

Theoretical insights into the regiodivergence in Ni-catalyzed [2+2+2] cycloaddition of unsymmetric diynes and CO₂

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DFT-Computed Energies of All Stationary Points

Table S1. Sum of electronic and zero-point energies (E , in Hartree), Sum of electronic and thermal free energies (G , in Hartree), thermal correction to Gibbs free energy ($CGFE$, in Hartree), electronic energy in THF (E_{THF} , in Hartree), and free energies in THF (G_{THF} , in Hartree). For transition state structures, one imaginary frequency (Ifreq) was observed and given below. For all minimum structures, no imaginary frequency was observed.

Structure	E	G	$CGFE$	E_{THF}	G_{THF}	Ifreq
Ni(COD) ₂	-793.033336	-793.075393	0.322693	-795.227883	-794.90519	
COD	-311.839767	-311.871559	0.148956	-312.121644	-311.972688	
1	-679.880041	-679.925313	0.181370	-680.269821	-680.088451	
CO ₂	-188.565952	-188.586668	-0.009098	-188.648113	-188.657211	
L1=PMe ₃	-460.980413	-461.008634	0.085314	-461.167696	-461.082382	
Ni(L1) ₂	-1091.291264	-1091.338712	0.182243	-1093.312542	-1093.130299	
INT1-1a	-1771.220996	-1771.291021	0.388564	-1773.628765	-1773.240201	
INT2-1a	-1498.776314	-1498.841912	0.289769	-1501.078851	-1500.789082	
TS1-1a	-1498.752067	-1498.815148	0.293472	-1501.066239	-1500.772767	-202.89
INT3-1a	-1498.786339	-1498.848197	0.297690	-1501.107387	-1500.809697	
INT4-1a	-1498.803852	-1498.860759	0.303186	-1501.111351	-1500.808165	
TS2-1a	-1498.780468	-1498.836295	0.304112	-1501.086307	-1500.782195	-238.33
INT5-1a	-1498.815044	-1498.872822	0.303387	-1501.114615	-1500.811228	
TS3-1a	-1498.802405	-1498.858540	0.304194	-1501.098606	-1500.794412	-338.34
2	-868.525878	-868.567861	0.205519	-868.985488	-868.779969	
TS4-1a	-1959.758881	-1959.830556	0.400016	-1962.253030	-1961.853014	-243.04
INT6-1a	-1959.798039	-1959.867514	0.406921	-1962.302345	-1961.895424	
TS5-1a	-1959.746266	-1959.808764	0.413850	-1962.246786	-1961.832936	-291.21
INT7-1a	-1959.828979	-1959.893644	0.412874	-1962.318400	-1961.905526	
TS6-1a	-1959.806770	-1959.870468	0.412303	-1962.284688	-1961.872385	-374.87
INT1-1b	-1771.209431	-1771.275161	0.393121	-1773.617551	-1773.224430	
TS1-1b	-1498.738262	-1498.797881	0.296878	-1501.048474	-1500.751596	-157.58
TS4-1b	-1959.745537	-1959.815336	0.401020	-1962.237903	-1961.836883	
INT8-1cd	-1310.229684	-1310.282994	0.290872	-1312.446911	-1312.156039	
TS7-1cd	-1310.191840	-1310.245105	0.291023	-1312.498086	-1312.207063	-203.48
INT9-1cd	-1310.221455	-1310.277073	0.289161	-1312.440748	-1312.151587	
TS8-1c	-1498.770298	-1498.828762	0.298817	-1501.068095	-1500.769278	-287.95
TS8-1d	-1498.783309	-1498.839431	0.301993	-1501.080347	-1500.778354	-196.89
INT5-1b	-1498.820280	-1498.877679	0.304010	-1501.128174	-1500.824164	
TS3-1b	-1498.796762	-1498.852991	0.304231	-1501.091555	-1500.787324	-389.06
3	-868.526166	-868.569341	0.203728	-868.988979	-868.785251	
INT1-1e	-1596.525017	-1596.590389	0.377519	-1598.929683	-1598.552164	
TS4-1e	-1785.067899	-1785.137215	0.386480	-1787.559367	-1787.172887	-260.42
INT6-1e	-1785.114915	-1785.181407	0.393931	-1787.617899	-1787.223968	
INT4-1e	-1785.098983	-1785.165437	0.392571	-1787.589398	-1787.196827	
INT4-1e'	-1785.100997	-1785.168007	0.391707	-1787.591045	-1787.199338	

TS5-1e	-1785.074862	-1785.135097	0.398988	-1787.564430	-1787.165442	-328.50
INT7-1e	-1785.142978	-1785.204668	0.400186	-1787.631155	-1787.230969	
TS6-1e	-1785.118181	-1785.179119	0.399228	-1787.596209	-1787.196981	-389.55
INT2-1e	-1785.072237	-1785.146461	0.380122	-1787.554192	-1787.174070	
TS1-1e	-1785.044230	-1785.116096	0.383591	-1787.531962	-1787.148371	-249.63
TS1-1e'	-1785.051325	-1785.124698	0.382063	-1787.547264	-1787.165201	-186.38
INT3-1e	-1785.092373	-1785.162753	0.388325	-1787.587970	-1787.199645	
TS2-1e	-1785.071351	-1785.136315	0.393618	-1787.559548	-1787.165930	-253.71
TS2-1e'	-1785.075877	-1785.141622	0.393099	-1787.566361	-1787.173262	-236.59
INT5-1e	-1785.116505	-1785.182146	0.395078	-1787.595346	-1787.200268	
TS3-1e	-1785.100422	-1785.164736	0.394791	-1787.571996	-1787.177205	-363.66
INT1-1f	-1596.518033	-1596.581768	0.378611	-1598.921828	-1598.543217	
TS4-1f	-1785.055018	-1785.121728	0.388451	-1787.541868	-1787.153417	-220.76
TS1-1f	-1785.031853	-1785.100990	0.385799	-1787.515403	-1787.129604	-187.63
INT8-1gh	-1596.521063	-1596.583782	0.380017	-1598.917357	-1598.537340	
INT8-1gh'	-1596.526667	-1596.590158	0.379599	-1598.928182	-1598.548583	
TS7-1gh	-1596.479069	-1596.541559	0.380187	-1598.875984	-1598.495797	-249.09
TS7-1gh'	-1596.489152	-1596.551913	0.380462	-1598.892262	-1598.511800	-200.79
INT9-1gh	-1596.523380	-1596.586972	0.380409	-1598.922054	-1598.541645	
INT9-1gh'	-1596.518641	-1596.583020	0.379324	-1598.921435	-1598.542111	
TS8-1g	-1785.077498	-1785.141805	0.393223	-1787.550665	-1787.157442	-183.32
TS8-1g'	-1785.073771	-1785.140694	0.389790	-1787.553672	-1787.163882	-176.70
TS8-1h	-1785.081051	-1785.146247	0.391772	-1787.555634	-1787.163862	-227.46
TS8-1h'	-1785.081631	-1785.149167	0.389019	-1787.561957	-1787.172938	-195.65
INT5-1f	-1785.121490	-1785.186301	0.395831	-1787.601640	-1787.205809	
INT7-1f	-1785.145677	-1785.208010	0.399267	-1787.634244	-1787.234977	
TS5-1f	-1785.117751	-1785.179896	0.398028	-1787.594173	-1787.196145	-449.43
4	-719.164883	-719.212228	0.207901	-719.595569	-719.387668	
INT1-4a	-1810.505456	-1810.576452	0.416306	-1812.954219	-1812.537913	
TS4-4a	-1999.043758	-1999.116710	0.427580	-2001.579063	-2001.151483	-243.94
INT6-4a	-1999.083092	-1999.154721	0.433298	-2001.627930	-2001.194632	
INT3-4a	-1538.071709	-1538.137810	0.321828	-1540.433105	-1540.111277	
INT4-4a	-1538.088522	-1538.146776	0.330728	-1540.436573	-1540.081380	
TS2-4a	-1538.066298	-1538.122722	0.332509	-1540.412436	-1540.079927	-255.01
INT5-4a	-1538.108841	-1538.166088	0.333771	-1540.457636	-1540.123865	
TS3-4a	-1538.087545	-1538.143951	0.333749	-1540.423962	-1540.090213	-347.98
5	-907.809706	-907.853131	0.233646	-908.310191	-908.076545	
6	-907.810930	-907.855661	0.231805	-908.314752	-908.082947	
INT2-4a	-1538.061188	-1538.129393	0.315817	-1540.404240	-1540.088423	
TS1-4a	-1538.037020	-1538.101497	0.320876	-1540.391812	-1540.070936	-205.35
INT1-4b	-1810.494158	-1810.562379	0.419073	-1812.942849	-1812.523776	
TS1-4b	-1538.023327	-1538.085524	0.322668	-1540.373680	-1540.051012	-157.43
TS4-4b	-1999.029889	-1999.100343	0.429604	-2001.562029	-2001.132425	-199.88
INT8-4cd	-1349.504751	-1349.560686	0.316617	-1351.760895	-1351.444278	

TS7-4cd	-1349.469730	-1349.524255	0.319297	-1351.730156	-1351.410859	-189.05
INT9-4cd	-1349.513122	-1349.569120	0.318098	-1351.771234	-1351.453136	
TS8-4c	-1538.063169	-1538.122706	0.327155	-1540.398778	-1540.071623	-325.53
TS8-4d	-1538.073106	-1538.131065	0.329351	-1540.410276	-1540.080925	-205.35
INT5-4b	-1538.106118	-1538.163839	0.333214	-1540.455603	-1540.122389	
TS3-4b	-1538.081682	-1538.138918	0.332837	-1540.416851	-1540.084014	-395.02
INT1-4e	-1635.809503	-1635.876940	0.404180	-1638.254979	-1637.850799	
TS4-4e	-1824.352965	-1824.424696	0.412448	-1826.885400	-1826.472952	-257.84
INT6-4e	-1824.399998	-1824.468484	0.420477	-1826.943380	-1826.522903	
INT4-4e	-1824.385392	-1824.452589	0.421127	-1826.911268	-1826.490141	
INT4-4e'	-1824.388650	-1824.456282	0.420207	-1826.916969	-1826.496762	
TS2-4e	-1824.360457	-1824.425843	0.422404	-1826.887021	-1826.464617	-283.55
TS2-4e'	-1824.364052	-1824.429300	0.423009	-1826.890814	-1826.467805	-257.47
INT7-4e	-1824.430099	-1824.492523	0.429116	-1826.957442	-1826.528326	
TS6-4e	-1824.404086	-1824.46615	0.427703	-1826.921003	-1826.493300	-386.73
INT2-4e	-1824.357552	-1824.431188	0.409338	-1826.879503	-1826.470165	
TS1-4e	-1824.329242	-1824.403148	0.410178	-1826.857684	-1826.447506	-252.96
INT3-4e	-1824.377237	-1824.448399	0.416406	-1826.913471	-1826.497065	
TS5-4e	-1824.352461	-1824.415687	0.424171	-1826.880884	-1826.456713	-299.43
INT1-4f	-1635.801946	-1635.869173	0.403679	-1638.246442	-1637.842763	
TS1-4f	-1824.339665	-1824.408294	0.415336	-1826.867321	-1826.451985	-225.24
TS4-4f	-1824.316411	-1824.386682	0.413536	-1826.841088	-1826.427552	-178.58
INT8-4gh	-1635.797520	-1635.863509	0.404950	-1638.362874	-1637.957924	
INT8-4gh'	-1635.801799	-1635.866959	0.406445	-1638.241251	-1637.834806	
TS7-4gh	-1635.762344	-1635.824774	0.410266	-1638.200796	-1637.790530	-79.05
TS7-4gh'	-1635.765376	-1635.830426	0.407538	-1638.210220	-1637.802682	-179.58
INT9-4gh	-1635.814319	-1635.878627	0.409142	-1638.252699	-1637.843557	
INT9-4gh'	-1635.810402	-1635.876578	0.406807	-1638.252332	-1637.845525	
TS8-4g	-1824.365371	-1824.431776	0.420247	-1826.880182	-1826.459935	-231.04
TS8-4g'	-1824.359751	-1824.430403	0.414699	-1826.879868	-1826.465169	-319.59
TS8-4h	-1824.371388	-1824.438204	0.419381	-1826.885341	-1826.465960	-215.63
TS8-4h'	-1824.371021	-1824.4392	0.418017	-1826.891543	-1826.473526	-208.86
INT7-4e	-1824.413681	-1824.477938	0.426595	-1826.935024	-1826.508429	
INT7-4f	-1824.407814	-1824.474702	0.423107	-1826.932119	-1826.509012	
TS6-4e	-1824.376911	-1824.442004	0.423995	-1826.893842	-1826.469847	-365.62
TS6-4f	-1824.390372	-1824.45267	0.427588	-1826.908446	-1826.480858	-431.19
L2=PN	-747.276741	-747.316472	0.172688	-747.649458	-747.476770	
NiL2	-916.578845	-916.619005	0.173541	-918.591827	-918.418286	
Ni(L2) ₂	-1663.883895	-1663.951417	0.359392	-1666.273225	-1665.913833	
Ni(L2) ₂ -1	-1663.879767	-1663.943369	0.363492	-1666.260560	-1665.897068	
Ni(L2) ₂ -2	-1663.886638	-1663.947167	0.366244	-1666.265648	-1665.899404	
Ni(L2) ₂ -3	-1663.897574	-1663.958157	0.366725	-1666.278026	-1665.911301	
Ni(L2) ₂ -4	-1663.898475	-1663.955549	0.370222	-1666.278606	-1665.908384	

The coordinates of all stationary points (Å)

Ni(COD) ₂			COD		
Ni	0.00008700	-0.00019300	0.00015700	C	-0.87309700 -1.63360600 -0.20854700
C	1.53780300	0.47059100	-1.48151300	C	0.39074000 -1.81376400 0.19254400
C	2.63624300	-0.58340500	-1.42080700	C	-0.39074000 1.81376400 -0.19254400
C	2.24542000	-1.83708700	-0.60252800	C	1.26912000 -0.81582000 0.91607500
C	2.63612100	0.58355300	1.42081100	C	0.87309700 1.63360600 0.20854700
C	1.39444800	-1.53794400	0.61504800	C	1.71931200 0.39152400 0.03045500
C	1.53768600	-0.47051300	1.48151000	H	0.86089300 -2.76724000 -0.04890000
H	1.00341700	0.53401200	-2.42642100	H	0.75613100 -0.42566300 1.80528800
H	3.55335400	-0.14105000	-1.01811200	H	-0.86089300 2.76724000 0.04890000
H	3.55327900	0.14122200	1.01821000	H	-1.34730200 -2.45289900 -0.74923000
H	3.15436100	-2.39358400	-0.31809500	H	2.16058900 -1.33964500 1.27968700
H	2.88566800	-0.89525300	-2.44260800	H	1.34730200 2.45289900 0.74923000
H	1.67322300	-2.51441000	-1.24947200	H	2.75774200 0.64250700 0.27577800
H	2.88543100	0.89541900	2.44263400	H	1.71838500 0.07278800 -1.02043800
H	0.78103600	-2.36978000	0.95781900	C	-1.71931200 -0.39152400 -0.03045500
H	1.00376200	-0.53431800	2.42665000	H	-1.71838500 -0.07278800 1.02043800
C	1.39438800	1.53792600	-0.61507300	H	-2.75774200 -0.64250700 -0.27577800
H	0.78021800	2.36929500	-0.95761000	C	-1.26912000 0.81582000 -0.91607500
C	2.24541100	1.83719600	0.60243900	H	-0.75613100 0.42566300 -1.80528800
H	3.15441500	2.39349300	0.31783700	H	-2.16058900 1.33964500 -1.27968700
H	1.67331600	2.51469000	1.24926200		
C	-1.53772700	-0.47099700	-1.48136400	I	
C	-2.63604600	0.58318000	-1.42100300	C	3.98183300 -0.67072100 0.07832700
C	-2.24519800	1.83705300	-0.60304000	C	2.53475500 -0.14189400 -0.00227000
C	-2.63644100	-0.58290400	1.42060200	H	4.14371900 -1.14506400 1.05697000
C	-1.39452200	1.53827500	0.61482200	H	4.12376100 -1.46328600 -0.67040700
C	-1.53787400	0.47102300	1.48133800	C	1.50569300 -1.27054800 0.21799500
H	-1.00354800	-0.53489600	-2.42636400	H	2.38742600 0.64109700 0.74933200
H	-3.55328400	0.14105800	-1.01833600	H	2.36719800 0.32233700 -0.98007200
H	-3.55331700	-0.14056800	1.01736700	H	1.66252000 -2.05947900 -0.53224600
H	-3.15414000	2.39374400	-0.31896400	H	1.68464500 -1.74222500 1.19540800
H	-2.88526000	0.89480500	-2.44291900	C	4.98281500 0.37641400 -0.12630500
H	-1.67281100	2.51412600	-1.25006400	C	5.79465900 1.25385400 -0.29754600
H	-2.88629900	-0.89432600	2.44242600	H	6.51393600 2.02606700 -0.44836300
H	-0.78067600	2.36993500	0.95721100	C	0.12164500 -0.80408200 0.14993700
H	-1.00386200	0.53473900	2.42643700	C	-1.02564000 -0.39801900 0.08996800
C	-1.39460400	-1.53824700	-0.61474500	Si	-2.76333100 0.19556200 -0.00199800
H	-0.78070200	-2.36988400	-0.95706400	C	-3.90461800 -1.29695000 -0.22635000
C	-2.24551000	-1.83694900	0.60297100	H	-4.95425100 -0.98192600 -0.28278000
H	-3.15438600	-2.39367700	0.31877300	H	-3.66935200 -1.84267900 -1.14731100
H	-1.67321600	-2.51390100	1.25020300	H	-3.81071000 -1.99877100 0.61029900
				C	-2.93583500 1.36850500 -1.47560100

H -3.96396100 1.74298800 -1.55755300
H -2.27136700 2.23451700 -1.37623800
H -2.68771300 0.86398800 -2.41647900
C -3.19285200 1.10098900 1.60206600
H -4.22784600 1.46463000 1.57851600
H -3.09007000 0.44108000 2.47116000
H -2.53814700 1.96564700 1.76049000

CO₂

C 0.00000000 0.00000000 0.00000000
O 0.00000000 0.00000000 1.16958300
O 0.00000000 0.00000000 -1.16958300

PMe₃

P 0.00000000 0.00000000 0.60595600
C 0.00000000 1.64353800 -0.28096300
C -1.42334500 -0.82176900 -0.28096300
C 1.42334500 -0.82176900 -0.28096300
H -0.88358700 2.22041900 0.01454800
H 0.00000000 1.53646600 -1.37309700
H 0.88358700 2.22041900 0.01454800
H -2.36473300 -0.34500000 0.01454800
H -1.33061900 -0.76823300 -1.37309700
H -1.48114600 -1.87541900 0.01454800
H 1.33061900 -0.76823300 -1.37309700
H 1.48114600 -1.87541900 0.01454800
H 2.36473300 -0.34500000 0.01454800

