423300
H	-2.26379900	-4.66245100	2.49626400
H	-2.06313700	-5.00177200	0.77709500
H	-1.53853200	-2.62938700	3.55197500
H	-2.55367000	-1.62501300	2.50449700
H	-0.81579000	-1.27998400	2.66973700
H	0.15191700	2.60077900	-3.75858800
H	-1.20072100	1.90261400	-2.85111100
H	0.43212100	1.23475300	-2.66125700
H	-1.66482100	4.33805700	-2.06971800
H	-0.21695500	4.87288300	-2.94594900

H	-0.40911300	5.26225000	-1.23319600
H	2.03515300	3.66347900	-2.61297900
H	2.22850600	2.56181500	-1.23366100
H	1.91222900	4.28923700	-0.96805200
H	-0.32129700	1.44939600	2.74638000
H	-1.77124800	2.45989800	2.51157600
H	-0.48454600	2.98528800	3.60757300
H	-1.47930400	4.81706300	1.29907300
H	0.15706200	5.32496000	0.82291100
H	-0.24282700	5.13074400	2.52980200
H	1.74716600	3.54247800	2.80376400
H	2.12789200	3.81050700	1.10059300
H	1.95757500	2.16153200	1.71642300
H	-5.58123900	-1.06189200	-0.18963600
C	-5.28967300	1.09080900	-0.16676800
H	-4.67378700	3.17357000	-0.15472800
H	-6.35179600	1.31870100	-0.18883400
C	3.79121600	-1.38061300	-0.79846200
C	4.18315400	0.09620700	-0.40115400
C	3.34720400	-1.49622800	-2.26598800
H	4.18075100	-1.32663600	-2.95590000
H	2.95897500	-2.50261200	-2.44901600
H	2.55475300	-0.77737500	-2.49736800
C	4.86078500	-2.43477200	-0.50449900
H	4.48567100	-3.42626900	-0.78008100
H	5.77197600	-2.24576500	-1.08431700
H	5.12201400	-2.45883000	0.55610300
C	4.77688900	0.93180700	-1.53934100
H	5.00821100	1.93851700	-1.17469500
H	5.70903200	0.48794000	-1.90898900
H	4.08275700	1.02962000	-2.37732000
O	2.65524500	-1.64166400	0.05038800
O	2.91413200	0.66117200	-0.02089600
B	2.03558800	-0.39756700	0.38044900
H	0.90243800	-0.23913300	-0.35152200
C	5.12675900	0.17308600	0.81191300
H	6.14328200	-0.14857600	0.55900100
H	5.17139300	1.21128600	1.15628500
H	4.77254400	-0.43990000	1.64522800

IMA5-3

	x	y	z
C	4.73952800	1.36668200	0.11675100
C	3.34620800	1.29579300	0.08823500
C	2.63614200	0.08971100	0.03271200
C	3.41603700	-1.07194300	-0.00839700
C	4.81162300	-1.06171100	0.01917600
C	5.46254000	0.17210000	0.08408700
H	5.23500800	2.33115300	0.16094900
H	5.36359700	-1.99557200	-0.01123000
H	6.54841700	0.20341900	0.10640300
O	2.77141600	-2.29554600	-0.08371900
O	2.62709100	2.48045400	0.11043500
P	1.09064900	-2.18860200	-0.09175600
P	0.96287900	2.25457700	-0.00545000
C	0.70610000	-3.05844300	-1.73634300
C	0.71664500	-3.23684600	1.44691100
C	0.61602800	3.11348800	-1.65898600