Ni(PMe₃)₂

Ni -0.00004700 0.01053000 -0.03080100
P 2.14414300 -0.00163800 -0.01772200
C 2.99846900 0.92707100 1.34997700
H 2.67591100 0.52987200 2.31769900
H 4.09090200 0.85142700 1.27861000
H 2.71081100 1.98253400 1.30874500
C 2.98542800 -1.65545600 0.12177200
H 4.07883100 -1.56293100 0.12478100
H 2.66716800 -2.14873400 1.04574200
H 2.68341700 -2.29016000 -0.71742800
C 3.02370900 0.70118700 -1.49945800
H 2.72731900 0.14825100 -2.39658100
H 2.72738600 1.74597500 -1.63726700
H 4.11456000 0.65053400 -1.39251100
P -2.14424400 -0.00148500 -0.01800700

C -3.02261800 0.70302800 -1.49965700
H -4.11356500 0.65277400 -1.39347300
H -2.72572100 1.74779700 -1.63634800
H -2.72588300 0.15074900 -2.39706900
C -2.99902500 0.92627100 1.35004900
H -2.71085900 1.98164100 1.31005700
H -4.09144300 0.85119200 1.27788300
H -2.67730100 0.52796200 2.31759400
C -2.98622300 -1.65510400 0.11956700
H -2.66874000 -2.14925500 1.04333800
H -4.07959100 -1.56216000 0.12196900
H -2.68392800 -2.28924500 -0.71995500

INT1-1a

Ni 2.47435900 0.23527100 -0.00005400
C 0.87917600 1.24330000 0.00081100
C 0.57268400 -0.00292300 0.00074100
H 0.49935200 2.25541600 0.00119500
C -0.53137900 -1.00366300 0.00090900
H -0.43072100 -1.66370300 -0.87431600
H -0.43080000 -1.66328500 0.87646200
P 3.32264400 -1.80655300 -0.00032200
P 4.08242000 1.75314800 -0.00017900
C 2.80200900 -2.86631400 1.43331500
H 1.70939400 -2.89274700 1.48294400
H 3.18391500 -3.89114500 1.35115700
H 3.16708500 -2.42354300 2.36571500
C 2.80198900 -2.86633100 -1.43394100
H 3.18381300 -3.89118800 -1.35172400
H 1.70937200 -2.89268900 -1.48362700
H 3.16714600 -2.42363000 -2.36634300
C 5.15475400 -2.14131700 -0.00032900
H 5.61317700 -1.68935900 0.88579300
H 5.37698500 -3.21521800 -0.00019300
H 5.61311900 -1.68960000 -0.88660200
C 5.26662800 1.78006600 1.43397800
H 5.80915400 0.83059400 1.48708700
H 5.99259500 2.59826400 1.35388700
H 4.70288200 1.89661600 2.36537600
C 5.26951500 1.77801600 -1.43199700
H 5.99519300 2.59645300 -1.35173000
H 5.81230500 0.82855800 -1.48249100
H 4.70765500 1.89300900 -2.36472900
C 3.52877600 3.52331100 -0.00204300

H 2.90946600 3.70773300 0.88144500
 H 4.37345000 4.22261000 -0.00170300
 H 2.91124400 3.70644700 -0.88704600
 C -1.93391900 -0.37173100 0.00069400
 H -2.04304100 0.27307600 -0.87878500
 H -2.04313900 0.27348800 0.87985900
 C -3.05462000 -1.43452700 0.00087700
 H -2.93913000 -2.08664300 0.87937300
 H -2.93892000 -2.08716000 -0.87720800
 C -4.39894800 -0.85895300 0.00053400
 C -5.51116300 -0.36011100 0.00022200
 Si -7.18782900 0.38661800 -0.00029700
 C -8.47966100 -0.99647300 -0.00015100
 H -8.37788800 -1.63473500 0.88511500
 H -9.49632100 -0.58352000 -0.00051700
 H -8.37748000 -1.63529600 -0.88496500
 C -7.39040800 1.45619500 1.54758700
 H -7.26939300 0.86216600 2.46077600
 H -6.64703600 2.26125300 1.57319000
 H -8.38558700 1.91761200 1.57724300
 C -7.38982500 1.45531600 -1.54886600
 H -6.64641300 2.26033200 -1.57466600
 H -7.26851000 0.86076400 -2.46167400
 H -8.38497600 1.91675500 -1.57913500

INT2-Ia

Ni -2.91841300 -0.74725900 -0.47665200
 C -1.31021300 -1.72165200 -0.71424600
 C -1.01679800 -0.55448900 -0.30408300
 O -4.20804600 -2.04071300 1.74728400
 O -4.54457100 -2.16457400 -0.56826300
 C -4.15617000 -1.92023300 0.56207600
 C -0.05300900 0.49435100 0.11544800
 H -0.22526900 1.40915600 -0.46951100
 H -0.25291800 0.76536100 1.16219200
 H -1.00713300 -2.70668200 -1.03165700
 P -4.08334700 1.15582900 -0.04904500
 C -3.67866200 2.01166100 1.54057700
 H -4.27507300 2.92117200 1.67667600
 H -3.86880900 1.32822300 2.37397600
 H -2.61659700 2.27512800 1.55596100
 C -3.85622400 2.50513400 -1.29725100
 H -4.41479300 3.40891300 -1.02772200
 H -2.79347400 2.75418900 -1.37945500

H -4.19593800 2.15530200 -2.27729200
 C -5.92757900 1.02055100 0.04845900
 H -6.39874100 1.99638000 0.21195500
 H -6.31329200 0.58467200 -0.87824300
 H -6.19924100 0.35289600 0.87233600
 C 1.41518200 0.05486100 -0.03239700
 C 2.39403700 1.16226200 0.41471100
 H 1.61553000 -0.21030200 -1.07645500
 H 1.58795100 -0.84832700 0.56307800
 H 2.21081700 2.07202800 -0.17596100
 H 2.18641500 1.43239200 1.46056000
 C 3.79746800 0.77351000 0.28350100
 C 4.96118000 0.43115300 0.16722500
 Si 6.72001500 -0.07670200 -0.00014100
 C 7.81940400 1.45022600 0.19936200
 H 8.87953600 1.18203000 0.10855900
 H 7.59808900 2.20263900 -0.56636000
 H 7.67605600 1.91957800 1.17942500
 C 7.12388200 -1.34459300 1.34415800
 H 6.97102700 -0.92493900 2.34510800
 H 6.49012400 -2.23444900 1.25547200
 H 8.16947700 -1.66989200 1.27360200
 C 6.98175000 -0.84004400 -1.71087700
 H 6.34709400 -1.72183200 -1.85576900
 H 6.74506400 -0.12446900 -2.50670300
 H 8.02510300 -1.15342900 -1.84201800

TSl-Ia

Ni 3.16165300 0.62362900 -0.00058200
 C 1.29741100 1.66869800 0.01039200
 C 1.36398400 0.34175500 0.01269900
 H 0.36721100 2.23122500 0.01526100
 C 0.36291200 -0.76409000 0.02211400
 H 0.53698200 -1.41332900 -0.84950900
 H 0.53658500 -1.39772300 0.90527600
 O 1.99025800 3.97766200 0.00291900
 O 3.74148300 2.53322000 -0.00747400
 C 2.51503100 2.88159500 0.00053900
 P 4.10973900 -1.28392300 -0.00645400
 C 3.78047800 -2.38247600 1.43985300
 H 2.71449300 -2.62343300 1.48791400
 H 4.35436400 -3.31331100 1.36885000
 H 4.05313900 -1.86169300 2.36252600
 C 3.76857300 -2.37645000 -1.45462700

H 4.03487400 -1.85214200 -2.37716200
 H 4.34193700 -3.30820000 -1.39179400
 H 2.70200100 -2.61615200 -1.49587300
 C 5.95033100 -1.13124200 -0.01370500
 H 6.27254200 -0.57404400 0.87117700
 H 6.43495600 -2.11430900 -0.01830800
 H 6.26520000 -0.56935400 -0.89826300
 C -1.10009400 -0.28553000 0.01715900
 C -2.09386000 -1.46749700 0.02734200
 H -1.28110800 0.33333000 -0.86863300
 H -1.28226000 0.34929600 0.89134400
 H -1.90461400 -2.11152100 -0.84398900
 H -1.90976200 -2.09216400 0.91370700
 C -3.48977000 -1.03243400 0.01805000
 C -4.64413700 -0.64266100 0.00918500
 Si -6.38501600 -0.04728500 -0.00715800
 C -6.57427400 1.32789600 1.27709100
 H -5.91240400 2.17313000 1.05634100
 H -7.60445500 1.70533400 1.29357800
 H -6.33314300 0.96978100 2.28452900
 C -7.52960000 -1.49260700 0.41611500
 H -7.43221100 -2.30532300 -0.31285400
 H -7.30265300 -1.90357200 1.40655700
 H -8.57852100 -1.17055000 0.41990500
 C -6.78794700 0.61643900 -1.73166900
 H -6.12836000 1.44923800 -2.00123200
 H -6.67303500 -0.16119600 -2.49551000
 H -7.82206700 0.98047400 -1.77729000

INT3-1a

Ni 3.36188600 0.64000000 0.00106000
 O 3.47324700 2.43183500 0.00283700
 O 2.23420200 4.31441700 0.00217400
 C 2.31637800 3.10010600 0.00062700
 C 1.16114400 2.15815200 -0.00415600
 C 1.48010700 0.85480000 -0.00535100
 H 0.14556600 2.55140900 -0.00663900
 C 0.53632800 -0.31468700 -0.01093600
 H 0.74361300 -0.94193600 -0.89195100
 H 0.74350400 -0.95055400 0.86387600
 P 3.81831800 -1.57501000 0.00255100
 C 3.30795900 -2.60378400 -1.44461500
 H 3.71205000 -3.61941300 -1.36988500
 H 2.21694500 -2.65903900 -1.49756700

H 3.66921400 -2.14053800 -2.36777900
 C 5.66091700 -1.77210900 0.00431300
 H 6.08579900 -1.28985100 0.89050500
 H 5.94686600 -2.82979200 0.00575300
 H 6.08726000 -1.29181600 -0.88223600
 C 3.30562000 -2.60014300 1.45152800
 H 2.21449900 -2.65529100 1.50285400
 H 3.70985700 -3.61596300 1.38013700
 H 3.66527200 -2.13447200 2.37409600
 C -0.95759900 0.05672000 -0.00897900
 C -1.85792000 -1.19838900 -0.01467800
 H -1.18965900 0.67102600 -0.88577900
 H -1.18913400 0.66282400 0.87365900
 H -1.62434900 -1.81176900 -0.89745600
 H -1.62153800 -1.82164100 0.86041300
 C -3.28437100 -0.87689600 -0.01035900
 C -4.46750700 -0.58542500 -0.00614100
 Si -6.25315600 -0.14415200 0.00300400
 C -7.27095600 -1.72291400 0.23040600
 H -8.34415900 -1.49510700 0.24895000
 H -7.09374500 -2.43252200 -0.58594700
 H -7.01984700 -2.22635000 1.17107100
 C -6.58212000 1.04934600 1.43256400
 H -6.33145600 0.59389800 2.39749700
 H -5.98798300 1.96479700 1.33158600
 H -7.64009900 1.33874200 1.46360300
 C -6.69186500 0.67783600 -1.64273300
 H -6.10517900 1.59001900 -1.80061300
 H -6.49947100 0.00691900 -2.48786300
 H -7.75348200 0.95401100 -1.66932500

INT4-1a

Ni 0.56791700 -0.15350100 0.09957100
 O 1.99629500 0.45042000 -0.90839500
 O 3.66922900 -0.25127600 -2.23398100
 C 2.73950700 -0.50312900 -1.48614600
 C 2.30667000 -1.86649300 -1.07576700
 C 1.24115600 -1.92036000 -0.26420100
 H 2.88423600 -2.72986500 -1.41041400
 C 0.75417700 -3.17089400 0.41674300
 H 1.39325600 -4.02114100 0.13665900
 H -0.26975100 -3.42637700 0.10629200
 P 0.50574800 2.17729900 0.64904200
 C 0.79199200 -2.99709100 1.94958700

C -0.31761800 -2.04369000 2.49021200
 H 1.77469900 -2.60040100 2.22619100
 H 0.68240200 -3.96602200 2.44994300
 H -1.18112500 -2.63268600 2.82936500
 H 0.04429900 -1.49118500 3.36527800
 C -0.81498400 -1.12249700 1.45911500
 C -1.45307300 -0.58795400 0.54179000
 C -0.67082700 2.97365900 1.83975600
 H -1.69641400 2.91119300 1.46537000
 H -0.62979300 2.44392400 2.79733600
 H -0.41985200 4.02682000 2.00983100
 C 0.47733800 3.30126200 -0.81605400
 H 1.21201200 2.91910200 -1.53020900
 H -0.50999800 3.28593000 -1.28940900
 H 0.72508900 4.33399600 -0.54529400
 C 2.14575700 2.55555800 1.41006800
 H 2.23042400 2.05169300 2.37867800
 H 2.91659000 2.16104900 0.74366500
 H 2.28729800 3.63262700 1.55496300
 Si -2.71650600 -0.18567100 -0.77093200
 C -3.47413300 1.51615300 -0.45153900
 H -2.74288700 2.32099800 -0.58216300
 H -4.29119900 1.69819900 -1.16089100
 H -3.88934300 1.59209100 0.55995900
 C -1.87351900 -0.23980900 -2.45496100
 H -1.06285300 0.49384000 -2.52556700
 H -1.43530500 -1.22565300 -2.64536200
 H -2.59530300 -0.02847000 -3.25411800
 C -4.05335300 -1.51619400 -0.63288000
 H -4.53170900 -1.50410000 0.35318400
 H -4.83453800 -1.35529000 -1.38633400
 H -3.63578200 -2.51661900 -0.79285300

TS2-1a

Ni 0.66664900 -0.00715500 -0.01582900
 O 2.44616500 -0.20742000 -0.62332700
 O 4.35337400 0.97550700 -0.83135700
 C 3.19222000 0.86761900 -0.46380900
 C 2.47653800 1.95908200 0.26347800
 C 1.15440400 1.94289500 0.50911700
 H 3.09211800 2.76356100 0.67081600
 C 0.50218800 3.03387800 1.32543700
 H 1.27002800 3.64968800 1.80796200
 H -0.10099900 2.58237300 2.12324800

P 0.80512000 -2.24294600 0.21827300
 C -0.40291300 3.87933200 0.39646600
 C -0.81293500 2.96687700 -0.78977500
 H 0.13832300 4.75498900 0.02509700
 H -1.28575900 4.24185300 0.93307700
 H -1.85844900 3.10945800 -1.08200900
 H -0.19045700 3.17587500 -1.66724900
 C -0.61688900 1.54857600 -0.37115700
 C -1.21353400 0.44261000 -0.07373500
 Si -2.96200200 -0.20087000 -0.13150200
 C -4.15117000 1.22006200 -0.53816400
 H -3.93810000 1.65845000 -1.52023000
 H -5.18748500 0.85929500 -0.55782400
 H -4.09655800 2.02160300 0.20800200
 C -3.11814800 -1.50602800 -1.49571000
 H -2.43858800 -2.35348800 -1.35582300
 H -4.14044300 -1.90266700 -1.53489000
 H -2.89499200 -1.06564000 -2.47479200
 C -3.43999700 -0.91145500 1.55657700
 H -4.47588500 -1.27304300 1.54322400
 H -2.79858900 -1.74644100 1.85566700
 H -3.36791500 -0.14274900 2.33524800
 C -0.49380400 -3.34154500 0.94152200
 H -0.72581200 -3.01263800 1.95924600
 H -1.41235500 -3.30324200 0.35121700
 H -0.14125700 -4.37861200 0.97881700
 C 1.20859900 -3.03494500 -1.39556600
 H 2.03351900 -2.46881900 -1.83606600
 H 1.49938300 -4.08372800 -1.26818600
 H 0.34575500 -2.97819000 -2.06645700
 C 2.26812700 -2.64406800 1.26705900
 H 2.09220200 -2.30910800 2.29435200
 H 2.46877300 -3.72167600 1.27106300
 H 3.12613500 -2.10245300 0.86365100

INT5-1a

Ni 0.66304400 -0.22668400 0.00176600
 O 0.85137800 1.47333200 -0.58087300
 O 1.01863300 3.66174000 -0.38451600
 C 0.31709000 2.65082000 -0.31848500
 C -1.11820300 2.81481600 0.01153100
 C -2.13375800 1.93930500 0.17541300
 H -1.35556400 3.87023200 0.12824500
 C -3.54329400 2.43990700 0.47513100

H -3.73966400 3.42689900 0.04545000
 H -3.67801000 2.52676900 1.56445200
 P 3.07428200 -0.13227500 0.16859700
 C -4.45534500 1.33047500 -0.06940200
 C -3.66240100 0.05217100 0.24849900
 H -4.56702200 1.44107300 -1.15534300
 H -5.45713700 1.33617600 0.37255700
 H -3.86008000 -0.26114800 1.28422800
 H -3.92809500 -0.79046300 -0.39803800
 C -2.18505500 0.46134000 0.10771400
 C -1.16725000 -0.41597800 -0.00278900
 Si -1.27046600 -2.29621400 -0.09997800
 C -2.22685100 -3.06332200 1.34717800
 H -3.28639200 -2.78703400 1.33090100
 H -2.16633300 -4.15868000 1.30873600
 H -1.81277400 -2.73817900 2.30884800
 C -1.96400300 -2.89145000 -1.75979200
 H -3.00795600 -2.58724400 -1.89650100
 H -1.38689600 -2.47635000 -2.59401000
 H -1.92348900 -3.98587000 -1.83128400
 C 0.52815700 -2.94902000 0.03085600
 H 1.07402800 -2.60420800 0.92062000
 H 0.47448000 -4.04275700 0.12044300
 H 1.13926700 -2.73592200 -0.85491600
 C 4.21048700 -1.45131200 0.81012500
 H 3.96321800 -1.67900100 1.85256000
 H 4.08760200 -2.36859000 0.22456200
 H 5.25998300 -1.13974300 0.75965700
 C 3.54665900 1.34700100 1.16641600
 H 4.62578700 1.53284200 1.12020900
 H 3.00575100 2.21177300 0.76929200
 H 3.25473000 1.20181400 2.21184500
 C 3.79587700 0.26277000 -1.48551900
 H 3.22027600 1.09142700 -1.90709000
 H 4.85075900 0.54967100 -1.40934300
 H 3.70783300 -0.60093300 -2.15293800