C	0.41467900	3.25835500	1.51272500
H	-1.85265400	-0.54819100	3.82663800
Ni	0.72530100	0.03394300	-0.01622000
C	1.14624200	-2.33555900	2.62972200
H	0.54344400	-1.42413500	2.67498200
H	1.00204100	-2.88976500	3.56617300
H	2.20227300	-2.05286000	2.56776300
C	1.54476700	-4.53667500	1.48046500
H	1.41429200	-5.00907200	2.46282000
H	1.20968800	-5.25806500	0.72911600
H	2.61147600	-4.34851100	1.33313600
C	-0.78296400	-3.57185700	1.58027700
H	-0.97445000	-3.90601300	2.60814200
H	-1.43615300	-2.72156600	1.37732500
H	-1.07810200	-4.38801700	0.91613400
C	1.69728800	-4.19654700	-2.04837900
H	1.61074100	-5.02816400	-1.34432500
H	1.47483000	-4.58846300	-3.04954900
H	2.73296800	-3.84777600	-2.04001800
C	-0.73927000	-3.59292900	-1.75112900
H	-1.02503800	-3.81210800	-2.78826400
H	-0.82764500	-4.52592900	-1.18730200
H	-1.45925200	-2.87660400	-1.34458400
C	0.85678100	-1.96292600	-2.81763200
H	0.13180200	-1.15433900	-2.67696400
H	1.86252800	-1.52858700	-2.82157200
H	0.68027700	-2.40837900	-3.80536200
C	1.48765800	2.37952400	-2.70355300
H	2.55599300	2.49532300	-2.49990800
H	1.26044100	1.30910000	-2.74229400
H	1.28241900	2.80439700	-3.69443400
C	-0.86628400	2.93678900	-2.03735700
H	-1.03148800	3.37403900	-3.03102400
H	-1.14981500	1.88180300	-2.07676500
H	-1.54352600	3.42943400	-1.33660900
C	0.99409500	4.60588600	-1.65553600
H	0.91016400	4.99563300	-2.67843300
H	0.32465300	5.19933800	-1.02607500
H	2.02397900	4.76441700	-1.32126400
C	1.30377000	4.49915800	1.74147200
H	0.99809700	4.96707400	2.68624200
H	2.36065600	4.23342600	1.81987300
H	1.19565600	5.24897500	0.95462200
C	-1.06334000	3.68164500	1.40860500
H	-1.37310600	4.09998300	2.37534300
H	-1.20627800	4.46696800	0.65822800
H	-1.73339400	2.85063000	1.17060100
C	0.59817600	2.29928700	2.71172500
H	-0.05443700	1.42664600	2.63192600
H	1.63514500	1.95585300	2.79973200
H	0.34595300	2.83591800	3.63567100
O	-3.62706100	-0.81916700	2.88449900
C	-2.44872400	-0.54344600	2.89605000
O	-1.66781200	-0.20941000	1.86960500
C	-4.09686100	0.76881400	-0.46644800
C	-3.86999400	-0.72925500	-0.94014900
C	-4.39631100	1.75736100	-1.59869000
H	-5.34642100	1.51371700	-2.08872800

H	-4.48553100	2.76705600	-1.18350700
H	-3.61023900	1.77263700	-2.35645000
C	-5.17632900	0.91985300	0.61733000
H	-5.15671300	1.95153800	0.98611100
H	-6.17769100	0.72364600	0.21702300
H	-4.98790900	0.25444900	1.46109600
C	-3.39865000	-0.83454200	-2.40020100
H	-3.15056000	-1.87642500	-2.62426800
H	-4.17572600	-0.51519900	-3.10316700
H	-2.50364100	-0.22890500	-2.57561300
O	-2.82316800	1.11469200	0.12368100
O	-2.80102200	-1.19193800	-0.08868300
B	-2.13240200	-0.07595500	0.46343800
H	-0.86820700	0.01983100	-0.15247900
C	-5.07111300	-1.65362300	-0.72293300
H	-5.94269800	-1.31355000	-1.29477100
H	-4.81990500	-2.66541100	-1.05995900
H	-5.33766900	-1.70659200	0.33431700

TSA2-3

	x	y	z
C	4.42106800	1.06445200	-1.56560600
C	3.14895300	1.07769400	-0.99108600
C	2.46392500	-0.07864700	-0.59401400
C	3.16149700	-1.27911200	-0.79226000
C	4.43414300	-1.35091200	-1.36030500
C	5.05715900	-0.16392900	-1.74779300
H	4.89348200	1.99956800	-1.84843700
H	4.91406900	-2.31592900	-1.48693700
H	6.04795300	-0.19624600	-2.19228500
O	2.56182500	-2.46380600	-0.40117100
O	2.54730300	2.30709800	-0.79475700
P	0.96677400	-2.27630400	0.08534200
P	1.07104900	2.23590800	0.00128500
C	0.06743100	-3.10752400	-1.38386400
C	1.00973000	-3.36179900	1.64047500
C	0.00362000	3.18906200	-1.26288900
C	1.50138800	3.27061500	1.53783600
H	-1.35009400	0.10589900	3.76162100
Ni	0.78122200	-0.01455700	0.30835700
C	1.98494900	-2.64517900	2.60498200
H	1.62954600	-1.64577100	2.86934300
H	2.06295500	-3.23577600	3.52706200
H	2.98781200	-2.55952000	2.17557000
C	1.54419800	-4.77833600	1.35221500
H	1.70097400	-5.29702600	2.30721200
H	0.83661600	-5.37651100	0.77074000
H	2.50120700	-4.75280000	0.82303900
C	-0.38108800	-3.45107200	2.30066200
H	-0.26949300	-3.90556000	3.29360300
H	-0.84240700	-2.47111500	2.43436100
H	-1.07607700	-4.07178600	1.73134900
C	0.94352200	-4.20625700	-2.02226500
H	1.13998000	-5.03839100	-1.34206300
H	0.40569100	-4.60827900	-2.89067300
H	1.90374300	-3.81595300	-2.36750000
C	-1.29328800	-3.69925300	-0.97061400
H	-1.81294300	-4.02817300	-1.88073900

H	-1.17726000	-4.58261500	-0.33461800
H	-1.94126000	-2.97114500	-0.47300700
C	-0.16089900	-1.99497000	-2.43188100
H	-0.82191100	-1.21341400	-2.05061200
H	0.77922300	-1.53109900	-2.74895600
H	-0.63194500	-2.43807400	-3.31894800
C	-0.48841600	2.13611100	-2.28153100
H	0.34328500	1.58056400	-2.72940100
H	-1.18382100	1.43179800	-1.82063900
H	-1.01765900	2.65401000	-3.09225400
C	-1.21233400	3.86315700	-0.60005800
H	-1.84237100	4.28764600	-1.39277500
H	-1.83360700	3.15398200	-0.04643100
H	-0.91519400	4.69009500	0.05265100
C	0.83714900	4.24592900	-2.02045300
H	0.18651800	4.71295200	-2.77099800
H	1.21171000	5.03983000	-1.37036200
H	1.68906100	3.79970400	-2.53840500
C	2.05447100	4.66132000	1.17125400
H	2.44816600	5.13405900	2.08067100
H	2.87072600	4.59908300	0.44569200
H	1.27888100	5.32187500	0.77238600
C	0.29319700	3.41950300	2.48383300
H	0.61312500	3.98425700	3.36948800
H	-0.54006400	3.96191100	2.03173500
H	-0.06643400	2.44756000	2.82340300
C	2.60260400	2.46734200	2.27004000
H	2.24673300	1.47611900	2.56621400
H	3.49905800	2.34776100	1.65435200
H	2.88899600	3.01184000	3.17923600
O	0.00223100	0.07557600	2.26884600
C	-1.17674100	0.06612600	2.67366700
O	-2.25223600	0.00997400	1.98733200
C	-4.40201900	0.85201000	-0.22590800
C	-4.32458400	-0.67032500	-0.63965700
C	-4.97508700	1.78396900	-1.29688000
H	-6.00964700	1.51613300	-1.54323600
H	-4.97518300	2.81483700	-0.92547800
H	-4.38027600	1.75733600	-2.21316500
C	-5.15371600	1.07815900	1.09867000
H	-4.98535000	2.11060800	1.42378100
H	-6.23349700	0.92667500	0.98640600
H	-4.78408000	0.41440100	1.88391900
C	-4.08438200	-0.86415800	-2.14723400
H	-3.85160300	-1.91723400	-2.33719700
H	-4.96429600	-0.59699100	-2.74365800
H	-3.23677600	-0.26338300	-2.49165500
O	-3.01574000	1.18283900	-0.03203900
O	-3.15969600	-1.13456800	0.06175300
B	-2.34343000	-0.00533400	0.41127600
H	-1.16499500	-0.05266200	-0.00145500
C	-5.52486700	-1.51596600	-0.20342100
H	-6.45300400	-1.15972500	-0.66708400
H	-5.37308900	-2.55637200	-0.51184900
H	-5.64861400	-1.50372000	0.88202000

TSA3-3

x

y

z

Ni	-0.66677000	-0.08491400	-0.08122100
P	-1.36685400	2.07923100	0.05641800
P	-0.54956500	-2.36044300	0.05075600
O	1.16293700	0.19382500	-1.25771600
C	-2.51329300	-0.42109600	0.21937900
O	-3.02350900	1.92086400	0.26538400
C	-0.92876900	3.03031600	1.64639400
C	-1.34707900	3.14266700	-1.51494100
O	-2.16535500	-2.79269700	0.19059600
C	0.13806300	-3.12642000	1.65874200
C	-0.10326400	-3.33954200	-1.50994300
C	1.55065800	0.43981900	-2.50448400
C	-3.45858100	0.60834000	0.33163700
C	-3.03329000	-1.72141700	0.29263500
C	-1.97815000	4.10644700	1.99159400
C	0.47212600	3.66513500	1.55037100
C	-0.93447100	1.97098200	2.77295000
C	0.07669800	3.64021100	-1.84152000
C	-2.31148000	4.34242500	-1.42571000
C	-1.84221500	2.19561500	-2.63527100
C	-0.05142800	-2.05301200	2.75437700
C	-0.65401100	-4.38554600	2.06921900
C	1.63680000	-3.46286200	1.53881200
C	-0.90925400	-2.66523000	-2.64631400
C	-0.52629600	-4.81807100	-1.40206600
C	1.40294200	-3.24753500	-1.83246900
O	0.85336500	0.25176200	-3.47977300
H	2.57034300	0.84769500	-2.57001700
C	-4.82514500	0.38556500	0.50435000
C	-4.39020700	-1.99982900	0.46332000
H	-1.74721500	4.50828900	2.98672700
H	-2.99051900	3.69506100	2.01842400
H	-1.96393300	4.94488100	1.29156200
H	0.78055600	3.98491300	2.55448400
H	0.46918000	4.55627400	0.91533900
H	1.23088100	2.97510200	1.16894400
H	-1.90264900	1.46561400	2.85680600
H	-0.73605500	2.47334200	3.72859200
H	-0.16123700	1.21326500	2.62170400
H	0.36377000	4.48922700	-1.21509000
H	0.10177100	3.97786000	-2.88505000
H	0.84114200	2.86946700	-1.72125700
H	-3.31112200	4.04013600	-1.10145900
H	-2.40078500	4.79211800	-2.42301500
H	-1.94419700	5.12130200	-0.75195700
H	-1.90112900	2.76634100	-3.57091900
H	-2.84258500	1.80489600	-2.42101100
H	-1.16323400	1.35607000	-2.80357400
H	0.25814800	-2.47411200	3.71983500
H	-1.09676400	-1.73879700	2.84717300
H	0.55910400	-1.16789000	2.55704200
H	-1.71813000	-4.17458600	2.19889000
H	-0.25618800	-4.74266800	3.02812400
H	-0.55460000	-5.20082000	1.34869500
H	2.01761500	-3.70557400	2.53990000
H	2.22654100	-2.62801500	1.14799400
H	1.80480000	-4.34254800	0.90944400
H	-0.58326900	-1.63714100	-2.82759400