TS3-1a

Ni -0.86409500 -0.26555600 -0.79588500
 O 0.71287500 -0.15350200 -1.77469100
 O 1.34247400 -1.73903300 -3.23769100
 C 1.20492800 -1.41103100 -2.07114100
 C 1.60464100 -2.24413500 -0.93548100
 C 1.78357300 -1.76673600 0.33084500

H 1.93825800 -3.24215500 -1.20432600
 C 2.48551200 -2.48237700 1.46835400
 H 3.19336900 -3.24534500 1.12887700
 H 1.74496200 -2.98616300 2.10825500
 P -2.65390500 -0.49466800 0.43212000
 C 3.15788300 -1.32425000 2.23993800
 C 2.19587300 -0.12468300 2.06225400
 H 4.12153700 -1.09120300 1.77147200
 H 3.34958500 -1.56349000 3.29125600
 H 1.46625300 -0.09385100 2.88521800
 H 2.72017700 0.83778900 2.07316800
 C 1.49793600 -0.41388700 0.73504200
 C 0.72811500 0.44176600 -0.00695000
 Si 0.76682400 2.33860800 -0.08413900
 C 0.12689200 3.01808300 1.57052900
 H 0.12709600 4.11548200 1.55770500
 H -0.90109000 2.69136200 1.76888200
 H 0.74733500 2.69782400 2.41537500
 C 2.54430900 2.92713800 -0.37603000
 H 2.58452500 4.02097200 -0.45559600
 H 3.21998300 2.62731800 0.43329100
 H 2.93621200 2.50838800 -1.30999100
 C -0.32520200 2.95146400 -1.49723500
 H -0.25672700 4.04314100 -1.58958200
 H -0.00822500 2.50680500 -2.44648000
 H -1.37849500 2.68984600 -1.34360500
 C -3.76744500 0.97001700 0.65625000
 H -3.21003300 1.79281600 1.11485000
 H -4.12710500 1.30988900 -0.32007600
 H -4.62886200 0.72820900 1.28959300
 C -2.35118400 -1.01656400 2.18151700
 H -3.28853700 -1.14096900 2.73562500
 H -1.80125900 -1.96249000 2.18731700
 H -1.73393400 -0.26547200 2.68378500
 C -3.84433300 -1.78571000 -0.16054200
 H -3.33580800 -2.75323400 -0.21638000
 H -4.71185700 -1.87456300 0.50395000
 H -4.19144800 -1.53012600 -1.16671000

2

O -1.03494800 2.40381800 0.03796500
 O 1.19005900 2.42842800 0.08136400
 C 0.20098700 1.72417100 0.03717800
 C 0.17897200 0.26019600 -0.00775300

C -1.04771100 -0.35071200 -0.05813200
 C -1.41011700 -1.82578600 -0.10930700
 H -0.77169900 -2.44995400 0.51851100
 H -1.29553800 -2.18905700 -1.14103700
 C -2.89700800 -1.86375800 0.31694700
 C -3.48022500 -0.50978000 -0.15473700
 H -2.95987000 -1.92679200 1.40990900
 H -3.43317800 -2.72408900 -0.09439700
 H -3.84008000 -0.58794600 -1.19065700
 H -4.32574600 -0.17404900 0.45483500
 C -2.27911400 0.40500400 -0.07849500
 C -2.21300300 1.74962500 -0.02468400
 H -3.05693700 2.43248900 -0.02002700
 Si 1.92620900 -0.51240500 -0.00677900
 C 1.87393500 -2.40978800 -0.06995900
 H 2.90530000 -2.77803900 -0.14746300
 H 1.44306000 -2.85487700 0.83424000
 H 1.32659900 -2.79830000 -0.93608600
 C 2.82693000 -0.00483300 1.57715000
 H 2.31564500 -0.38672800 2.46931600
 H 3.84890800 -0.40444800 1.58492400
 H 2.88304700 1.08471300 1.65540900
 C 2.84994600 0.09516000 -1.54207600
 H 2.36152000 -0.24271900 -2.46429300
 H 2.89199900 1.18806300 -1.55790400
 H 3.87761300 -0.28955900 -1.55179900

TS4-1a

Ni -2.23817200 -0.01662900 -0.02616500
 C -0.63812100 -1.03692300 0.71888400
 C -0.43258500 0.21912900 0.37190100
 H 0.00497400 -1.90595100 0.61871400
 O -2.03732800 -2.74385500 1.90096700
 O -2.47555700 -0.55968000 2.44207800
 C -1.95786300 -1.52564300 1.88230000
 P -3.03265200 2.03188100 -0.05619300
 P -3.78990000 -1.47281500 -0.85652500
 C 0.70067800 1.16359300 0.18365100
 H 0.66135100 1.89589600 1.00711600
 H 0.55671800 1.74716700 -0.73661300
 C 2.08910400 0.49891200 0.16895200
 H 2.23909300 -0.05950300 1.09928600
 H 2.14072800 -0.22752400 -0.65011400
 C 3.21838100 1.53889600 0.00079100

H 3.17891900 2.25642300 0.83351400
 H 3.04062800 2.12482100 -0.91318900
 C 4.55046500 0.93955600 -0.06258000
 C 5.65354100 0.42466900 -0.11832500
 Si 7.32320400 -0.33873300 -0.21025500
 C 7.46221600 -1.31753200 -1.82341500
 H 8.45045000 -1.78615900 -1.91194100
 H 6.70942700 -2.11268700 -1.87220900
 H 7.31994900 -0.66945800 -2.69590800
 C 7.55843400 -1.49348500 1.26868900
 H 8.54847000 -1.96579000 1.24081400
 H 7.47354900 -0.94992300 2.21662600
 H 6.80709100 -2.29143300 1.27373600
 C 8.62420400 1.03471700 -0.17524600
 H 8.55700100 1.62319000 0.74701400
 H 9.63684300 0.61599000 -0.23240100
 H 8.49836500 1.72225500 -1.01953400
 C -4.86308100 2.28537000 -0.20421400
 H -5.37320300 1.70296600 0.56956400
 H -5.13119900 3.34158600 -0.08551000
 H -5.21399400 1.94220400 -1.18234800
 C -2.39417000 3.23109800 -1.31500800
 H -1.30341300 3.28431300 -1.25048700
 H -2.65637300 2.88518100 -2.32002300
 H -2.80881300 4.23458500 -1.16394200
 C -2.67282500 2.87820500 1.54597600
 H -3.17373300 3.85033300 1.61951700
 H -2.99424500 2.22430500 2.36151800
 H -1.59256200 3.01968400 1.64464300
 C -5.12373200 -2.02961600 0.29552200
 H -5.73532300 -1.17597600 0.60396200
 H -5.76740100 -2.78522700 -0.16985800
 H -4.64777000 -2.45208800 1.18509900
 C -4.73110600 -1.04674300 -2.39639900
 H -5.33886500 -1.89242200 -2.73812700
 H -5.39245500 -0.19404400 -2.21278200
 H -4.03108600 -0.77171300 -3.19217900
 C -2.98474700 -3.06943300 -1.31729600
 H -2.23610700 -2.89340000 -2.09635000
 H -2.48008900 -3.45096200 -0.42450300
 H -3.71438500 -3.80509300 -1.67561000

INT6-1a

Ni -2.39694400 0.16916600 -0.05598100

O -2.48302600 2.00689700 -0.33982800
 O -1.24022600 3.78922600 -0.90415600
 C -1.32244100 2.60698000 -0.60950000
 C -0.17386800 1.67851500 -0.47075200
 C -0.45232500 0.39936000 -0.16456100
 H 0.82649500 2.09606400 -0.57429600
 C 0.63535800 -0.59779100 0.17144000
 H 0.47219800 -0.94395300 1.20514100
 H 0.53904700 -1.50014200 -0.44988800
 P -2.41854800 -2.06812100 -0.27404400
 C -1.59874200 -3.18075600 0.95901700
 H -1.69602200 -4.23048800 0.65976500
 H -0.54080800 -2.93424100 1.05976900
 H -2.07473200 -3.04588200 1.93582200
 C -4.07058900 -2.89789400 -0.40093100
 H -4.68058700 -2.40238400 -1.16206800
 H -3.95006700 -3.95150400 -0.67713500
 H -4.59853200 -2.84358400 0.55450900
 C -1.68777100 -2.58249600 -1.89568000
 H -0.66477600 -2.21499900 -1.99615500
 H -1.69614200 -3.67294700 -2.00507300
 H -2.28116000 -2.13959800 -2.70200700
 C 2.08589500 -0.10010400 0.05535900
 C 3.09995200 -1.20393000 0.43004400
 H 2.24000300 0.76417300 0.71025700
 H 2.28681100 0.23912200 -0.96726100
 H 2.90164200 -1.54923600 1.45563300
 H 2.94587600 -2.07882600 -0.21923100
 C 4.49183800 -0.76692500 0.32795000
 C 5.64471300 -0.38264300 0.23579300
 Si 7.38102400 0.20139300 0.09732200
 C 8.54654200 -1.23595700 0.49424500
 H 9.59498000 -0.92019500 0.42196600
 H 8.38045300 -1.61414900 1.50955600
 H 8.40029200 -2.07092600 -0.20068500
 C 7.68808700 0.81092200 -1.66694600
 H 7.52390400 0.01171300 -2.39892700
 H 7.01841000 1.63996200 -1.92284800
 H 8.71998200 1.16533800 -1.78387900
 C 7.65759700 1.61266500 1.32619500
 H 6.98834000 2.45584600 1.12029300
 H 7.47412800 1.28578600 2.35620900
 H 8.68928100 1.98240400 1.27074900
 P -4.66810500 0.67467400 0.44481000

C -5.45837100 1.63850800 -0.91579700
 H -6.37673900 2.13242800 -0.57850100
 H -4.72944900 2.38171800 -1.24608000
 H -5.69687000 0.97656300 -1.75517100
 C -6.06067000 -0.42558200 0.99961300
 H -5.75645300 -1.01602100 1.87048600
 H -6.93322200 0.17582800 1.27934000
 H -6.35767700 -1.11272200 0.20226100
 C -4.59353300 1.88385800 1.83822200
 H -4.25928200 1.38033800 2.75143900
 H -3.86172500 2.64778300 1.56797400
 H -5.57171300 2.34293300 2.02113100

TS5-1a

Ni -0.46672000 0.02516100 -0.13096400
 O -0.54960200 -0.40723300 2.04056400
 O -0.22720400 0.92182600 3.85061200
 C -0.50042300 0.72619400 2.66279100
 C -0.83861600 1.91672300 1.79571800
 C -0.72580100 1.97184400 0.45201000
 H -1.18939500 2.80386800 2.33085300
 C -1.03355700 3.26153100 -0.28258800
 H -1.64327600 3.91653300 0.35198800
 H -1.59680300 3.07810300 -1.20380500
 P -0.16882400 -2.25605000 -0.02079400
 C 0.29572000 3.91889500 -0.65930400
 C 1.10557100 2.80755600 -1.32593700
 H 0.80644800 4.26524200 0.24691300
 H 0.16726700 4.77786800 -1.32804900
 H 0.73609500 2.64500000 -2.34925100
 H 2.17003100 3.04937800 -1.40458300
 C 0.96498100 1.51870500 -0.57180800
 C 1.54750200 0.40738600 -0.32660300
 P -2.67477100 -0.04705700 -0.77103900
 Si 3.34445400 -0.10206700 -0.37143900
 C 4.35498900 1.33282900 -1.09936600
 H 5.41880200 1.06207200 -1.11183000
 H 4.06424400 1.56774700 -2.12989200
 H 4.25885800 2.24600200 -0.50075200
 C 3.64902300 -1.58430900 -1.51769700
 H 4.73016800 -1.73279000 -1.63555900
 H 3.22935500 -2.52873500 -1.15920400
 H 3.23578100 -1.38964800 -2.51514800
 C 3.99483700 -0.40555000 1.37744000

H 5.06043000 -0.66753200 1.34783800
 H 3.89199300 0.50857200 1.97383100
 H 3.46314800 -1.19789900 1.91042700
 C 1.18357300 -2.78283400 1.11437000
 H 2.16474000 -2.58421700 0.68694500
 H 1.05717800 -2.19855200 2.02929200
 H 1.10138300 -3.85431200 1.33081400
 C 0.10590800 -3.30073900 -1.52933600
 H 0.22310400 -4.35908300 -1.26843400
 H -0.73830800 -3.19868900 -2.21807900
 H 1.00611200 -2.96241100 -2.05046600
 C -1.56311500 -3.12539500 0.83449600
 H -2.50019900 -3.08474900 0.27561000
 H -1.30509100 -4.17729400 1.00145700
 H -1.69230300 -2.62154300 1.79600700
 C -3.79956100 -0.26381400 0.67901500
 H -3.62714300 0.57027100 1.36518100
 H -4.85180200 -0.27715300 0.37271800
 H -3.56076200 -1.18164800 1.21794200
 C -3.50307500 1.39005800 -1.60489600
 H -4.52734800 1.11337200 -1.87937100
 H -3.54526000 2.24901100 -0.93262100
 H -2.96256100 1.67806500 -2.51162400
 C -3.22575500 -1.36689200 -1.96062400
 H -2.76250500 -1.17849000 -2.93524600
 H -2.92644800 -2.36348100 -1.63219100
 H -4.31497100 -1.35170800 -2.08259900

INT7-1a

Ni -0.57614500 0.00382200 0.05747700
 O -0.45679900 1.51818100 1.16659000
 O -0.79240900 3.71025000 0.93039000
 C -0.21906000 2.67271300 0.58210200
 C 0.79226600 2.79045900 -0.51888100
 C 1.81952100 1.97037200 -0.83562200
 H 0.75879400 3.77227000 -0.98699200
 C 2.98777800 2.39843200 -1.70468200
 H 3.01417100 3.47501600 -1.89930200
 H 2.95219500 1.88395700 -2.67826600
 P -0.68342900 -1.37185400 -1.70616700
 C 4.19651300 1.88696800 -0.89210300
 C 3.70821200 0.54942300 -0.28971600
 H 4.41444200 2.60091300 -0.08872800
 H 5.10516100 1.77771900 -1.49403400

H 3.98655100 -0.28781700 -0.94491200
 H 4.16102600 0.34630100 0.68708700
 C 2.17223800 0.67179800 -0.21792300
 C 1.30943900 -0.24210600 0.27024400
 P -2.92711400 0.32050900 0.48284100
 Si 1.75723400 -1.62659800 1.47005600
 C 2.59888500 -0.89724200 3.00752400
 H 3.56813300 -0.44028900 2.77936700
 H 1.96490300 -0.12065200 3.45094000
 H 2.76689900 -1.67285100 3.76590400
 C 2.89812100 -2.95198000 0.70967600
 H 2.40205200 -3.51767700 -0.08916200
 H 3.81056500 -2.51469200 0.28902800
 H 3.20226300 -3.67649500 1.47646100
 C 0.18691400 -2.50623600 2.08053800
 H 0.44183800 -3.26637800 2.83049400
 H -0.49743900 -1.79152600 2.55256100
 H -0.36139300 -3.00914000 1.27570800
 C 0.88470100 -1.79320700 -2.58599700
 H 0.68052700 -2.34765200 -3.50905000
 H 1.42188700 -0.87133000 -2.82412000
 H 1.52881600 -2.39306500 -1.93853700
 C -1.50308300 -3.02891700 -1.58211800
 H -2.50512100 -2.91813100 -1.15840300
 H -1.58115000 -3.50872400 -2.56419400
 H -0.92403600 -3.67831100 -0.91827200
 C -1.64735300 -0.55693400 -3.06270800
 H -1.67773000 -1.18044900 -3.96354800
 H -2.67046200 -0.36064600 -2.73055200
 H -1.18143800 0.40258300 -3.30766800
 C -3.55452100 2.00268800 0.04787300
 H -2.86499500 2.75354300 0.44852000
 H -3.59953300 2.11606600 -1.04084200
 H -4.55693700 2.16419400 0.46157400
 C -4.35096200 -0.76605600 -0.02556200
 H -4.46319400 -0.77469700 -1.11520100
 H -4.17730100 -1.79441400 0.30976600
 H -5.29230800 -0.41479500 0.41301400
 C -3.08580900 0.29606200 2.32229100
 H -2.90516000 -0.71543800 2.70136300
 H -2.32177100 0.96734000 2.72143600
 H -4.08048500 0.62591700 2.64288300

TS6-1a

Ni 0.67812400 0.11484300 0.09318300
 O -0.08468800 -1.63782700 -0.00444000
 O 0.80515100 -2.95768900 -1.57898700
 C 0.00245800 -2.05611700 -1.31639400
 C -0.89670200 -1.45928500 -2.27748300
 C -1.93664800 -0.61664200 -1.94164200
 H -0.84016700 -1.88869800 -3.27357400
 C -3.11225500 -0.26910000 -2.83596000
 H -3.32316800 -1.03567300 -3.58960300
 H -2.91395700 0.66861000 -3.37857900
 P 0.68386500 2.29469100 -0.27801300
 C -4.26782200 -0.07773300 -1.82774400
 C -3.59013500 0.43049100 -0.53080200
 H -4.73527100 -1.05029700 -1.63228900
 H -5.05062600 0.59654200 -2.19297000
 H -3.61024900 1.53181300 -0.49202000
 H -4.11789000 0.08476200 0.36672300
 C -2.16042900 -0.09804200 -0.64050800
 C -1.20018200 -0.17986400 0.36302600
 Si -1.58664500 -0.45730600 2.21027100
 C -2.49280100 1.04215200 2.95047500
 H -2.76851700 0.82295100 3.99044300
 H -1.86337200 1.93883000 2.96277900
 H -3.41485700 1.28600700 2.41154100
 C -2.67289800 -1.99779400 2.39400600
 H -2.87013200 -2.21997600 3.45054300
 H -3.63943700 -1.87864400 1.89108200
 H -2.17215500 -2.86571400 1.95096400
 C 0.01393400 -0.71595100 3.18807700
 H -0.20826800 -0.86648600 4.25261700
 H 0.54983300 -1.59923200 2.82568100
 H 0.68556500 0.14700300 3.10324800
 C -0.39823200 3.38143700 0.75909300
 H -1.42198800 2.99844400 0.73424700
 H -0.05473500 3.36760300 1.79841900
 H -0.39238800 4.41617800 0.39744500
 C 0.03613200 2.63392100 -1.97745000
 H -0.08503500 3.70803900 -2.15939400
 H 0.72139700 2.21674700 -2.72152900
 H -0.92773000 2.12940100 -2.09021200
 C 2.26467600 3.26582200 -0.27580700
 H 2.97213300 2.82044200 -0.98238700
 H 2.09555400 4.31080500 -0.56041300
 H 2.71660800 3.23970100 0.72100300