H	-1.98482000	-2.66947200	-2.44167100
H	-0.74382400	-3.23271500	-3.57124300
H	-1.57809900	-4.92406300	-1.12099600
H	0.08722300	-5.37224600	-0.68522600
H	-0.38972300	-5.29354200	-2.38206900
H	1.55859300	-3.59354400	-2.86210700
H	2.00357300	-3.88242500	-1.17671500
H	1.78846900	-2.22997100	-1.75463200
H	-5.50296000	1.22941000	0.58170000
C	-5.28153000	-0.93152200	0.56853100
H	-4.72635600	-3.03057500	0.50904000
H	-6.34185600	-1.12714300	0.70142500
C	4.06534700	1.38711900	0.53568700
C	4.31411100	-0.14875900	0.24778400
C	3.98257500	1.70134400	2.04033100
H	4.95314200	1.59576300	2.53746100
H	3.64574000	2.73511700	2.16987800
H	3.26375400	1.04625200	2.54256600
C	5.06492600	2.33769100	-0.12752800
H	4.80077800	3.37388200	0.11029700
H	6.08418300	2.15767100	0.23450600
H	5.05859200	2.23249700	-1.21524700
C	5.11768500	-0.88008000	1.32912000
H	5.23623100	-1.93318500	1.05080400
H	6.11977400	-0.44872200	1.44105700
H	4.61200200	-0.84463600	2.29688100
O	2.77023200	1.61140500	-0.04376400
O	2.98076000	-0.68460800	0.23119900
B	2.03352200	0.37756100	0.01822500
H	1.09338300	0.33577000	0.85738400
C	4.97112800	-0.41755500	-1.11757900
H	6.02800200	-0.12776100	-1.12667300
H	4.90928800	-1.48952100	-1.33269700
H	4.46791300	0.11581400	-1.92883900

TSA4-3

	x	y	z
C	4.73582100	1.53261500	0.10218100
C	3.34596700	1.40782100	0.07620500
C	2.68209300	0.17728100	0.01382600
C	3.50386700	-0.95326600	-0.03220200
C	4.89852000	-0.89305300	-0.00796900
C	5.50248300	0.36498900	0.06087800
H	5.19679100	2.51398300	0.15114900
H	5.48663500	-1.80459700	-0.04293400
H	6.58665800	0.43681100	0.08054300
O	2.89711900	-2.19819400	-0.10686700
O	2.57568000	2.56230500	0.10907800
P	1.20972500	-2.13690500	-0.08508900
P	0.92076800	2.25619000	-0.01238000
C	0.83719600	-3.06766300	-1.70049400
C	0.90331700	-3.16900400	1.48194000
C	0.54478500	3.13231100	-1.65103100
C	0.32570900	3.21975900	1.51433400
H	-1.98587300	-0.58546200	3.90002400
Ni	0.76239700	0.05107400	-0.03813600
C	1.33313000	-2.23471200	2.63840200
H	0.70972300	-1.33600600	2.67660100