P 2.93711800 -0.62985000 0.01666000
 C 4.35641700 0.26781700 0.81219400
 H 4.14605300 0.41976600 1.87635400
 H 5.28954100 -0.30009600 0.71810600
 H 4.49684900 1.24977300 0.34971500
 C 3.58382400 -0.95612900 -1.68805100
 H 4.57905500 -1.41560500 -1.66083800
 H 2.88424000 -1.63919600 -2.17973100
 H 3.63706900 -0.02597700 -2.26410500
 C 3.06466100 -2.30662800 0.78168300
 H 2.34707200 -2.94973900 0.26325200
 H 4.07769400 -2.71522300 0.68669700
 H 2.79440100 -2.25478900 1.84129700

INT1-1b

Ni 0.92727500 -0.31421700 0.03003200
 C -0.60469100 0.90894400 0.16219800
 C -0.95871300 -0.32735200 0.25017600
 C -2.09886300 -1.27489300 0.42997200
 H -1.88992900 -2.22130800 -0.08844000
 H -2.17078700 -1.53649900 1.49765200
 P 1.40742700 -2.47816600 0.07281400
 P 2.80078400 0.87613700 -0.21079300
 C 0.72202500 -3.41559000 1.52496300
 H -0.35945600 -3.26913400 1.58683700
 H 0.93580700 -4.48921800 1.45484400
 H 1.16526400 -3.02562700 2.44728300
 C 0.71356500 -3.45567600 -1.34868500
 H 0.88851400 -4.53205900 -1.23098400
 H -0.36183600 -3.27491200 -1.43477200
 H 1.18195400 -3.12010300 -2.27979800
 C 3.14173700 -3.15823000 0.08504800
 H 3.68710500 -2.77225300 0.95295800
 H 3.14158800 -4.25391200 0.13156100
 H 3.67464200 -2.84622300 -0.81810600
 C 3.46033000 1.62414500 1.35813500
 H 3.70922300 0.82424200 2.06358400
 H 4.35650600 2.23056200 1.17882800
 H 2.69047600 2.24827300 1.81998100
 C 4.36225100 0.09378900 -0.85851900
 H 5.17100200 0.82902000 -0.94723800
 H 4.68989300 -0.70583800 -0.18834600
 H 4.17636200 -0.34320300 -1.84556100
 C 2.75680700 2.36025000 -1.32804700

H 1.97537300 3.05008000 -1.00304700
 H 3.71854700 2.88755800 -1.34104200
 H 2.51522200 2.03717800 -2.34616400
 C -3.45876600 -0.73949000 -0.04935700
 H -3.38783800 -0.44935000 -1.10412200
 H -3.71907900 0.16366100 0.51040700
 C -4.58228500 -1.78541000 0.11847900
 H -4.65294300 -2.07907000 1.17590000
 H -4.31671900 -2.69946800 -0.43254500
 C -5.88691100 -1.30620400 -0.33968600
 C -6.95498000 -0.89300800 -0.72393500
 Si -1.12022700 2.68272900 0.16183900
 H -7.89836300 -0.52968200 -1.06179400
 C -2.88677600 2.91298800 0.82729000
 H -3.63336900 2.45374900 0.16979900
 H -3.00271900 2.47346400 1.82533100
 H -3.12898800 3.98106100 0.90582700
 C 0.01325000 3.71691300 1.28188200
 H 1.05271300 3.72929500 0.93721400
 H -0.33275400 4.75763100 1.32473600
 H 0.00830600 3.32319800 2.30575700
 C -1.07948300 3.38093800 -1.60366400
 H -1.35804800 4.44265700 -1.61250500
 H -0.09005000 3.28845000 -2.06404900
 H -1.79029200 2.84539900 -2.24444400

TS1-1b

Ni 0.36750100 -1.43847400 -0.09518800
 C -1.48178800 -0.22929400 -0.07971300
 C -0.28762300 0.21705400 0.30958400
 O -2.75629700 -1.30849000 -1.81175400
 O -1.01191500 -2.54158000 -1.07420600
 C -1.77464100 -1.52601500 -1.11311400
 P 2.47552200 -1.56733500 0.26625500
 Si -3.18779900 0.55509400 0.35551300
 C -3.03022900 1.65875600 1.89925400
 H -4.03962800 1.86747400 2.27798700
 H -2.47530900 1.17078600 2.70930700
 H -2.56208700 2.62961100 1.70010900
 C -3.81399700 1.62137700 -1.07252300
 H -3.92988300 1.01163000 -1.97164400
 H -4.78343500 2.07015500 -0.81939300
 H -3.11789800 2.43913000 -1.29567400
 C -4.38605300 -0.83318900 0.81200900

H -4.55738700 -1.49860300 -0.03735800
 H -4.00005900 -1.43065400 1.64709000
 H -5.34823600 -0.40912200 1.12708100
 C 0.28275500 1.47340400 0.87636800
 H -0.52502500 2.10462900 1.26514800
 H 0.93417400 1.23579300 1.72793700
 C 3.56415800 -1.06515100 -1.14037400
 H 3.45207300 0.00498800 -1.33797200
 H 4.61710100 -1.28025700 -0.92478100
 H 3.26259200 -1.60837400 -2.04096900
 C 1.08389800 2.27280400 -0.17081200
 H 1.89772500 1.65569100 -0.56859500
 H 0.43723300 2.51603700 -1.02106800
 C 3.25684800 -0.72047800 1.71147200
 H 2.74614700 -1.01854900 2.63225800
 H 4.31878600 -0.97862400 1.79174800
 H 3.16615800 0.36443100 1.60557100
 C 2.94761700 -3.33591500 0.53475500
 H 2.45932800 -3.71348200 1.43840200
 H 2.60305700 -3.93704300 -0.31225500
 H 4.03294500 -3.44838800 0.63930300
 C 1.67068700 3.57224400 0.42046600
 H 0.85277200 4.20771800 0.78795500
 H 2.28440500 3.33139800 1.30093400
 C 2.47697000 4.32066200 -0.54395400
 C 3.14190800 4.91928400 -1.35512700
 H 3.72341700 5.45689600 -2.06892800

TS4-1b

Ni 0.87359700 -0.38588200 -0.10975300
 C -0.59084300 1.15241600 0.08180200
 C -0.93079200 -0.03391700 -0.38501800
 O 1.01677700 2.37216600 1.63691800
 O 0.44770700 0.24378700 2.25296400
 C 0.50195400 1.26196500 1.56259100
 P 0.92647800 -2.58353000 -0.06200000
 P 3.06982500 0.29720600 -0.23293600
 C -2.12379100 -0.67647600 -1.01530400
 H -1.86537500 -1.65683700 -1.43650600
 H -2.44394700 -0.05658300 -1.86517200
 C -3.30760300 -0.83246100 -0.03935600
 H -3.00087700 -1.41988200 0.83316800
 H -3.60096000 0.15218600 0.33943600
 C -4.52008900 -1.50874100 -0.71462100

H -4.21747400 -2.48656100 -1.11722900
 H -4.83562000 -0.90998300 -1.58112500
 C -5.65343500 -1.68824700 0.19300600
 C -6.57756300 -1.82907700 0.95764000
 C 2.37572500 -3.34663800 0.80608100
 H 2.43988800 -2.93497700 1.81823700
 H 2.27261900 -4.43615400 0.87045100
 H 3.30654000 -3.11330000 0.28131300
 C 0.90096700 -3.51971600 -1.66121100
 H 0.00738100 -3.24669600 -2.23158300
 H 1.77607100 -3.24945300 -2.26079300
 H 0.90159300 -4.60356500 -1.49655800
 C -0.46280700 -3.36280300 0.87820700
 H -0.31789800 -4.44375600 0.98879400
 H -0.51816100 -2.89726200 1.86670800
 H -1.41192200 -3.18315500 0.36698100
 C 4.00936500 0.29292000 1.36085200
 H 4.05984300 -0.72201100 1.76670900
 H 5.02658000 0.68122200 1.23196200
 H 3.46665300 0.91903300 2.07499400
 C 4.21903300 -0.59427700 -1.38697500
 H 5.21627200 -0.13939000 -1.38174900
 H 4.31643600 -1.64756300 -1.10619300
 H 3.81851100 -0.54969500 -2.40528700
 C 3.29399400 2.04254200 -0.79261100
 H 2.87440700 2.16884600 -1.79541000
 H 2.74467500 2.68712200 -0.10258000
 H 4.35339200 2.32424300 -0.80661400
 Si -1.27566900 2.87576000 -0.31042700
 C 0.04729000 3.98644900 -1.08030900
 H 0.85926600 4.16748100 -0.37184700
 H 0.46997100 3.53924000 -1.98785500
 H -0.39182700 4.95324800 -1.35894900
 C -2.68843000 2.73117000 -1.57771400
 H -3.07512300 3.73285900 -1.80691500
 H -2.35230000 2.29029800 -2.52433500
 H -3.53221300 2.13781200 -1.20627600
 C -1.97128600 3.65210700 1.26710800
 H -2.78005800 3.04431600 1.69054500
 H -1.18504100 3.74809100 2.02130200
 H -2.37843700 4.65016400 1.06025200
 H -7.39476200 -1.95137100 1.63117300

INT8-1cd

C 2.68879500 -2.82924000 -0.16488300
 C 1.52423600 -3.52905400 0.55441400
 H 3.64042200 -3.11231200 0.30551200
 H 2.73484500 -3.18798900 -1.20418200
 C 0.17008800 -3.15471900 -0.06694400
 H 1.66332700 -4.61585000 0.50460500
 H 1.52922700 -3.24640100 1.61458500
 H 0.14714000 -3.50787800 -1.10933200
 H -0.63831500 -3.68065100 0.45892400
 C 2.56563000 -1.35518600 -0.17273100
 C 2.96586100 -0.16206200 -0.20103400
 C -0.10932100 -1.69765900 -0.05405800
 C -0.90614600 -0.70826000 -0.02738500
 Si -2.70723200 -0.29124500 -0.02604500
 H 3.77327900 0.54724600 -0.25276300
 Ni 1.01986800 -0.09827500 -0.09747400
 P 0.86112200 2.10853900 0.03883200
 C -3.68759500 -1.85001300 0.43530200
 H -4.76785500 -1.65632800 0.42135700
 H -3.48770900 -2.66870100 -0.26612400
 H -3.42570300 -2.20122200 1.44055600
 C -3.13422500 1.05375300 1.24160900
 H -2.69485600 2.02606000 0.99274900
 H -4.22164600 1.19143800 1.29769000
 H -2.78467000 0.77527000 2.24313300
 C -3.24641000 0.26916400 -1.75563300
 H -4.31765400 0.50739300 -1.77532800
 H -2.69937700 1.15673500 -2.09238900
 H -3.06745700 -0.52444000 -2.49079000
 C 0.41694500 2.73225100 1.72774900
 H 0.35353500 3.82660400 1.75915200
 H -0.54117900 2.30532500 2.03514600
 H 1.17698400 2.39808100 2.44144600
 C 2.38723800 3.11101300 -0.29742000
 H 2.19614000 4.18505500 -0.19098500
 H 3.18006900 2.82523600 0.40108100
 H 2.74299000 2.91254300 -1.31371800
 C -0.34766300 3.01584000 -1.03742900
 H -0.10882500 2.82346400 -2.08861600
 H -1.36021700 2.65017700 -0.85200200
 H -0.31898000 4.09721900 -0.85762800

TS7-1cd
 C 1.43081302 3.90686464 -0.26127943

C 2.65999437 3.37379838 0.53410862
 H 0.99977579 4.78073181 0.18083264
 H 1.68834185 4.13923902 -1.27349534
 C 2.89934811 1.95407699 -0.06185306
 H 3.51668180 4.01146532 0.46802136
 H 2.38698308 3.27352007 1.56382173
 H 3.29141751 2.00579290 -1.05608997
 H 3.56943248 1.36543542 0.52923749
 C 0.52717456 2.66894009 -0.21875171
 C -0.82806402 2.45392707 -0.26320224
 C 1.45881226 1.42969527 -0.08997778
 C 0.87662061 0.18670169 -0.02853133
 Si 1.74770087 -1.54659705 -0.00629017
 H -1.61336023 3.17650311 -0.34126456
 Ni -0.97098434 0.57251350 -0.14642997
 C 1.19685119 -2.52692861 1.57456867
 H 1.67729236 -3.48292328 1.58683571
 H 1.47400102 -1.97721516 2.44972757
 H 0.13544104 -2.66134574 1.55905973
 C 1.24520492 -2.54327378 -1.59302686
 H 1.54902407 -2.00257544 -2.46494384
 H 1.72564609 -3.49926844 -1.58075982
 H 0.18379477 -2.67769090 -1.60853580
 C 3.67212675 -1.30288750 0.02182886
 H 4.15256792 -2.25888217 0.03409589
 H 3.97594590 -0.76218917 -0.85008813
 H 3.94927658 -0.75317405 0.89698775
 P -2.73208743 -0.73439644 0.02821917
 C -2.19781133 -2.47417730 0.03878362
 H -1.54536430 -2.64187891 0.87010128
 H -3.05434783 -3.10981077 0.12372660
 H -1.67961447 -2.69368041 -0.87126605
 C -3.84185715 -0.44914696 -1.38579778
 H -4.69839365 -1.08478044 -1.30085479
 H -4.15596453 0.57369123 -1.39200875
 H -3.32366029 -0.66865008 -2.29584745
 C -3.61350638 -0.36103600 1.57615412
 H -3.92761376 0.66180219 1.56994315
 H -4.47004288 -0.99666947 1.66109711
 H -2.96105935 -0.52873762 2.40747178

INT9-1cd

C 1.48990500 3.51723200 -0.13487600
 C 2.91566200 3.13890600 0.35549500

H 1.02061500 4.29696000 0.47587800
 H 1.53879500 3.90115300 -1.16532900
 C 3.14505300 1.68720600 -0.14711700
 H 3.68471600 3.83980800 0.01223100
 H 2.93072800 3.14601800 1.45280400
 H 3.52316000 1.70581900 -1.18123100
 H 3.88245700 1.14074800 0.45199900
 C 0.76659600 2.18577000 -0.10221200
 C -0.51838000 1.80015400 -0.03338300
 C 1.75046100 1.08338500 -0.10903700
 C 1.23174300 -0.16110800 -0.04862700
 Si 2.02200200 -1.84063300 0.00511000
 H -1.36538200 2.49219200 0.00877500
 Ni -0.70364700 -0.09643600 -0.01548100
 P -3.01220700 -0.11842000 0.01290700
 C 3.08308100 -2.10740700 1.56184700
 H 3.48639000 -3.12757500 1.60529100
 H 3.93172300 -1.41300600 1.58658700
 H 2.49499800 -1.93928700 2.47211100
 C 3.08108400 -2.21645900 -1.53009100
 H 3.48047000 -3.23885000 -1.50468500
 H 2.49282200 -2.10856400 -2.44944700
 H 3.93204900 -1.52841500 -1.60273600
 C 0.59038200 -3.10351300 0.04866200
 H -0.04742000 -2.95584900 0.93190900
 H -0.04396800 -3.01918000 -0.84520700
 H 0.95675400 -4.13721000 0.08620800
 C -3.93610200 -1.72665900 0.01824900
 H -3.67597600 -2.30611800 -0.87357300
 H -3.65218900 -2.31408800 0.89749800
 H -5.02045300 -1.56846400 0.03347300
 C -3.74401400 0.75479700 1.47063000
 H -3.32261100 1.76226600 1.53699100
 H -4.83566200 0.82296000 1.40017900
 H -3.47689900 0.21986900 2.38748600
 C -3.78267400 0.76801000 -1.41661700
 H -4.87146000 0.84066400 -1.31342900
 H -3.35790100 1.77364400 -1.48854500
 H -3.54534600 0.23797300 -2.34444100

TS8-1c

C 1.64194100 3.18239200 -0.94119700
 C 3.04952300 3.00714400 -0.30297400
 H 1.07930700 4.03974800 -0.55748000

H 1.70899700 3.29881200 -2.03409900
 C 3.31336100 1.47445000 -0.28277800
 H 3.82734400 3.56688400 -0.83174000
 H 3.01859300 3.38298500 0.72628200
 H 3.84079500 1.15747700 -1.19474800
 H 3.93634800 1.17019400 0.56538400
 C 0.95954700 1.88717900 -0.60747800
 C -0.39052300 1.52262800 -0.53997900
 C 1.91092200 0.88288700 -0.24604900
 C 1.35817000 -0.35590100 -0.05400200
 Si 2.18688100 -2.02297000 0.20111000
 H -1.09513100 2.00054600 -1.22710100
 Ni -0.53730700 -0.34852500 -0.12607400
 P -2.85121500 -0.67417600 -0.28638600
 C -1.06639700 2.29297400 1.04304100
 O -1.52884900 1.38962600 1.72652900
 O -0.95738400 3.49738900 1.00103400
 C 3.44415600 -1.98659500 1.62280600
 H 3.86075600 -2.98610200 1.80223400
 H 4.28022300 -1.31250200 1.40333600
 H 2.97801100 -1.64634500 2.55484800
 C 3.03376900 -2.58496900 -1.40264400
 H 3.85814100 -1.91427000 -1.67222100
 H 3.44597500 -3.59676100 -1.29972900
 H 2.32724500 -2.59518600 -2.24115700
 C 0.80628600 -3.25850300 0.63375500
 H 0.29043000 -2.97329400 1.56004200
 H 0.05681600 -3.31936200 -0.16806800
 H 1.20218700 -4.27135200 0.77945700
 C -3.64942400 -1.13902400 1.31403100
 H -3.24539000 -2.09341800 1.66780300
 H -3.40732600 -0.36718700 2.04939200
 H -4.73692900 -1.22918400 1.21294900
 C -3.84464300 0.79012400 -0.81476000
 H -3.66459200 1.60939400 -0.11393500
 H -3.53643200 1.11170800 -1.81454800
 H -4.91516600 0.55685800 -0.82936100
 C -3.45400600 -1.99531100 -1.43966200
 H -3.13623000 -1.76539500 -2.46186600
 H -3.01748600 -2.95997400 -1.15972000
 H -4.54625800 -2.08431400 -1.41879000

TS8-1d

C 1.30618800 3.65155300 -0.10882300

C 2.77199700 3.31624200 0.26651000
 H 0.85291500 4.38540900 0.56715700
 H 1.25713100 4.07651000 -1.12221200
 C 2.99493000 1.87293600 -0.25543000
 H 3.49547100 4.03111200 -0.13959500
 H 2.87824100 3.32349700 1.35829900
 H 3.24557400 1.89866100 -1.32632900
 H 3.80996500 1.35238400 0.25525500
 C 0.62675200 2.29287400 -0.06635800
 C -0.65436400 1.88533700 -0.15707700
 C 1.63443000 1.22578000 -0.04085100
 C 1.23131900 -0.06930500 0.08796400
 Si 2.16899100 -1.60402700 -0.48303100
 H -1.47661200 2.59961500 -0.26863100
 Ni -0.80692400 0.00247200 0.05328300
 P -3.04580700 -0.03467600 -0.29150100
 C 0.14526700 -0.88613000 1.76110900
 O -0.63138000 -1.68092700 1.21092500
 O 0.67145300 -0.55745500 2.77305700
 C 2.66100100 -2.75614000 0.94381900
 H 1.78729000 -3.18369300 1.44758100
 H 3.26515700 -3.59052400 0.56463200
 H 3.25501100 -2.22815000 1.69877900
 C 1.03855600 -2.55951500 -1.67615100
 H 1.55368100 -3.44461800 -2.07111500
 H 0.12682000 -2.90029400 -1.17317300
 H 0.74508600 -1.93631900 -2.53015800
 C 3.75619700 -1.16718800 -1.43646500
 H 3.56040200 -0.48442200 -2.27126800
 H 4.51551600 -0.70513300 -0.79608200
 H 4.19329800 -2.08355700 -1.85442800
 C -3.82412200 -1.70905500 -0.25673400
 H -4.91505000 -1.65358700 -0.34277500
 H -3.43080500 -2.31329800 -1.08042000
 H -3.55699400 -2.20592800 0.68079900
 C -3.99735100 0.89602100 0.98878000
 H -5.07362700 0.88048500 0.78330800
 H -3.81363700 0.44923500 1.97085600
 H -3.65029100 1.93304300 1.02028000
 C -3.64972600 0.68926600 -1.87921100
 H -3.23937200 0.11910600 -2.71859300
 H -4.74380300 0.67884500 -1.94072000
 H -3.29327100 1.71991400 -1.96676800

INT5-1b

Ni -1.61087000 -0.66732700 -0.47402200
O -0.12801200 -1.34591600 -1.15628400
O 1.93373700 -1.77293900 -1.84922000
C 1.16912000 -1.12623900 -1.13492300
C 1.77004100 -0.11279600 -0.19962900
C 1.26914300 1.13689700 -0.02544300
C 2.04585900 2.30386000 0.58282900
H 3.12554700 2.14906900 0.58915100
H 1.72941400 2.47574000 1.62308300
P -3.63310900 -0.33188300 0.40105200
C 1.62749900 3.49795300 -0.29424000
C 0.13462100 3.24423700 -0.57099300
H 2.19195900 3.47201200 -1.23417300
H 1.81628600 4.46631000 0.18111200
H -0.48494000 3.72533600 0.19813300
H -0.19266100 3.63924900 -1.53921000
C -0.01995400 1.71444000 -0.49266900
C -1.21087200 1.12477000 -0.67631800
H -2.05764400 1.73716400 -1.00091000
Si 3.42995100 -0.74855900 0.51184800
C 3.76630200 -0.01327400 2.23928600
H 4.55828800 -0.59914000 2.72391600
H 4.09503600 1.03078600 2.23002900
H 2.87835200 -0.07695100 2.88068200
C 4.87328200 -0.33254700 -0.64239800
H 4.99499000 0.74947700 -0.77490900
H 5.81877300 -0.72841800 -0.25008900
H 4.69441000 -0.77576400 -1.62723500
C 3.31501400 -2.61922000 0.78575000
H 2.47809200 -2.87327000 1.44900300
H 3.17195400 -3.15085800 -0.15782200
H 4.23274400 -2.98674900 1.26280900
C -3.62440700 0.58691500 1.99993400
H -3.14145000 1.55714800 1.85203600
H -4.63880600 0.73884200 2.38480100
H -3.03836500 0.02930800 2.73683900
C -4.84521000 0.60938600 -0.62534500
H -5.02137600 0.07720900 -1.56513900
H -5.79806200 0.73698000 -0.10012600
H -4.43823700 1.59621200 -0.86563800
C -4.54711600 -1.88937100 0.80316700
H -5.51833100 -1.67793900 1.26420900
H -4.70696400 -2.46920500 -0.11147900

H -3.95308500 -2.49852600 1.49187200

TS3-1b

C 0.91454000 3.60331800 -0.13396200
C 2.32636400 3.31660300 0.40220600
H 0.37480500 4.36960900 0.43179500
H 0.97456200 3.94834400 -1.17678400
C 2.65095300 1.92178600 -0.14283700
H 3.05088900 4.07753700 0.09192800
H 2.30950600 3.29570300 1.49927300
H 2.97656200 2.00089000 -1.19158200
H 3.44805100 1.41593000 0.40645400
C 0.20387100 2.25701100 -0.09580500
C -1.10610600 2.02701900 -0.08005600
C 1.33793300 1.12014000 -0.07646600
C 1.15947600 -0.21031200 -0.02274100
Si 2.28968100 -1.66256300 0.00222000
H -1.92040900 2.74397000 -0.07585200
Ni -0.79008500 0.20838300 -0.03993000
C 1.89742900 -2.70199400 1.54558300
H 2.50487200 -3.61547400 1.58255900
H 2.09344500 -2.13388900 2.46352200
H 0.84131800 -2.99634400 1.56017500
C 1.94075400 -2.71553700 -1.54288900
H 2.17603600 -2.16203800 -2.46046400
H 2.53903800 -3.63577100 -1.54563200
H 0.88271400 -2.99903900 -1.59147900
C 4.16568700 -1.30733100 0.02993800
H 4.73807600 -2.24452100 0.01634200
H 4.48317700 -0.71658200 -0.83797800
H 4.46335700 -0.75797500 0.93189000
P -2.79597600 -0.46045500 0.02395300
C -2.98188400 -2.29859400 0.08005300
H -2.47020800 -2.68651200 0.96586900
H -4.03680200 -2.59707700 0.10980700
H -2.50615200 -2.73714700 -0.80221200
C -3.85274500 0.01634300 -1.41475000
H -4.86790300 -0.38492700 -1.31684400
H -3.90034500 1.10681400 -1.48599100
H -3.40426800 -0.36376400 -2.33747200
C -3.78956000 0.09886000 1.47764200
H -3.83095500 1.19182000 1.49125800
H -4.80895000 -0.30229700 1.44334200
H -3.30421100 -0.23315400 2.40024500

3

O -0.12587500 1.51468600 0.03175600
O 1.04414000 3.42613500 0.06843000
C 1.09499300 2.21749300 0.02334800
C 2.28126600 1.38674700 -0.03624500
C 2.16922500 0.03496500 -0.08203500
H 3.23363500 1.90652800 -0.03662800
C 3.25852800 -1.01180100 -0.15161400
H 4.13954700 -0.75473900 0.44532800
H 3.59519300 -1.11515100 -1.19348300
C 2.54474800 -2.30106500 0.31876300
C 1.06935700 -2.11928200 -0.11946800
H 2.59427700 -2.36541900 1.41232100
H 2.99797100 -3.21067000 -0.08641300
H 0.92936100 -2.49017900 -1.14517700
H 0.37496600 -2.67325600 0.51739200
C 0.87950000 -0.61340000 -0.06709000
C -0.24839500 0.14400600 -0.01358000
Si -2.10695700 -0.29574100 0.00088400
C -2.38358100 -2.16565400 -0.07772900
H -2.01535700 -2.68107000 0.81646600
H -3.45985100 -2.36748400 -0.14976300
H -1.90682400 -2.62105000 -0.95293100
C -2.83496100 0.41407100 1.59337800
H -3.92409000 0.28573500 1.61831000
H -2.42042400 -0.07781400 2.48119300
H -2.61890000 1.48509600 1.67208800
C -2.87423300 0.53895200 -1.51094900
H -2.65189600 1.61151100 -1.51525300
H -2.49039800 0.11272100 -2.44536000
H -3.96461300 0.41886400 -1.51262700

INT1-le

Ni -2.10527300 0.12620200 0.06210400
C -0.57315100 1.21709000 -0.08632500
C -0.22365600 -0.00690800 0.11099800
H -0.18866500 2.21507700 -0.26094500
C 0.90296100 -0.96831000 0.27868600
H 0.82929400 -1.44827900 1.26666300
H 0.80114000 -1.78629400 -0.45093200
P -3.06578500 -1.84711100 0.17146000
C -2.48072700 -3.11849000 -1.04952500
H -1.43782000 -3.37052700 -0.83254200

H -3.08298600 -4.03481200 -1.02160500
H -2.51381600 -2.69683400 -2.05922300
C -3.17812500 -2.87607400 1.71292200
H -3.76969300 -3.78807600 1.56698700
H -2.16830200 -3.15707200 2.02911500
H -3.62627400 -2.28315800 2.51669700
C -4.86454600 -1.66793700 -0.30783300
C 2.29137300 -0.32359200 0.12838700
H 2.40466900 0.47719900 0.86810300
H 2.37135000 0.14639500 -0.85852400
C 3.43286900 -1.34964500 0.30284900
H 3.31309100 -2.15645100 -0.43534400
H 3.34521600 -1.82762100 1.28978800
C 4.76629800 -0.76493200 0.16651100
C 5.86943000 -0.25938600 0.04995300
Si 7.53109200 0.49956000 -0.12084200
C 8.84921700 -0.79445500 0.29244100
H 8.79071500 -1.65181300 -0.38800400
H 9.85655800 -0.36747500 0.20772100
H 8.73049200 -1.17181300 1.31467000
C 7.76135000 1.09957500 -1.90075300
H 7.67603700 0.27108600 -2.61340800
H 7.00696500 1.84813500 -2.16895300
H 8.74994600 1.55655900 -2.03519500
C 7.67001100 1.96085600 1.07368800
H 6.90930600 2.72089600 0.86144100
H 7.53679900 1.63784700 2.11262300
H 8.65401800 2.44029600 0.99524500
C -5.05686400 -0.46887200 -1.26721800
C -4.95652600 0.87911900 -0.58689800
C -6.07622400 1.71652000 -0.52576600
C -5.99371200 2.95427600 0.10604000
C -4.77408000 3.32863500 0.66744900
C -3.69999000 2.45185700 0.56926700
N -3.77184600 1.24655800 -0.03721300
H -6.85851800 3.61001100 0.15481800
H -7.00668100 1.38900200 -0.97977100
H -4.64643400 4.28269300 1.16888800
H -2.72777800 2.70181000 0.97756900
H -5.45805800 -1.51173800 0.60154900
H -5.23327800 -2.58701700 -0.78029400
H -6.04100900 -0.54105800 -1.74438500
H -4.30967900 -0.51967400 -2.07053100

TS4-1e

Ni -1.90843300 0.05228200 -0.06805500
C -0.32294000 -0.95689500 0.73977000
C -0.10548200 0.24671400 0.25041800
H 0.31825600 -1.83233900 0.78402000
C 1.03166700 1.14936100 -0.08292900
H 0.88581100 1.57921000 -1.08442200
H 0.99737900 2.00499500 0.61166900
P -2.77998200 2.03849800 -0.22880300
C -2.41888000 3.04562800 1.27578100
H -1.36980400 3.35728300 1.25480700
H -3.05545500 3.93534400 1.34659600
H -2.55612200 2.40874700 2.15420500
C -2.52917400 3.24426900 -1.61029500
H -3.12900900 4.15141900 -1.47230300
H -1.47227900 3.52456800 -1.66032800
H -2.80097000 2.77686600 -2.56196700
C -4.63320400 1.84121800 -0.17426400
C 2.41535900 0.48293200 0.00630200
H 2.46102800 -0.36487300 -0.68697900
H 2.56213800 0.07630900 1.01293300
C 3.55452600 1.47223100 -0.32302300
H 3.51637700 2.31858400 0.37855800
H 3.38867600 1.89986700 -1.32298900
C 4.88162900 0.86024200 -0.27385000
C 5.97909600 0.33209400 -0.23050400
Si 7.63479500 -0.46146800 -0.16378100
C 8.81514300 0.65726200 0.80326900
H 8.45823800 0.82001200 1.82675700
H 9.81514700 0.20967600 0.86474000
H 8.91636100 1.63849700 0.32537700
C 7.48136500 -2.13731900 0.70001500
H 7.09841900 -2.02552700 1.72084300
H 6.79826900 -2.80262200 0.15953700
H 8.45675900 -2.63643400 0.76069400
C 8.27499700 -0.70212300 -1.92797500
H 7.60385400 -1.34345000 -2.51081600
H 8.36196400 0.25536600 -2.45436400
H 9.26636000 -1.17246700 -1.92219100
C -5.05009300 0.55637700 0.58119700
C -4.80802800 -0.71596400 -0.19871600
C -5.86999300 -1.55795300 -0.54559500
C -5.62558900 -2.73956600 -1.24012500
C -4.31143600 -3.05930200 -1.57577900

C -3.30300000 -2.17809700 -1.20427500
N -3.53682900 -1.02902800 -0.54075100
H -6.44512500 -3.40075200 -1.50727800
H -6.88004900 -1.28369500 -0.25775400
H -4.06353900 -3.97339800 -2.10473700
H -2.26193300 -2.38627600 -1.42614900
H -5.01122500 1.80990100 -1.20384500
H -5.08211500 2.71797900 0.30839300
H -6.11702000 0.61546800 0.82267900
H -4.50355700 0.48314600 1.53036800
C -1.69687800 -1.33455800 1.96426400
O -2.23764300 -0.31268500 2.39126000
O -1.72545800 -2.53460500 2.12469200

INT6-1e

Ni -2.12324400 0.32350900 -0.10514800
C 0.10039500 1.80776000 -0.55753600
C -0.19872700 0.54537900 -0.20585300
H 1.10661900 2.21024800 -0.66618200
C 0.86242700 -0.46680600 0.16778100
H 0.68169400 -0.78656600 1.20709600
H 0.75139600 -1.38012300 -0.43630600
P -2.16734000 -1.91556800 -0.10738600
C -1.52228600 -2.62830800 -1.69010800
H -0.47810400 -2.34600500 -1.83985100
H -1.60672700 -3.72091400 -1.69952700
H -2.09697000 -2.21804700 -2.52656200
C -1.41535400 -2.99573700 1.19250600
H -1.65143800 -4.05049700 1.01178500
H -0.33038400 -2.87149800 1.20621100
H -1.80448200 -2.70590500 2.17371700
C -3.92152600 -2.53137100 -0.13856700
C 2.32447300 -0.00466300 0.05378600
H 2.49130300 0.87295600 0.68756800
H 2.54241900 0.30357300 -0.97504000
C 3.30799500 -1.12203000 0.46767500
H 3.13478600 -2.01152700 -0.15660000
H 3.09418600 -1.43159400 1.50156100
C 4.71238000 -0.72788600 0.36282900
C 5.87777300 -0.38406400 0.26832500
Si 7.63497600 0.13273200 0.12771600
C 8.62318100 -1.26173900 -0.68528100
H 8.23928400 -1.48987300 -1.68630500
H 9.67969600 -0.98342100 -0.78749100

H 8.57566200 -2.18226200 -0.09204600
 C 7.73652600 1.69663500 -0.93081400
 H 7.33918400 1.52215100 -1.93730400
 H 7.16263000 2.51691200 -0.48479000
 H 8.77615800 2.03224300 -1.03445200
 C 8.31661900 0.47653400 1.85902700
 H 7.75507600 1.27581800 2.35616100
 H 8.25938700 -0.41558200 2.49335300
 H 9.36822300 0.78613500 1.81037100
 C -4.85065600 -1.56878500 -0.90557300
 C -5.17603400 -0.32413600 -0.11383400
 C -6.50027500 -0.03549000 0.22869300
 C -6.79159700 1.10231500 0.97699900
 C -5.74141900 1.93134100 1.35997600
 C -4.44770700 1.59195900 0.97635100
 N -4.15988300 0.48340000 0.26268500
 H -7.81725000 1.33646300 1.24813000
 H -7.29137000 -0.70327100 -0.09796300
 H -5.90920600 2.83604300 1.93465700
 H -3.60286100 2.23151100 1.19643800
 H -4.27373400 -2.64396400 0.89390000
 H -3.94087400 -3.52686000 -0.59891400
 H -5.78591900 -2.08397000 -1.14857800
 H -4.39369900 -1.28444200 -1.86312800
 C -1.04740800 2.73235600 -0.74441000
 O -2.20769600 2.13500100 -0.48787400
 O -0.95191800 3.90823900 -1.06383000

INT4-1e

Ni 0.94093100 0.63721200 -0.45177000
 O 1.23225100 0.88688900 -2.25526900
 O 2.27751100 2.22156500 -3.73094600
 C 1.91637900 1.98342900 -2.58930900
 C 2.15212100 2.86030900 -1.41145400
 C 1.71615700 2.37837800 -0.23851000
 H 2.62372600 3.83461400 -1.55061700
 C 1.71646400 3.17325300 1.04098400
 H 2.10420800 4.18333800 0.84491700
 H 2.37665000 2.72017800 1.79555000
 C 0.29048900 3.28179200 1.61590300
 C -0.21609600 1.94304500 2.22815400
 H -0.38459700 3.59371200 0.81142600
 H 0.24340500 4.05332500 2.39291000
 H -0.03071400 1.93726800 3.31121900

H -1.30077800 1.84049900 2.10117300
 C 0.48418700 0.77234300 1.68136500
 C 1.24662800 -0.18488900 1.49593700
 Si 2.44753800 -1.58325900 1.77838700
 C 1.53643900 -3.23279300 1.64597600
 H 1.12649800 -3.39583900 0.64401900
 H 2.22241400 -4.06065200 1.86564000
 H 0.70999100 -3.28692200 2.36401900
 C 3.85744900 -1.46795100 0.53222700
 H 3.51353900 -1.62339800 -0.49537100
 H 4.33854300 -0.48435900 0.57225300
 H 4.61994700 -2.22658200 0.74919600
 C 3.10504000 -1.34802500 3.53652700
 H 2.29583500 -1.37889600 4.27507500
 H 3.81888900 -2.14224500 3.78877300
 H 3.62226500 -0.38784800 3.64331800
 C -1.22925300 -1.55245300 -0.77871800
 C -1.72344400 -2.75992600 -1.28452000
 C -0.92441600 -3.54848400 -2.10913600
 C 0.35296600 -3.10003400 -2.43548200
 C 0.78145600 -1.88949200 -1.90008600
 N 0.02798800 -1.14719800 -1.06884500
 H -1.30321800 -4.48691000 -2.50478500
 H -2.73362700 -3.07021500 -1.04374100
 H 1.00333400 -3.65943300 -3.09964800
 H 1.74241200 -1.46271300 -2.16180300
 C -2.06408400 -0.62751600 0.08440400
 C -3.58557200 -0.81401700 -0.00302200
 P -4.50232900 0.49885300 0.98150000
 C -4.42290000 1.92218700 -0.22438800
 C -6.25060600 -0.07152700 0.66662400
 H -1.79374900 0.39571400 -0.20292800
 H -1.74449500 -0.73552900 1.12882000
 H -3.92003300 -0.80431900 -1.04958600
 H -3.87840300 -1.78229600 0.42340800
 H -6.43851700 -1.00267900 1.21214200
 H -6.95090100 0.68080500 1.04509300
 H -6.45831000 -0.23756400 -0.39770300
 H -4.75955900 1.64267300 -1.23033000
 H -5.05320300 2.74012500 0.14129000
 H -3.39865200 2.30402200 -0.29330700