H	1.21965600	-2.77187700	3.58918300
H	2.37975000	-1.92664000	2.54994800
C	1.76200800	-4.44818700	1.52316700
H	1.67424400	-4.89928000	2.52035100
H	1.42094000	-5.19587300	0.80043700
H	2.81865600	-4.23890600	1.33687700
C	-0.58259800	-3.53441600	1.66262400
H	-0.72859900	-3.90310100	2.68659100
H	-1.24620000	-2.68100800	1.51644400
H	-0.89722700	-4.33144400	0.98493600
C	1.86311500	-4.17716400	-2.00080600
H	1.81863500	-4.99179700	-1.27359100
H	1.64064800	-4.60356800	-2.98796400
H	2.88478500	-3.79007800	-2.01743700
C	-0.58730200	-3.65487100	-1.68315800
H	-0.88085400	-3.90876000	-2.71034500
H	-0.63527100	-4.57740000	-1.09695800
H	-1.32741900	-2.95597700	-1.28268500
C	0.93402200	-1.99355400	-2.80878200
H	0.18875500	-1.20368900	-2.66971800
H	1.92576000	-1.52904400	-2.83853000
H	0.75522900	-2.46541600	-3.78399200
C	1.44713200	2.45068100	-2.70517700
H	2.50907600	2.60852600	-2.49684900
H	1.26589100	1.37203800	-2.75768400
H	1.22568100	2.87995200	-3.69085300
C	-0.92724300	2.89799800	-2.03712100
H	-1.10955900	3.33233000	-3.02918200
H	-1.15909100	1.83035300	-2.08212500
H	-1.62669500	3.35967400	-1.33628200
C	0.86100600	4.63855700	-1.62607700
H	0.76105100	5.04087300	-2.64284300
H	0.16955300	5.19603200	-0.98722700
H	1.88402400	4.83225100	-1.28935300
C	1.16865900	4.48493800	1.78001700
H	0.83211100	4.92852800	2.72620000
H	2.23203700	4.25167300	1.87169900
H	1.05032000	5.24260200	1.00196400
C	-1.16341000	3.59797500	1.40003900
H	-1.49910100	3.99228800	2.36836000
H	-1.32442200	4.38811800	0.65865000
H	-1.80403000	2.74959000	1.14474500
C	0.52191700	2.24586500	2.69918100
H	-0.09927700	1.35291800	2.59193100
H	1.56776700	1.93372900	2.79603300
H	0.23769700	2.75483100	3.62975600
O	-3.80817600	-0.70797000	3.00882500
C	-2.61101400	-0.54985900	2.99276600
O	-1.83653700	-0.31667400	1.92396000
C	-4.23140300	0.62040100	-0.53007500
C	-3.88330100	-0.84355100	-1.02761500
C	-4.44064200	1.64575600	-1.64507600
H	-5.31793000	1.38608200	-2.24919700
H	-4.61943400	2.63145200	-1.20284300
H	-3.57508400	1.72236200	-2.30533000
C	-5.42098600	0.67268700	0.44029100
H	-5.49243100	1.68524500	0.85145700
H	-6.36367400	0.44493500	-0.06960500

H	-5.28274100	-0.01695500	1.27523100
C	-3.19732700	-0.87056800	-2.40059300
H	-2.88063500	-1.89288400	-2.62617000
H	-3.87926900	-0.54677100	-3.19399300
H	-2.31044300	-0.23081500	-2.41831800
O	-3.04654900	0.98576400	0.23111800
O	-2.92925800	-1.30361600	-0.03388800
B	-2.40602400	-0.18946500	0.60300200
H	-0.80004800	-0.01517600	-0.12735600
C	-5.06312700	-1.81662600	-1.02272300
H	-5.84929700	-1.48272200	-1.70991700
H	-4.72461200	-2.80491600	-1.35136400
H	-5.48986700	-1.92079300	-0.02316300

TSA5-3

	x	y	z
Ni	-0.74181700	0.08000800	-0.09822700
P	-1.40407200	-2.03753800	-0.16709800
P	-0.69343400	2.30048700	0.01649300
O	1.97735400	-0.47333200	1.92682300
C	-2.64214600	0.39270500	-0.18774100
O	-3.08808000	-1.95329800	-0.20980900
C	-1.10752200	-3.00387600	-1.77128900
C	-1.17329100	-3.06643800	1.40846600
O	-2.30692000	2.75624600	-0.18496600
C	0.07065700	3.25981900	-1.43805400
C	-0.36258100	3.10737000	1.70463600
C	2.44964500	-1.37531300	2.80816300
C	-3.57048100	-0.65268400	-0.24188200
C	-3.18193700	1.68265400	-0.23135300
C	-1.95361100	-4.28621400	-1.87176900
C	0.38683600	-3.33409700	-1.93361000
C	-1.52888500	-2.03050200	-2.89724900
C	0.22087900	-3.72353700	1.43607600
C	-2.26419200	-4.14012600	1.59357100
C	-1.29038500	-2.04386300	2.56386200
C	-0.02789300	2.30352900	-2.64871600
C	-0.70286400	4.55183100	-1.77162700
C	1.55018900	3.58794300	-1.16835800
C	-1.32902600	2.40641600	2.68846600
C	-0.66591100	4.61752000	1.69611000
C	1.08100800	2.85431900	2.17917700
O	2.00905300	-1.49064300	3.92345700
H	3.26995200	-1.99335500	2.40735900
C	-4.94964100	-0.45657200	-0.33029600
C	-4.55081200	1.94308500	-0.31794500
H	-1.86788700	-4.69247800	-2.88842500
H	-3.01169900	-4.09239400	-1.67366200
H	-1.60515800	-5.06164700	-1.18301000
H	0.57108300	-3.66364900	-2.96484400
H	0.70763000	-4.14048700	-1.26935000
H	1.01737800	-2.46476300	-1.73593700
H	-2.58434900	-1.75179800	-2.82293400
H	-1.37489100	-2.52033800	-3.86751800
H	-0.93102700	-1.11283300	-2.88131100
H	0.26177200	-4.61214800	0.79769000
H	0.44644400	-4.04322900	2.46078100
H	1.01509100	-3.04168200	1.11911500