INT4-1e'

Ni -1.38767800 -0.59192700 0.17212700

P 1.93443800 -1.79534000 -0.01415300
 C 1.73784400 -3.45536600 0.76687200
 H 1.16213500 -4.10987800 0.10604600
 H 2.71030900 -3.91671100 0.97196100
 H 1.17841500 -3.34242000 1.69956800
 C 3.00928200 -2.17181300 -1.47716100
 H 3.92222400 -2.70637800 -1.19005400
 H 2.45210300 -2.78524900 -2.19281700
 H 3.28448700 -1.23717600 -1.97622600
 C 3.10592100 -0.91759100 1.15629900
 C 2.56155200 0.45544500 1.61661700
 C 2.37686100 1.41444600 0.46897300
 C 3.20282500 2.53411400 0.30769400
 C 3.02961700 3.37865100 -0.78476500
 C 2.02577100 3.08216000 -1.70724000
 C 1.23649200 1.95967500 -1.48479100
 N 1.39702400 1.14468300 -0.42564100
 H 3.66472100 4.25053300 -0.91421100
 H 3.97179100 2.73375100 1.04740300
 H 1.84892200 3.70558600 -2.57760300
 H 0.42487700 1.69622700 -2.15553200
 H 4.08711100 -0.80605800 0.67832700
 H 3.24470600 -1.55383900 2.03723900
 H 3.26108700 0.89136300 2.33884800
 H 1.59639400 0.30162300 2.11473600

INT7-1e

Ni -0.37777300 0.00168800 0.18709700
 O -0.16448000 1.57075600 1.18739800
 O -0.48509700 3.76384400 0.88960300
 C -0.03742500 2.68528700 0.50111100
 C 0.73696600 2.68857700 -0.79078800
 C 1.74138600 1.86795400 -1.17412300
 H 0.57758100 3.60489600 -1.35618500
 C 2.74729700 2.21572700 -2.25544500
 H 2.67673200 3.25175900 -2.60084900
 H 2.61789400 1.56083100 -3.13158100
 C 4.08618600 1.89006600 -1.55669500
 C 3.77799100 0.63853900 -0.69996400
 H 4.36105100 2.72866500 -0.90601900
 H 4.91135500 1.73189300 -2.25964400
 H 4.04406400 -0.27576300 -1.24784300
 H 4.35667900 0.62382600 0.23088600
 C 2.25710100 0.68166000 -0.44858900

C 1.51946800 -0.19120400 0.27027600
 Si 2.18637100 -1.28538500 1.65095500
 C 3.48136400 -2.55945200 1.07011900
 H 4.34628900 -2.07242500 0.60592800
 H 3.84983000 -3.14199800 1.92466200
 H 3.07514700 -3.27249500 0.34198500
 C 2.97430900 -0.17064000 2.96920600
 H 3.85631500 0.35840900 2.59007500
 H 2.25144900 0.58727600 3.29212100
 H 3.28386800 -0.74874300 3.84947800
 C 0.77214000 -2.22845000 2.50039400
 H 0.28192400 -2.95244600 1.84013100
 H 1.15137000 -2.78115700 3.36973000
 H 0.00493200 -1.53238500 2.86004400
 P -0.53379000 -1.63223900 -1.31615500
 C 0.34693500 -1.19558900 -2.88067300
 H 1.40910800 -1.06921600 -2.65749100
 H 0.21845500 -1.97064500 -3.64462500
 H -0.02693400 -0.24150900 -3.26378600
 C 0.01585800 -3.37491000 -1.03979400
 H -0.15262100 -3.98413500 -1.93498300
 H 1.08114100 -3.39287900 -0.79587800
 H -0.53479400 -3.81318900 -0.20231900
 C -2.28512400 -1.86481800 -1.89564300
 C -3.05565500 -0.52903700 -1.91282000
 C -3.44535300 -0.03755800 -0.53650100
 C -4.79465700 0.12419400 -0.20826800
 C -5.15147500 0.59238500 1.05438100
 C -4.13984600 0.90398100 1.95767600
 C -2.81631700 0.72692600 1.56427300
 N -2.46758700 0.24924900 0.35256400
 H -6.19737500 0.72191000 1.31857200
 H -5.55418900 -0.10947500 -0.94801400
 H -4.35803800 1.29244200 2.94689700
 H -1.98535200 1.01554000 2.19767100
 H -2.78272800 -2.57301400 -1.22180000
 H -2.28301000 -2.31375900 -2.89671800
 H -3.96667500 -0.64673100 -2.50942700
 H -2.45535100 0.24283400 -2.41353400

TS6-1e

Ni 0.40207500 0.06365000 0.12579500
 O -0.39978900 -1.66018800 0.06183000
 O 0.47323000 -3.17774800 -1.33653200

C -0.25916600 -2.19857200 -1.21601000
 C -1.03578800 -1.59330300 -2.27139500
 C -2.03396400 -0.66436800 -2.05121500
 C -3.09793800 -0.26521200 -3.05674400
 H -3.29579000 -1.03849600 -3.80736500
 H -2.78420000 0.63919500 -3.60108000
 C -4.32234300 0.03707600 -2.16301100
 C -3.72756900 0.53861100 -0.82334400
 H -4.87307000 -0.89465300 -1.98589600
 H -5.02013900 0.75103700 -2.61527200
 H -3.67660700 1.64000600 -0.81264600
 H -4.35550000 0.25635100 0.03160200
 C -2.33631900 -0.08900200 -0.79181300
 C -1.47518000 -0.19779300 0.29961300
 Si -2.03718500 -0.36543600 2.10995000
 C -3.31665800 -1.75652300 2.25125700
 H -3.62571700 -1.90667000 3.29357200
 H -4.21691800 -1.54901600 1.66146200
 H -2.89107600 -2.69795500 1.88557700
 C -2.80597900 1.26436700 2.72035400
 H -2.06160400 2.06634900 2.78356000
 H -3.61963300 1.61061200 2.07332600
 H -3.22128100 1.12689500 3.72728400
 C -0.56290100 -0.78415800 3.22214200
 H 0.21014500 -0.00708400 3.18588700
 H -0.88612700 -0.88802800 4.26612300
 H -0.10221600 -1.72940100 2.91572100
 H -0.93317400 -2.07033800 -3.24162700
 P 0.71452100 2.21437500 -0.05398600
 C 0.00952900 2.90073300 -1.62133300
 H -1.06275800 2.68408900 -1.64465800
 H 0.16908300 3.98163200 -1.71029500
 H 0.46264800 2.39596200 -2.47997500
 C 0.15866200 3.46769300 1.18978300
 H 0.48486400 4.47763000 0.91525700
 H -0.93322700 3.45607000 1.25440100
 H 0.56025600 3.21984200 2.17740200
 C 2.52811700 2.59641600 -0.20980600
 C 3.26577000 1.54685500 -1.06834400
 C 3.49335500 0.20376000 -0.40358500
 C 4.79144900 -0.30145200 -0.28426900
 C 4.99761200 -1.56693700 0.26248400
 C 3.89074600 -2.30600200 0.66830100
 C 2.62633200 -1.73913800 0.53160900

N 2.42496900 -0.50636300 0.02581500
 H 6.00282700 -1.96901500 0.35484400
 H 5.63029000 0.29452200 -0.63102100
 H 3.99009000 -3.30690900 1.07492000
 H 1.72849000 -2.28616700 0.79655600
 H 2.95779400 2.62288800 0.79938600
 H 2.66322200 3.59437000 -0.64648900
 H 4.24165800 1.95116400 -1.35905500
 H 2.71341600 1.38311200 -2.00441900

INT2-1e

Ni -2.01640600 0.78752400 0.99763500
 C -0.40925200 0.47157200 1.91270900
 C -0.14099800 0.72244100 0.69043500
 O -2.71309500 3.25245400 2.28056000
 O -3.61700800 1.09504000 2.40772300
 C -2.94770000 2.08877300 2.16185300
 C 0.81338900 0.90748800 -0.43310800
 H 0.51191600 0.27730200 -1.28201600
 H 0.74499500 1.94381800 -0.79514200
 H -0.06536400 0.24656500 2.91101900
 C 2.26900600 0.59311900 -0.04251200
 C 3.24194600 0.80227500 -1.22318500
 H 2.33914300 -0.44262000 0.30858000
 H 2.56907100 1.23198100 0.79544000
 H 2.92969100 0.17323000 -2.06982000
 H 3.17031500 1.84181600 -1.57535800
 C 4.63087500 0.50039200 -0.87982100
 C 5.78164500 0.24365800 -0.57168400
 Si 7.52021600 -0.13639100 -0.11219500
 C 8.53843600 -0.35561800 -1.69185900
 H 9.58575900 -0.57996200 -1.45337900
 H 8.15104500 -1.17869800 -2.30330500
 H 8.52212900 0.55223900 -2.30575300
 C 8.21358800 1.29560200 0.91085300
 H 8.19882600 2.23336200 0.34362800
 H 7.63007400 1.45031000 1.82567600
 H 9.25208900 1.09852500 1.20533000
 C 7.55464500 -1.73258800 0.90250600
 H 6.96191600 -1.63485400 1.81925600
 H 7.14938700 -2.57595600 0.33162100
 H 8.58153200 -1.98760300 1.19319300
 C -3.05805400 2.33107600 -1.24501000
 C -4.09661800 0.25357600 -1.09424000

C -3.80186100 2.69080600 -2.36262000
 H -2.33234100 3.01049200 -0.81025200
 C -4.87779200 0.55315600 -2.21669700
 C -4.73186500 1.77840700 -2.86028500
 H -3.65526300 3.66315000 -2.82099500
 H -5.59811700 -0.17813800 -2.57039800
 H -5.33732800 2.01977700 -3.72945700
 C -4.21543400 -1.07696500 -0.39021200
 C -3.12527200 -2.07503900 -0.83646400
 H -3.19865800 -2.23586100 -1.92031800
 H -2.13058300 -1.65544100 -0.63376700
 P -3.29967500 -3.75719600 -0.01517100
 C -1.75121800 -4.55187500 -0.69120000
 H -0.85614400 -3.93756600 -0.53180700
 H -1.59983400 -5.52189700 -0.20532300
 H -1.86737700 -4.73427900 -1.76513000
 C -2.70076300 -3.34382300 1.70356100
 H -1.77202500 -2.76043900 1.69633200
 H -3.46475300 -2.77600900 2.24429900
 H -2.53144200 -4.27455000 2.25637400
 N -3.19164400 1.14275500 -0.62223600
 H -4.15038800 -0.90645000 0.68985300
 H -5.20468500 -1.50335300 -0.59263000

TS1-le

Ni 1.70418700 -0.01473400 0.69711100
 C -0.03337200 -1.22969200 0.84805400
 C -0.09533900 0.03020800 0.44610600
 H -0.86788000 -1.92029100 0.92168200
 O 0.87272900 -3.31835700 1.68069600
 O 2.49252200 -1.75506000 1.38762700
 C 1.31333800 -2.22906500 1.38027400
 C 1.98797200 2.76170500 1.02793500
 C 3.47049400 1.85372500 -0.53719900
 C 2.53091000 4.03130700 0.89455000
 H 1.16304700 2.56740200 1.70323000
 C 4.05108800 3.11486000 -0.71640900
 C 3.58629600 4.21265200 -0.00021400
 H 2.12920000 4.85294000 1.47769900
 H 4.86819600 3.21793500 -1.42326100
 H 4.03526100 5.19179600 -0.13921600
 C 3.99376200 0.64299800 -1.26933100
 H 3.14740000 0.00203600 -1.54388200
 H 4.47044700 0.97133700 -2.20060000

C 5.00638000 -0.16449400 -0.42605500
 H 5.82236200 0.49650600 -0.10517500
 H 4.51835700 -0.55882200 0.47345600
 P 5.78793800 -1.57741800 -1.39495300
 C 6.69839300 -2.38689100 0.01903500
 H 6.04155500 -2.58919800 0.87322900
 H 7.13012400 -3.33326100 -0.32428500
 H 7.52359100 -1.74495700 0.34652900
 C 4.32753700 -2.73456100 -1.51065400
 H 3.78670200 -2.81387100 -0.56095600
 H 3.63598700 -2.39365100 -2.28901200
 H 4.68524800 -3.72692000 -1.80706900
 N 2.44147800 1.69307700 0.33457800
 C -1.15930400 0.96529100 -0.01874700
 C -2.57739400 0.36842100 0.02012600
 H -0.92069700 1.29106400 -1.04228600
 H -1.13049500 1.87977700 0.59311800
 C -3.64184400 1.37178800 -0.47400400
 H -2.61348300 -0.53323000 -0.60153900
 H -2.81817700 0.05805500 1.04312800
 H -3.59727000 2.28397800 0.13910400
 H -3.40154500 1.68380300 -1.50091100
 C -4.99733600 0.82467100 -0.43486100
 C -6.11669800 0.34515800 -0.39170900
 Si -7.80407600 -0.38375800 -0.32470200
 C -8.13216500 -1.00951800 1.42959800
 H -9.13351700 -1.45186400 1.50470200
 H -7.40536900 -1.77616100 1.72160600
 H -8.07047600 -0.19560300 2.16114200
 C -7.90109900 -1.81809000 -1.55372500
 H -8.89473500 -2.28314500 -1.53313700
 H -7.71181800 -1.47848000 -2.57851200
 H -7.16406400 -2.59429400 -1.31803500
 C -9.06577900 0.94952400 -0.78222200
 H -10.08546400 0.54490900 -0.75900100
 H -9.02459900 1.79271000 -0.08313500
 H -8.88452500 1.34177900 -1.78951100

TS1-le'

Ni -1.27056600 0.56993800 0.24309500
 C 0.56600900 1.64497600 0.09490700
 C 0.52335200 0.31564600 0.11472700
 H 1.48535300 2.22233800 0.03758000
 O -0.16927200 3.93838300 0.06635700

O	-1.88875800	2.46769700	0.23543500	H	10.16033100	-0.12827500	1.50263600
C	-0.66814700	2.83212700	0.13860000	H	8.60315800	-0.00178100	2.33788700
C	-8.20448400	-1.09171800	-0.40876400	H	9.11492400	-1.55112800	1.65063200
C	-6.16495000	-0.03078100	-0.42886900	C	8.28780200	1.86547100	-0.37378500
C	-8.89307100	0.09632600	-0.15634700	H	9.31382900	2.25422700	-0.38809200
H	-8.74683800	-2.03095700	-0.50982300	H	7.80699800	2.15592800	-1.31489400
C	-6.76541300	1.20754400	-0.17273200	H	7.75266700	2.36526100	0.44175300
C	-8.15196200	1.27056200	-0.03554200				
H	-9.97441600	0.09527700	-0.05814400				
H	-6.15425600	2.10124400	-0.08532900	Ni	-2.06971700	-0.17438700	-0.87483400
H	-8.64211400	2.22015500	0.16187600	C	0.04773500	-1.77148500	-1.17974500
C	-4.66401200	-0.16271500	-0.59078100	C	-0.20331400	-0.49218200	-0.85806300
H	-4.45898800	-0.54906300	-1.59787500	H	1.03745100	-2.22295500	-1.23290600
H	-4.18960100	0.82182500	-0.51762500	C	0.80211200	0.56181200	-0.47716900
C	-4.06528400	-1.12077700	0.45812700	H	0.77045400	1.38603900	-1.20653700
H	-4.24496600	-0.72523800	1.46585100	H	0.49813900	1.01485100	0.47888400
H	-4.56141600	-2.09664000	0.39283900	C	2.25198900	0.06263600	-0.35803600
P	-2.23019500	-1.33302200	0.29289000	H	2.58671900	-0.35368500	-1.31471600
C	-1.80523900	-2.46630800	1.68671000	H	2.30552600	-0.74928100	0.37569400
H	-2.41425000	-3.37655600	1.65454600	C	3.21413200	1.19475700	0.06532100
H	-0.74802600	-2.74279500	1.63077300	H	2.87109400	1.62773000	1.01652000
H	-1.97385300	-1.95458000	2.63874100	H	3.16872800	2.00907300	-0.67280100
C	-2.01990100	-2.40643500	-1.19439100	C	4.59800900	0.74468400	0.20918000
H	-2.61191700	-3.32399100	-1.10385100	C	5.74364400	0.34619700	0.32659800
H	-2.33242900	-1.86500200	-2.09148000	Si	7.46953400	-0.25844300	0.51388100
H	-0.96441000	-2.67064800	-1.30923300	C	8.04189900	0.06475600	2.28802700
N	-6.87639300	-1.16583300	-0.54334900	H	7.40610000	-0.45775200	3.01200400
C	1.54018900	-0.77377500	0.06100900	H	9.07226700	-0.28256100	2.43568500
C	2.99579500	-0.27699100	0.00162500	H	8.01183800	1.13380900	2.52823100
H	1.33472000	-1.40988100	-0.81370100	C	7.51437300	-2.11296600	0.14628600
H	1.41289800	-1.42489900	0.93908800	H	6.86515300	-2.67098700	0.83066300
C	4.00076500	-1.44800700	-0.05522700	H	7.18013200	-2.32465000	-0.87584600
H	3.13198200	0.36156600	-0.87830000	H	8.53247100	-2.50792500	0.25395700
H	3.20873600	0.34219600	0.88012300	C	8.58268800	0.66929300	-0.70253700
H	3.84948200	-2.10163600	0.81646100	H	8.26272900	0.50645900	-1.73814800
H	3.79066700	-2.06694100	-0.93981300	H	8.56692800	1.74900000	-0.51424100
C	5.39261200	-1.00162900	-0.09123600	H	9.62252800	0.32962600	-0.61638100
C	6.54507100	-0.60696500	-0.11706300	C	-1.15086600	-2.61482100	-1.44559400
Si	8.28547900	-0.01196400	-0.14837600	O	-2.28031500	-1.91434300	-1.28771600
C	9.19036000	-0.84055100	-1.58807200	O	-1.12808000	-3.79412000	-1.74937400