H	-3.26625700	-3.70475100	1.56965900
H	-2.12079600	-4.61577100	2.57250100
H	-2.21400000	-4.92648500	0.83615000
H	-1.19699900	-2.57283100	3.52052500
H	-2.26108100	-1.53585400	2.55287600
H	-0.50079300	-1.28905800	2.52399000
H	0.37107000	2.80607400	-3.54000300
H	-1.06546100	2.02161500	-2.85992500
H	0.54748300	1.38678300	-2.48387600
H	-1.75415000	4.34994000	-1.98911500
H	-0.24885300	5.00806900	-2.66140100
H	-0.65821300	5.28772900	-0.96500700
H	2.01099100	3.94302200	-2.09997000
H	2.11198000	2.71719500	-0.82097200
H	1.65871000	4.38748500	-0.42865400
H	-1.14403700	1.32864700	2.73984700
H	-2.37758700	2.56578300	2.42088800
H	-1.16831800	2.82121900	3.69178600
H	-1.66660900	4.83150200	1.30890600
H	0.06638200	5.18128300	1.11000900
H	-0.61625800	4.99379500	2.72628300
H	1.19313100	3.27960400	3.18560400
H	1.82845000	3.32642300	1.53757900
H	1.30980300	1.78872700	2.24100900
H	-5.62200000	-1.30766300	-0.36941300
C	-5.42696200	0.85600400	-0.36710800
H	-4.91190400	2.96624500	-0.34439600
H	-6.49684900	1.03404500	-0.43502900
C	4.01284800	-1.02082600	-0.99205800
C	4.32877700	0.44306200	-0.49183800
C	3.34571800	-1.05106400	-2.37250000
H	4.03744900	-0.72175100	-3.15491500
H	3.04098800	-2.07536400	-2.60397400
H	2.45620700	-0.41483400	-2.39962000
C	5.20362700	-1.97994100	-0.97440700
H	4.87959300	-2.97326900	-1.30153700
H	5.98952400	-1.63875700	-1.65815900
H	5.63144200	-2.07851400	0.02601600
C	4.62530500	1.45202200	-1.60053900
H	4.80385600	2.43930900	-1.16225400
H	5.52575200	1.16313100	-2.15523400
H	3.79613300	1.53934400	-2.30541600
O	3.05177800	-1.48284400	-0.00355600
O	3.09878700	0.81691300	0.18312000
B	2.49220000	-0.36568300	0.60505400
H	0.80947800	-0.17991700	-0.10355600
C	5.44765400	0.49767600	0.56140200
H	6.43058000	0.29609100	0.12218300
H	5.46618100	1.49833600	1.00402300
H	5.27731600	-0.22158300	1.36870000

TSA6-3

	x	y	z
H	-3.48082400	0.64954700	-1.22555200
O	-3.86011600	0.16729800	0.71201500
C	-3.23541700	0.09493500	-0.30556400
O	-2.17832600	-0.75066600	-0.49369600
C	1.35321000	-0.68584300	0.05569300

C	0.99065600	0.85415600	0.02574100
C	2.53476000	-1.09284700	-0.82100500
H	3.45745600	-0.60972000	-0.48009400
H	2.67807100	-2.17622900	-0.76026200
H	2.37044800	-0.83373300	-1.86932000
C	1.52852600	-1.24071100	1.47516300
H	1.57135600	-2.33289500	1.42546500
H	2.45266100	-0.87954900	1.93816400
H	0.68727300	-0.96531600	2.11923800
C	1.30958100	1.52859300	-1.31446800
H	0.84704300	2.52019600	-1.33160500
H	2.38809200	1.64986300	-1.45830200
H	0.91106700	0.95354400	-2.15653700
O	0.14684000	-1.30152300	-0.48772000
O	-0.46490600	0.83077300	0.14500900
B	-0.86563600	-0.40969400	-0.27682200
C	1.55392300	1.67789600	1.18063600
H	2.64969900	1.66430100	1.16975400
H	1.22760700	2.71821600	1.08338200
H	1.20885900	1.30612400	2.14774000

TSB1-3

	x	y	z
C	4.91769700	-0.52813700	-1.28104000
C	3.62951000	-0.71926100	-0.78093100
C	2.75256800	0.33337700	-0.48791100
C	3.22406600	1.61861600	-0.78367700
C	4.50423400	1.86651800	-1.28250400
C	5.34664500	0.77906700	-1.52178800
H	5.55538700	-1.38334100	-1.48026100
H	4.81914300	2.88551400	-1.48313900
H	6.34652100	0.95153500	-1.91038000
O	2.37730600	2.69649500	-0.59076100
O	3.18970900	-2.02090000	-0.57798400
P	0.85832100	2.28481100	0.00943700
P	1.61875700	-2.10605600	0.00996200
C	0.89158600	3.26559700	1.63505300
C	-0.24183800	3.05697200	-1.33678100
C	1.95564600	-3.00613200	1.64946200
C	0.80807400	-3.15899900	-1.34312200
C	-1.04955900	-0.41397000	1.43014800
O	-0.21707000	-0.13287800	2.34862600
O	-2.22554100	0.45861300	1.35826800
H	-0.63683800	-0.23975700	0.22344000
Ni	0.97767300	0.03392500	0.11823600
C	-5.40954600	0.20352600	-0.24362100
C	-4.85958200	-1.27348700	-0.36245600
C	-5.26933000	1.00810800	-1.54413400
H	-5.97146200	0.66663000	-2.31235400
H	-5.47650200	2.06155800	-1.33157500
H	-4.25370300	0.93914600	-1.94737200
C	-6.83572400	0.32201800	0.29276600
H	-7.11316700	1.37873700	0.36301800
H	-7.54924700	-0.17211700	-0.37695300
H	-6.92970800	-0.11549900	1.28930900
C	-4.97278500	-1.90135100	-1.75029000
H	-4.53760800	-2.90613300	-1.73566000
H	-6.02191900	-1.99258900	-2.05436400

H	-4.44113600	-1.31483100	-2.50320500
O	-4.50518700	0.79772900	0.72161800
O	-3.45063400	-1.10250100	-0.04699100
B	-3.34341200	0.05624900	0.70627600
C	-5.44016600	-2.22179400	0.69572600
H	-6.49100300	-2.45732000	0.49672200
H	-4.87024500	-3.15631900	0.68679800
H	-5.36554100	-1.79019000	1.69893800
H	-1.41448900	-1.45390300	1.33436600
C	2.01134700	2.60214700	2.47224700
H	1.77168400	1.55724700	2.68678600
H	2.98655300	2.65529900	1.97795300
H	2.08993100	3.13673400	3.42767900
C	-0.43322900	3.13974200	2.41221900
H	-0.68879000	2.09451700	2.59608300
H	-0.30546300	3.64046100	3.38160800
H	-1.26920000	3.62606600	1.90301500
C	1.23937100	4.74918300	1.40364400
H	0.41218700	5.29962500	0.94439500
H	1.43513800	5.21559300	2.37783100
H	2.13348900	4.87483200	0.78555100
C	0.65049100	-3.37492700	2.38046100
H	0.91311100	-3.85116100	3.33432000
H	0.06386400	-2.48136400	2.60790400
H	0.03985800	-4.09087000	1.82102600
C	2.72007600	-1.97079700	2.50984000
H	3.66223100	-1.66617300	2.04329100
H	2.10576200	-1.08617600	2.69663900
H	2.95893700	-2.43344700	3.47626600
C	2.83902900	-4.25604700	1.46435100
H	3.18575600	-4.58248000	2.45328900
H	2.29142900	-5.09211500	1.02170700
H	3.72130800	-4.05097400	0.85152500
C	-0.66500900	-3.44956300	-0.99355900
H	-1.13552800	-3.95188200	-1.84914600
H	-0.76362100	-4.11778000	-0.13281800
H	-1.24114100	-2.54109400	-0.79087000
C	1.55547600	-4.47523900	-1.63174400
H	1.41626400	-5.21243800	-0.83706900
H	1.15545100	-4.91325500	-2.55553600
H	2.62797900	-4.31312100	-1.77477100
C	0.85594400	-2.27684200	-2.61312900
H	0.32554300	-1.33007900	-2.47045200
H	1.88391900	-2.05208800	-2.91349700
H	0.37268900	-2.81723400	-3.43717900
C	0.35965100	4.35195400	-1.92024000
H	-0.27974600	4.69259100	-2.74528300
H	0.40718200	5.15909700	-1.18589400
H	1.36604400	4.18865100	-2.31367200
C	-0.31171500	2.00227000	-2.46514600
H	0.68323600	1.73977200	-2.84106400
H	-0.80215100	1.08262800	-2.12975600
H	-0.88975000	2.41233600	-3.30367000
C	-1.66383700	3.32788000	-0.80837200
H	-1.69099600	4.19630000	-0.14370200
H	-2.32158600	3.54755500	-1.65953300
H	-2.08722800	2.47581700	-0.26831400