C -3.05464800 2.09109500 0.55393600
 N -2.26900900 1.71815400 -0.48866500
 H -3.02575700 5.46556500 0.10930500
 H -1.16690000 2.29672700 -2.13590100
 H -1.59955000 4.73715800 -1.83492200
 H -3.96073200 3.71491500 1.62686600
 C -3.62528300 0.99230400 1.41812300
 H -2.79768300 0.37489700 1.79000600
 H -4.11503700 1.43779600 2.29083200
 C -4.63665700 0.09952700 0.66570500
 H -4.16905300 -0.39077500 -0.20786700
 H -5.45619100 0.71793900 0.27772200
 P -5.38915800 -1.23824100 1.75737900
 C -3.92475700 -2.38375000 1.91095200
 H -3.19670700 -1.97619300 2.62088200
 H -4.27099800 -3.34092400 2.31633700
 H -3.43020600 -2.56028700 0.94856200
 C -6.34550900 -2.14396600 0.43635300
 H -5.71623600 -2.41560500 -0.41945100
 H -6.76660900 -3.05967700 0.86481500
 H -7.18031400 -1.52550200 0.08902300

TS2-1e

Ni 0.51959200 0.46998200 -0.70237000
 O -1.12695300 1.11551500 -1.38722700
 O -2.22263100 3.08477400 -1.52352800
 C -1.19512400 2.42376200 -1.41351700
 C 0.15807900 3.05889100 -1.32906000
 C 1.24291500 2.42786700 -0.84156900
 H 0.26617400 4.05025300 -1.77402200
 C 2.60241700 3.09394000 -0.90719100
 H 2.55963700 3.96781400 -1.56703900
 H 3.33007600 2.39548200 -1.33943900
 C 3.03174100 3.48025300 0.52826400
 C 2.29678600 2.50423000 1.48371100
 H 2.74575200 4.51280800 0.75073900
 H 4.11725400 3.40637300 0.65018400
 H 2.94248600 2.13251400 2.28622000
 H 1.43471300 2.99393300 1.95066100
 C 1.82755900 1.33749800 0.67562700
 C 1.96956100 0.06893100 0.49259500
 Si 2.89524400 -1.38549600 1.19916900
 C 4.16772500 -0.77607000 2.46628900
 H 3.68413800 -0.27689600 3.31438200

H 4.74789900 -1.61700300 2.86719300
 H 4.87681700 -0.06893100 2.01985300
 C 1.69408000 -2.57414200 2.05008800
 H 0.97255700 -2.99719300 1.34304700
 H 2.24189000 -3.40764900 2.50768100
 H 1.13104300 -2.07017500 2.84421700
 C 3.79179200 -2.27176500 -0.21283000
 H 4.38403200 -3.11316200 0.16800900
 H 3.08180100 -2.66820000 -0.94741600
 H 4.47532200 -1.59468300 -0.73887400
 C 0.48485000 -1.93700700 -2.19604400
 C 0.09154400 -3.17433700 -2.68683700
 C -0.93003000 -3.85425800 -2.02143300
 C -1.51100200 -3.26112800 -0.90762900
 C -1.07811400 -2.00220800 -0.46494300
 N -0.07689900 -1.36271300 -1.11279700
 H -1.26572800 -4.82815000 -2.36639400
 H 1.27660200 -1.36963800 -2.67340500
 H 0.57715500 -3.58833800 -3.56403100
 H -2.30959700 -3.75883800 -0.36628400
 C -1.74253800 -1.33049100 0.71145100
 H -1.94673700 -2.08560400 1.48175700
 H -1.04909500 -0.60315900 1.14444800
 C -3.04775800 -0.61110400 0.30004000
 H -3.79609400 -1.33554900 -0.05050600
 H -2.80654700 0.06358300 -0.52651200
 P -3.75000000 0.47176800 1.66424200
 C -4.99708600 -0.69935200 2.42297200
 H -4.47781500 -1.50175900 2.95950000
 H -5.60927300 -0.15935100 3.15398700
 H -5.66256500 -1.14914100 1.67486100
 C -4.87798500 1.51884900 0.61346400
 H -5.55777400 0.91623700 -0.00211800
 H -5.47542400 2.17671400 1.25436300
 H -4.26218400 2.14116500 -0.04576600

TS2-1e'

Ni 0.78523300 0.45679900 0.52003700
 O -0.33954400 1.31460600 1.77278100
 O -1.15470000 3.35845100 2.26119800
 C -0.54171900 2.59524700 1.52956000
 C 0.04439300 3.02686900 0.22481100
 C 0.90614800 2.27285500 -0.47953200
 H -0.31576300 3.97013100 -0.19027500

H	-0.80774800	-3.78128800	1.11638100
C	-0.27870500	-1.50821600	3.04979100
H	-1.01098100	-2.23103200	3.42663600
H	0.72431500	-1.81497200	3.36303400
H	-0.48574200	-0.51461800	3.45469500

Ni -0.36852800 -0.65060900 -0.24920300

S29

H 4.19142800 -4.08308900 -1.95041500
 H 0.08198600 -2.81869400 -2.06951900
 H 1.88019200 -4.30684100 -2.93700900
 H 4.56482900 -2.37166900 -0.17290500
 C 2.76264100 -0.62912700 0.86428900
 H 1.80285800 -0.33874000 1.30292200
 H 3.38048500 -1.05050800 1.66856100
 C 3.45934100 0.61511900 0.27116000
 H 2.80823500 1.07605500 -0.47856400
 H 4.39349300 0.31167700 -0.22105200
 P 3.93455600 1.87939600 1.57990800
 C 2.25566000 2.59447000 1.97892300
 H 1.66565400 1.87748200 2.56052600
 H 2.38964700 3.48723600 2.60051900
 H 1.70707100 2.86478000 1.07032300
 C 4.54174800 3.21724300 0.42715400
 H 3.80510700 3.44259700 -0.35255100
 H 4.74422700 4.12814500 1.00140500
 H 5.48087400 2.90512400 -0.04329300

TS3-1e

Ni 0.06256900 0.07573900 0.12601600
 O -0.61311500 -1.59509800 0.50313300
 O 0.41349800 -3.34607700 -0.46904800
 C -0.38015900 -2.42187700 -0.59282000
 C -1.16432800 -2.15810000 -1.78704700
 C -2.20876500 -1.27198400 -1.83561000
 C -3.22793500 -1.15540900 -2.95167900
 H -3.35481100 -2.08207600 -3.52110200
 H -2.91405100 -0.37679900 -3.66385900
 C -4.50836400 -0.71693300 -2.20589400
 C -3.99977200 0.12870800 -1.01276000
 H -5.02516800 -1.60629500 -1.82577600
 H -5.21233000 -0.17266700 -2.84452900
 H -3.95749200 1.19365700 -1.28903600
 H -4.66349200 0.06118200 -0.14279100
 C -2.60104500 -0.42609500 -0.74985200
 C -1.80801000 -0.22325800 0.35913200
 Si -2.35012000 0.24641200 2.11995700
 C -3.72242300 -0.92025700 2.71066900
 H -4.03590800 -0.66793200 3.73169300
 H -4.61068500 -0.87937700 2.07026600
 H -3.36413000 -1.95616700 2.71729100
 C -2.98413500 2.03616100 2.06828800

H -2.20391600 2.72083700 1.71409200
 H -3.85348200 2.14782700 1.40996200
 H -3.28364900 2.36716400 3.07084500
 C -0.89325700 0.12264000 3.31599000
 H -0.11217700 0.85580800 3.08420200
 H -1.22988300 0.30318800 4.34517700
 H -0.43889300 -0.87302200 3.27627400
 H -0.97030700 -2.83369400 -2.61473500
 C -0.10731100 2.67099300 -1.01014600
 C 0.32454000 3.89420400 -1.50764100
 C 1.66596500 4.24089900 -1.34911600
 C 2.51416600 3.34984900 -0.69558100
 C 2.02078100 2.13485000 -0.21227900
 N 0.71270300 1.80467000 -0.37820600
 H 2.04420600 5.18765500 -1.72384700
 H -1.13838700 2.34843900 -1.10756800
 H -0.37885500 4.55272300 -2.00629300
 H 3.56310100 3.58800400 -0.54988500
 C 2.90755700 1.14561300 0.50877700
 H 3.87187100 1.62495200 0.71335800
 H 2.45535300 0.91183300 1.48195000
 C 3.12861300 -0.17204800 -0.26362200
 H 3.57725900 0.02808100 -1.24699100
 H 2.15960500 -0.65990400 -0.45507000
 P 4.14467900 -1.42262300 0.70768800
 C 5.86468700 -0.89172400 0.19991300
 H 6.11069900 0.07647400 0.65057900
 H 6.59206600 -1.61994300 0.57540000
 H 5.97890200 -0.81536900 -0.88902400
 C 3.91262800 -2.89194000 -0.41081200
 H 4.18891600 -2.67785100 -1.45134700
 H 4.52970700 -3.72223700 -0.05005400
 H 2.86290600 -3.20465400 -0.37504500

INT1-1f

Ni 0.54997700 -0.38463800 -0.09096400
 C -0.95195800 0.84025500 0.06440600
 C -1.32100400 -0.39296700 -0.04787100
 C -2.46420900 -1.34844400 -0.11892300
 H -2.35307900 -1.97264000 -1.01851400
 H -2.39861000 -2.04744200 0.72928900
 C -3.85270000 -0.68871000 -0.12754300
 C -4.98814200 -1.72963000 -0.23290100
 H -3.92094200 0.00953200 -0.96975100

H -3.98491500 -0.09606400 0.78405400
 H -4.84975000 -2.32890400 -1.14461000
 H -4.91537800 -2.43582200 0.60712400
 C -6.32340900 -1.13054200 -0.24642300
 C -7.41782300 -0.61919900 -0.25677800
 H -8.38349700 -0.16818900 -0.26539400
 Si -1.32669700 2.62446400 0.31752200
 C -3.05101700 2.90125000 1.06813000
 H -3.14837900 2.39155000 2.03434100
 H -3.23967600 3.96980900 1.23574500
 H -3.84276900 2.52166600 0.41211300
 C -0.04912300 3.39280400 1.49185300
 H 0.96893000 3.29106500 1.09843100
 H -0.24490100 4.46087700 1.65204500
 H -0.07431100 2.89723100 2.46993600
 C -1.25756000 3.54718500 -1.34525400
 H -0.26499400 3.48591700 -1.80820200
 H -1.97848400 3.12902200 -2.05791200
 H -1.49471500 4.61104900 -1.21467700
 C 2.39166400 1.63645100 -1.00277000
 C 3.45450500 0.17212300 0.45081100
 C 3.56303700 2.34543700 -1.24375700
 H 1.45736500 1.91730100 -1.47435600
 C 4.66569100 0.84617900 0.25896600
 C 4.72958200 1.94534300 -0.59349700
 H 3.54964400 3.19503800 -1.91894100
 H 5.55170800 0.50157800 0.78389200
 H 5.66542400 2.47602200 -0.74407300
 C 3.39143200 -1.04746600 1.34219400
 H 4.34265600 -1.13568300 1.87994000
 H 2.60694600 -0.90187800 2.09617000
 C 3.12214800 -2.35798700 0.56232000
 H 3.80483800 -2.42299600 -0.29402700
 H 3.33151900 -3.22108100 1.20626900
 P 1.35320000 -2.42718900 -0.05844200
 C 0.59535000 -3.62895600 1.13901100
 H 1.14499000 -4.57729200 1.17967000
 H 0.57525500 -3.18344600 2.13888400
 H -0.43977000 -3.82938400 0.84482200
 C 1.52096100 -3.50782100 -1.56133000
 H 0.52390400 -3.73447700 -1.95308100
 H 2.06950900 -2.96644700 -2.33897200
 H 2.03894300 -4.45082000 -1.34799400
 N 2.31920000 0.57118400 -0.17539400

TS1-If

C 3.52162800 1.18842300 0.01773000
 H 4.02775400 0.27699300 -0.31849700
 H 3.15082400 1.68624500 -0.88655100
 C 4.53675600 2.10985000 0.72743700
 H 4.92139900 1.60512100 1.62510100
 H 4.02249400 3.01352700 1.08553200
 C 5.65467600 2.49473200 -0.13413000
 C 6.56718400 2.80202300 -0.86307900
 Si 2.27490600 -2.79401500 0.37912900
 C 1.18921000 -4.29303000 0.76230400
 H 0.65176500 -4.62839700 -0.12810900
 H 1.81010300 -5.12160500 1.12662000
 H 0.45425400 -4.06390200 1.54364800
 C 3.54865600 -3.15614400 -0.96893100
 H 3.04579900 -3.40117700 -1.90734900
 H 4.20245800 -2.29292300 -1.14305700
 H 4.18569300 -4.00112000 -0.67641000
 C 3.21332700 -2.36657400 1.97802700
 H 3.98819000 -1.60534500 1.83193500
 H 2.54366100 -2.02582600 2.77681400
 H 3.71916600 -3.27036600 2.34229400
 C 2.34094300 0.81793200 0.93788900
 H 1.86080000 1.73746800 1.29787000
 H 2.72276900 0.30090500 1.82798300
 C 1.32318600 -0.04038200 0.25995900
 C 1.16861000 -1.30671200 -0.11556500
 C -0.16422700 2.99856200 -0.61221600
 C -0.53659800 4.33451200 -0.56162100
 C -1.74647100 4.66597400 0.04897800
 C -2.52853400 3.64373000 0.57729300
 C -2.10598500 2.31266200 0.49226200
 N -0.92340900 2.00282500 -0.10106000
 H -2.07195600 5.70005700 0.11456000
 H 0.76730900 2.68996000 -1.07177100
 H 0.11225500 5.09064400 -0.99059600
 H -3.47469200 3.86201200 1.06241400
 Ni -0.37681500 0.19544300 -0.31864400
 C -2.96201300 1.18554000 1.01463600
 H -2.31120900 0.42985700 1.47168600
 H -3.61662300 1.57231000 1.80467100
 C -3.81893700 0.53462600 -0.09430900
 H -3.17369000 0.09288100 -0.86378200

H -4.43492200 1.30546500 -0.57622300
P -4.99749400 -0.77191100 0.57479500
C -3.78366700 -2.13413700 0.97296000
H -3.27296100 -1.91831500 1.91793200
H -4.33710200 -3.06999000 1.11002700
H -3.03416700 -2.26732700 0.18474000
C -5.63712900 -1.40691100 -1.05968500
H -4.82720000 -1.68659300 -1.74361300
H -6.26811800 -2.28492800 -0.88389700
H -6.25891800 -0.64170200 -1.53730600
C 0.00883700 -1.90765800 -1.27384200
O -1.16336800 -1.43077600 -1.29887900
O 0.52708400 -2.79603400 -1.93002000
H 7.37682300 3.07112700 -1.50234100

TS4-1f

C 3.53151800 -0.53925100 -0.08223100
H 3.75903500 0.29406400 0.59088500
H 3.14136000 -1.34615200 0.54865300
C 4.82470600 -1.00968800 -0.78234000
H 5.22309700 -0.19171600 -1.39930700
H 4.58731500 -1.82599200 -1.48017900
C 5.85304800 -1.45721900 0.15724600
C 6.68867300 -1.82465500 0.94806900
Si 0.71326400 3.22097600 -0.52969600
C -1.04615200 3.86365000 -0.80343800
H -1.60091800 3.85868800 0.13877300
H -1.02885400 4.89018800 -1.19154200
H -1.58609300 3.24100600 -1.52746600
C 1.64155300 4.29924600 0.71829800
H 1.15352900 4.25534300 1.69616100
H 2.67978300 3.96623900 0.83862200
H 1.66520600 5.34602400 0.38866700
C 1.62893200 3.31462700 -2.19601400
H 2.68707800 3.04038900 -2.10594900
H 1.17422700 2.65901100 -2.94869900
H 1.59461200 4.33952000 -2.58809400
C 2.45838000 -0.10251200 -1.10249100
H 2.25783500 -0.93226700 -1.79260000
H 2.85815600 0.72726600 -1.70279800
C 1.20496200 0.33061600 -0.42256500
C 0.64449100 1.42889100 0.05236700
C -3.07394200 0.80210400 0.65654400
C -4.44799900 1.02114900 0.68462600

C -5.28092900 0.14332600 -0.00197500
C -4.69774700 -0.91986800 -0.68660200
C -3.30972800 -1.08860800 -0.67454200
N -2.50162600 -0.22907200 -0.00367000
H -6.35872000 0.27996100 -0.00808500
H -2.39875200 1.47563900 1.17212400
H -4.84049100 1.86955500 1.23533600
H -5.31140600 -1.62707400 -1.23612600
Ni -0.45593400 -0.34417400 -0.00699100
C -2.69476700 -2.25942900 -1.41137100
H -3.49600100 -2.79167800 -1.93595600
H -2.00796700 -1.88345000 -2.18164500
C -1.94559200 -3.24569300 -0.48742100
H -1.78300200 -4.19680900 -1.00841900
H -2.55382600 -3.46203500 0.39881800
P -0.31124300 -2.52579000 0.05800000
C 0.89687300 -3.48660700 -0.96804200
H 0.75958800 -3.24821400 -2.02779100
H 1.91759300 -3.21041000 -0.68764300
H 0.77293100 -4.56661800 -0.82607900
C -0.04476800 -3.24327300 1.73884200
H -0.12478600 -4.33654900 1.73874900
H 0.94586300 -2.95004000 2.09851900
H -0.77903700 -2.81812700 2.42894900
C -0.02906200 1.32467300 1.81707800
O -0.63474600 2.35700800 2.06749300
O 0.31094200 0.29453600 2.37891200
H 7.42885200 -2.14341400 1.64584200

INT8-1gh

C 0.09529900 -3.71738900 1.56623400
C -1.34522000 -4.00367700 1.11010600
H 0.29064700 -4.22935500 2.51869100
H 0.79318000 -4.14926700 0.83266900
C -1.67554300 -3.30951400 -0.22119200
H -1.48386600 -5.08627600 1.00090200
H -2.04586300 -3.66014000 1.88138100
H -1.00492200 -3.69917500 -1.00225000
H -2.69727300 -3.56802800 -0.53101100
C 0.38471100 -2.27261300 1.71239800
C 0.95286300 -1.24484100 2.17131100
C -1.54109800 -1.83392500 -0.16730700
C -1.85770300 -0.65279700 -0.49630300
Si -2.93390000 0.54894800 -1.38826600