[Ni]OCH₂OBPin

	x	y	z
C	5.27932400	0.89854700	0.37030100
C	4.04320000	0.27257800	0.20719800
C	2.82616000	0.96470200	0.14355900
C	2.91648700	2.35684400	0.27124900
C	4.12413100	3.03736000	0.43727300
C	5.30375600	2.29094600	0.48278300
H	6.18913200	0.30825200	0.41189500
H	4.13165000	4.11875400	0.52950300
H	6.25491000	2.80064300	0.61091700
O	1.74635700	3.10066700	0.23257700
O	4.02081400	-1.11703500	0.10820000
P	0.35580000	2.17363200	0.00805000
P	2.46322800	-1.73505900	-0.02993900
C	-0.62666600	2.63476100	1.55829200
C	-0.31040000	2.99325100	-1.57874600
C	2.34801100	-2.82363000	1.51542200
C	2.64903900	-2.71941400	-1.64396700
C	-1.26144900	-1.29305100	-0.97690500
O	-0.45710000	-0.93131300	0.04552900
O	-2.38608700	-0.36999900	-1.15958400
H	-0.76966400	-1.28734500	-1.96401600
Ni	1.15202700	0.06714100	-0.03373400
C	-5.81820200	-0.33918300	-0.20195000
C	-5.28066100	-1.61466000	0.56252800
C	-6.56779900	-0.68418000	-1.49731100
H	-7.54494400	-1.13629200	-1.29580700
H	-6.72397700	0.23511800	-2.07051300
H	-5.98760900	-1.37426400	-2.11844400
C	-6.65101400	0.62123000	0.64550800
H	-6.94799200	1.48326000	0.03897000
H	-7.56260700	0.13315300	1.00947600
H	-6.08658100	0.99239300	1.50398400
C	-6.12935200	-2.87507400	0.40070200
H	-5.66286300	-3.70418600	0.94301700
H	-7.13522800	-2.72599000	0.81036200
H	-6.21956300	-3.16809700	-0.64789600
O	-4.59208400	0.33009700	-0.58803100
O	-3.99841500	-1.83874100	-0.07717600
B	-3.59882100	-0.63216100	-0.62192400
C	-5.00030700	-1.35564200	2.04972400
H	-5.92546400	-1.24096900	2.62486400
H	-4.44328300	-2.20492500	2.45773700
H	-4.39135600	-0.45648800	2.18729800
H	-1.69965500	-2.28902900	-0.80214200
C	0.26769600	2.21712400	2.74869500
H	0.49590900	1.14615000	2.72460600
H	1.21069000	2.77142200	2.76791100
H	-0.26865100	2.42516400	3.68351300
C	-1.92742200	1.80643700	1.60930900
H	-1.71928900	0.73721200	1.50740300
H	-2.41235600	1.97861200	2.58003300
H	-2.64050300	2.08315000	0.82907900
C	-0.92558000	4.14107300	1.66744300
H	-1.62943900	4.48098000	0.90224000
H	-1.38326900	4.34474900	2.64468600
H	-0.01276100	4.74126900	1.59466600

C	0.94001900	-3.45014900	1.61066300
H	0.82439600	-3.90624500	2.60279100
H	0.15576000	-2.69977800	1.47121100
H	0.78990200	-4.24116900	0.87009200
C	2.53911100	-1.85274500	2.70424000
H	3.52221800	-1.37261500	2.68803100
H	1.77312400	-1.07046500	2.71420600
H	2.45320200	-2.42041800	3.63959600
C	3.43478700	-3.91213000	1.58254900
H	3.40508100	-4.38580500	2.57271900
H	3.27385400	-4.70191600	0.84215100
H	4.43758700	-3.49683900	1.43951800
C	1.53092300	-3.76819300	-1.79616600
H	1.56487800	-4.17936600	-2.81340700
H	1.65858200	-4.60430600	-1.10219300
H	0.53420900	-3.34374900	-1.64292700
C	4.02851700	-3.39827100	-1.76928600
H	4.16696500	-4.20544300	-1.04580400
H	4.11311700	-3.83709900	-2.77226800
H	4.84266800	-2.68047000	-1.64189300
C	2.51793200	-1.66648000	-2.76929600
H	1.53023000	-1.19414400	-2.77199000
H	3.27147200	-0.87735200	-2.67631100
H	2.66245800	-2.15757000	-3.74048200
C	0.08595200	4.48202600	-1.66200900
H	-0.26545600	4.87911300	-2.62352900
H	-0.37212700	5.08061700	-0.87044000
H	1.16829400	4.61985400	-1.60856200
C	0.37212200	2.23388600	-2.73962800
H	1.46480800	2.28095900	-2.67331400
H	0.07321400	1.18098800	-2.76068600
H	0.07363200	2.68987100	-3.69267800
C	-1.83772000	2.84924700	-1.71179400
H	-2.37296300	3.46357400	-0.98093300
H	-2.13407400	3.20293400	-2.70848700
H	-2.16976200	1.81373000	-1.60962100