H 1.66396900 -0.78132200 2.83501000
 Ni -0.36117500 -0.64848500 0.86531900
 C -4.15065000 -0.39952900 -2.49419000
 H -4.80936100 0.28676200 -3.04194000
 H -3.62002400 -1.01236100 -3.23253100
 H -4.78539700 -1.06888600 -1.90130400
 C -3.91150000 1.58092800 -0.13510100
 H -3.24201400 2.16778600 0.50418900
 H -4.58909000 2.27975500 -0.64201800
 H -4.51746000 0.93892900 0.51520100
 C -1.89848300 1.70793800 -2.47364100
 H -2.54771900 2.36653900 -3.06468800
 H -1.24246100 2.34360200 -1.86829100
 H -1.26949700 1.14575200 -3.17389600
 C -0.71733300 1.94974000 2.06965800
 C -0.58507200 3.30633200 2.34066200
 C 0.27536000 4.06257600 1.54361400
 C 0.96272800 3.42144400 0.51871100
 C 0.78606300 2.04803500 0.30110200
 N -0.05615700 1.32312600 1.07436000
 H 0.40491700 5.12736300 1.71605500
 H -1.14803300 3.75265700 3.15403000
 H 1.64032300 3.97355500 -0.12600400
 H -1.37685500 1.32124500 2.65874000
 C 1.55319800 1.33354700 -0.78539500
 C 2.93992600 0.85670000 -0.30398500
 P 3.95383800 0.06503200 -1.67285500
 C 3.10075700 -1.59126400 -1.79721100
 C 5.43917100 -0.43748900 -0.65769400
 H 5.16318500 -0.99434800 0.24629500
 H 6.10159200 -1.06335000 -1.26567900
 H 6.00363800 0.45412100 -0.36329100
 H 3.70534500 -2.26223200 -2.41774300
 H 2.94289500 -2.05451000 -0.81593500
 H 2.12791000 -1.47536200 -2.28581900
 H 0.95715000 0.47638500 -1.11480200
 H 1.67812900 2.00669400 -1.64261700
 H 2.81755000 0.15722400 0.53233500
 H 3.51758400 1.71600400 0.06276700

INT8-Igh'

C 3.02941000 2.97126200 -1.66001600
 C 4.10610100 1.87928200 -1.76564500
 H 3.50288600 3.94195700 -1.45862000

H 2.52171400 3.06782400 -2.63166000
 C 3.48607500 0.49742400 -2.02339500
 H 4.80038400 2.12792700 -2.57742600
 H 4.68683100 1.84919100 -0.83518400
 H 2.96045700 0.51708000 -2.99035400
 H 4.28101500 -0.25508200 -2.11637900
 C 2.01626500 2.69472200 -0.61800900
 C 1.14045400 2.97211700 0.24281600
 C 2.53159700 0.07064100 -0.97086300
 C 1.95742400 -0.82198800 -0.27194600
 Si 1.94136900 -2.64628000 0.02892300
 H 0.56744200 3.70555500 0.78278400
 Ni 1.31211500 1.02995700 0.22383300
 C 2.86831900 -3.49683600 -1.39310200
 H 2.90768100 -4.58379400 -1.24595200
 H 2.37965000 -3.30827400 -2.35637400
 H 3.90069700 -3.13459000 -1.46765100
 C 2.83319100 -3.05675200 1.65136900
 H 2.36504600 -2.57598600 2.51706800
 H 2.83789500 -4.13954200 1.83104000
 H 3.87606600 -2.72018600 1.61362800
 C 0.17935500 -3.34696200 0.07331500
 H 0.20599100 -4.44214600 0.13973400
 H -0.39926500 -2.98172500 0.92898200
 H -0.37174500 -3.08354000 -0.83744500
 C -5.97135000 -0.06081100 -0.19612500
 C -6.16469600 -0.66827900 -1.43825400
 C -5.06828500 -0.77227800 -2.29258300
 C -3.83850400 -0.26864400 -1.87084500
 C -3.74057300 0.32542300 -0.60575200
 N -4.79784700 0.42577900 0.21989700
 H -5.16765200 -1.23528600 -3.27099200
 H -7.14337700 -1.04363700 -1.72189000
 H -2.96262200 -0.33020600 -2.51070600
 H -6.80301100 0.04262900 0.50002800
 C -2.42874400 0.87135300 -0.08439000
 C -1.86564500 0.00173000 1.05665200
 P -0.25744500 0.64187300 1.75046300
 C 0.05710800 -0.57763000 3.11219900
 C -0.85177800 2.08139800 2.76230000
 H -1.63254500 1.78056300 3.47005400
 H -0.01115700 2.50785200 3.31951000
 H -1.25467400 2.86248600 2.11081600
 H 0.92080000 -0.24686300 3.69835400

H -0.80876100 -0.67511100 3.77752300
H 0.29398800 -1.55589000 2.68811600
H -1.69345600 0.93595400 -0.89364600
H -2.60303000 1.89041600 0.28143800
H -1.67255700 -1.01020200 0.68224500
H -2.61080200 -0.07783300 1.85814400

TS7-lgh

C 1.95445200 1.62494500 3.13894500
C 3.42341200 1.45561900 2.72671700
H 1.76174100 1.38862800 4.19031500
H 1.64014000 2.66650600 2.97571300
C 3.36102800 1.30955200 1.20455600
H 4.04557200 2.29759700 3.04948800
H 3.83366600 0.54192600 3.17510000
H 3.24703200 2.30189200 0.74164800
H 4.25436800 0.85204700 0.77422400
C 1.16917100 0.71388000 2.20536200
C -0.04257700 0.20176100 2.36984300
C 2.11470300 0.45911100 0.89553700
C 1.86573000 -0.29307700 -0.18572300
Si 2.78424500 -0.71116300 -1.72467800
H -0.73221400 0.29847600 3.20186400
Ni 0.12064300 -0.61671700 0.71533900
C 2.89017600 -2.60357500 -1.86146900
H 3.38885300 -2.91333900 -2.78885700
H 3.45369000 -3.02886900 -1.02164100
H 1.88970900 -3.05193200 -1.84783200
C 1.79585100 -0.05294700 -3.21126200
H 1.71316400 1.04095700 -3.18244300
H 2.27555200 -0.32343400 -4.16068800
H 0.77921700 -0.46396100 -3.22087100
C 4.56113500 -0.03114800 -1.88417400
H 5.00188200 -0.32043300 -2.84756400
H 4.58684100 1.06391300 -1.82724000
H 5.21829700 -0.42007400 -1.09628800
C -2.42778700 -1.35406900 -0.32271600
C -3.52677700 -2.20804300 -0.46656900
C -3.62147000 -3.37175300 0.28948900
C -2.59790700 -3.66300700 1.19372600
C -1.53090100 -2.78376100 1.29676200
N -1.43409400 -1.65604100 0.55340800
H -4.47214500 -4.03733700 0.17651100
H -4.30085800 -1.94464400 -1.18078900

H -2.61851400 -4.55572000 1.80990600
H -0.71031800 -2.96541200 1.98096200
C -2.31995500 -0.07489400 -1.11183700
C -2.83472000 1.14978300 -0.32377800
P -2.82374000 2.72519100 -1.34857500
C -3.44340100 3.90638700 -0.04164100
C -1.00626400 3.14498600 -1.29732300
H -3.87637000 0.97634600 -0.02162200
H -2.24234400 1.27928100 0.59134500
H -0.43691600 2.43219800 -1.90237600
H -0.85565600 4.14056600 -1.72958500
H -0.60219800 3.13516400 -0.27797500
H -2.88159200 3.82938400 0.89763300
H -3.36268300 4.93361500 -0.41361900
H -4.50152900 3.71023600 0.16326300
H -1.26754500 0.07509100 -1.38486800
H -2.89490900 -0.17838200 -2.03962700

TS7-lgh'

C -1.94538900 3.52944500 -0.87504300
C -3.45315600 3.44603700 -0.58704100
H -1.70427900 4.00648100 -1.83044300
H -1.44668800 4.11010900 -0.08478800
C -3.56898100 2.31835500 0.44413000
H -3.86135800 4.39791700 -0.22983700
H -3.99125100 3.17205700 -1.50340700
H -3.31372000 2.70369000 1.44356800
H -4.57142500 1.88969300 0.50863800
C -1.45841600 2.08753600 -0.81700700
C -0.35399600 1.57903500 -1.35771200
C -2.53670200 1.25398700 0.02916200
C -2.51988700 -0.06196100 0.30120600
Si -3.62499600 -1.18971500 1.24740900
H 0.40123700 2.08080200 -1.95272600
Ni -0.80305300 -0.09265000 -0.71602500
C -4.09603000 -2.65527600 0.13125700
H -4.72016500 -3.38340500 0.66517800
H -4.65709100 -2.31757000 -0.74908500
H -3.20056700 -3.17559000 -0.22859000
C -2.65695000 -1.85769200 2.74300600
H -2.39298800 -1.04939400 3.43625500
H -3.24397500 -2.59769400 3.30205100
H -1.72363900 -2.33672300 2.42382600
C -5.25571000 -0.45200500 1.91468300

H	-5.82581900	-1.21039100	2.46774800
H	-5.07754200	0.38704500	2.59818500
H	-5.89940300	-0.08889700	1.10363200
C	4.21654400	0.41914300	0.47895600
C	4.28275800	1.04497400	1.72981700
C	5.49221400	1.04687700	2.42427400
C	6.59745800	0.42272700	1.84868200
C	6.43445000	-0.17747500	0.59852900
N	5.28110300	-0.18574600	-0.07717100
H	5.56828300	1.52787600	3.39588400
H	3.40036200	1.52212700	2.14677400
H	7.56050700	0.39887700	2.34960000
H	7.27363100	-0.67521200	0.11415200
C	2.93103900	0.37388900	-0.32067700
C	2.39934700	-1.06553300	-0.44964400
P	0.83918300	-1.21947100	-1.44422900
C	1.38356500	-0.92753800	-3.18632600
C	0.54117700	-3.04406100	-1.41768400
H	3.17306400	-1.70189700	-0.89681200
H	2.17529800	-1.46915700	0.54551700
H	0.29810800	-3.35374200	-0.39711900
H	-0.31570300	-3.28115900	-2.05536700
H	1.41906400	-3.60005400	-1.76761700
H	2.22407100	-1.57723500	-3.45496200
H	0.54584400	-1.12541600	-3.86209300
H	1.68101200	0.11641200	-3.31609200
H	2.16950800	1.01113800	0.14071400
H	3.13556200	0.77904200	-1.31957700

INT9-1gh

C	-2.13978400	0.32708700	-3.48606700
C	-3.63500000	0.16976900	-3.09079900
H	-1.86915600	-0.25495300	-4.37439400
H	-1.92305500	1.38191700	-3.71491700
C	-3.68762200	0.47718000	-1.56967200
H	-4.30184200	0.80730400	-3.68206800
H	-3.94159000	-0.87060600	-3.25807300
H	-3.78301200	1.56284900	-1.41107400
H	-4.54361300	0.00739600	-1.07160800
C	-1.41839900	-0.10089300	-2.22315600
C	-0.19175800	-0.56676400	-1.93334800
C	-2.33769000	-0.01318600	-1.06957400
C	-1.82963500	-0.40763100	0.11997700
Si	-2.64528400	-0.55230600	1.78555400

H	0.61225800	-0.72889700	-2.65716000
Ni	0.01584100	-0.91620700	-0.08070100
C	-3.93820900	-1.94857800	1.82510600
H	-4.36707600	-2.07587900	2.82766900
H	-4.76424400	-1.74299400	1.13330800
H	-3.49209100	-2.90512200	1.52672300
C	-1.28414100	-0.98829200	3.04995500
H	-0.53367100	-0.18946500	3.12332500
H	-1.69727400	-1.13766600	4.05547600
H	-0.76244200	-1.91637800	2.77587600
C	-3.47582400	1.06106500	2.36045100
H	-3.90907300	0.95615700	3.36379400
H	-2.75368200	1.88598900	2.39217500
H	-4.28275400	1.35742300	1.67929700
C	2.18841200	-2.71555500	-0.66153300
C	3.46257800	-3.26605000	-0.73586300
C	4.52792800	-2.53976200	-0.20359700
C	4.27371400	-1.29867000	0.37405400
C	2.96623500	-0.80152700	0.41598200
N	1.93830100	-1.51761300	-0.09732200
H	5.53994100	-2.93345200	-0.23758700
H	3.60907600	-4.23635300	-1.19860900
H	5.07974900	-0.70612900	0.79566600
H	1.32275700	-3.23183700	-1.06482900
C	2.65965700	0.55964700	0.99413700
C	2.47545900	1.63028600	-0.10283600
P	2.18582900	3.34912000	0.60027000
C	0.44822800	3.14759500	1.25537200
C	1.80872300	4.23070600	-1.00138900
H	3.38492700	1.68286500	-0.71622900
H	1.64556100	1.34115500	-0.76102200
H	1.03294300	3.72372900	-1.58777500
H	1.47555000	5.25148600	-0.78473200
H	2.71934100	4.30073100	-1.60646000
H	0.02664000	4.13919200	1.45502600
H	-0.20957600	2.61234200	0.55997100
H	0.46701700	2.60587500	2.20711600
H	3.47042100	0.85497300	1.67038200
H	1.74561700	0.49236300	1.59662000

INT9-1gh'

C	-1.88548000	-3.14835000	-1.99331100
C	-2.87064900	-3.76155800	-0.95872000
H	-0.98755300	-3.75886200	-2.14284300

H -2.62611200 4.65905400 -1.76991400
H -3.48112900 2.98716500 -0.12889500
H -0.40039300 4.22654300 -2.87704600
H 0.84257400 2.15827300 -2.25278400
C -2.31801200 0.66611000 0.64910800
C -3.55054400 -0.10505900 0.13018900
P -4.42504900 -1.06544800 1.49119400
C -5.61076200 -2.03485300 0.42375300
C -3.17034500 -2.40087700 1.84231900
H -2.58738200 1.19610100 1.57256000
H -1.51477600 -0.03038100 0.90626700
H -4.29118500 0.60205800 -0.26643700
H -3.25425500 -0.76436200 -0.69371400
H -2.32455900 -1.98477400 2.39990600
H -3.63497500 -3.16259200 2.47852800
H -2.78629400 -2.88532500 0.93725100
H -5.10396400 -2.56877500 -0.38920200
H -6.14279600 -2.76468400 1.04357100
H -6.35735900 -1.35968800 -0.00866200
H 1.36075000 -2.28197800 -2.57164800

TS8-1g'

C -3.69509100 1.82022700 -1.65703200
C -3.51390000 3.35783900 -1.54412500
H -4.69162200 1.49088900 -1.34407800
H -3.56750400 1.49603900 -2.70046400
C -1.99207600 3.56920000 -1.31765600
H -3.89355800 3.89845900 -2.41757400
H -4.05943900 3.72389600 -0.66597900
H -1.46562700 3.56221200 -2.28400700
H -1.75401800 4.51557900 -0.82111100
C -2.56306000 1.26373400 -0.79940900
C -2.27026700 0.04081600 -0.29126600
C -1.62703300 2.34665700 -0.50446300
C -0.67140500 2.10452600 0.42045200
Si -3.47009000 -1.40012600 -0.16027100
Ni -0.57431300 0.14677500 0.64115300
C -0.56810500 1.35536600 2.40812900
O 0.47560600 0.68762400 2.35600200
O -1.34298500 1.92211500 3.10946100
C -5.05053100 -0.81293800 0.71723800
H -5.57046100 -0.02528100 0.16104100
H -5.75420800 -1.64513700 0.84891100
H -4.81388100 -0.41313500 1.71035100

C -3.94231300 -2.10852500 -1.86252400
H -4.64437300 -2.94585000 -1.75732200
H -4.42616800 -1.34822500 -2.48721100
H -3.06714200 -2.47438700 -2.41236200
C -2.77371600 -2.80807500 0.90953300
H -2.00573500 -3.39927900 0.39906400
H -2.34165600 -2.42651200 1.84272700
H -3.58221800 -3.49879100 1.18045500
C 4.47773700 0.04776400 0.01432100
C 4.88588000 1.38218300 0.13100300
C 6.15099700 1.74782100 -0.32788000
C 6.96912200 0.77014100 -0.89117800
C 6.47489800 -0.53339600 -0.96808800
N 5.26496500 -0.89631100 -0.53094200
H 6.49013700 2.77708800 -0.24538100
H 4.22198100 2.11624300 0.57879300
H 7.96232800 1.00535600 -1.26159100
H 7.08280600 -1.32700300 -1.40089400
C 3.11835600 -0.41161200 0.50136800
C 2.28407600 -1.01497600 -0.64387200
P 0.61653200 -1.67450100 -0.13665300
C 0.09356700 -2.51771800 -1.69559600
C 1.05696000 -3.08354400 0.97964500
H 2.58192600 0.41783600 0.97090900
H 3.27389300 -1.17155100 1.27778800
H 2.10108000 -0.25470100 -1.41382700
H 2.85460800 -1.82536000 -1.11398700
H 1.45196800 -2.69336900 1.92210400
H 0.16149100 -3.66851800 1.20638700
H 1.80677500 -3.73598600 0.51800000
H 0.86525300 -3.21248300 -2.04535600
H -0.83727900 -3.06773000 -1.53719500
H -0.08782000 -1.76171300 -2.46550700
H 0.14221300 2.80433500 0.61989500

TS8-1h

C 1.32695000 1.94137900 3.10237400
C 2.84626200 2.14565100 2.86522300
H 1.10213400 1.59647000 4.11783100
H 0.78412100 2.88759300 2.95948900
C 3.05286700 1.89904400 1.34714900
H 3.20473500 3.12898300 3.18738200
H 3.40571200 1.38977200 3.42955800
H 2.83067300 2.81747900 0.78369000

H 4.07602400 1.60499000 1.09382400
 C 0.94893500 0.93715800 2.02587400
 C -0.16167800 0.22501100 1.73539400
 C 2.02180800 0.82701200 1.03992500
 C 1.91064700 -0.10989500 0.04570600
 Si 2.77162900 -0.04749800 -1.63698600
 H -1.06607600 0.26586100 2.35079300
 Ni 0.10835400 -0.94622100 0.26894800
 C 1.93032600 -2.15225200 0.42665200
 O 1.14401100 -2.59470500 -0.42546000
 O 2.76861700 -2.43455600 1.22184500
 C 4.17113000 -1.32163200 -1.78968800
 H 3.79438300 -2.34864900 -1.72843100
 H 4.68463300 -1.21313300 -2.75378400
 H 4.91650500 -1.19553400 -0.99586600
 C 1.48146900 -0.39911200 -2.98703500
 H 1.94887300 -0.36350000 -3.97951200
 H 1.03330600 -1.39075100 -2.86265900
 H 0.67459400 0.34484400 -2.97730700
 C 3.50429200 1.67168400 -1.99061000
 H 2.75631600 2.46561400 -1.87913800
 H 4.34766200 1.91197100 -1.33417400
 H 3.87276000 1.70832800 -3.02408300
 C -2.78236800 -1.22054700 -0.39139700
 C -4.02099900 -1.87442700 -0.38132500
 C -4.16230800 -3.09089600 0.27789300
 C -3.05068000 -3.64340300 0.91514800
 C -1.84931300 -2.94843300 0.86348700
 N -1.71461600 -1.76458500 0.23356200
 H -5.11977000 -3.60406400 0.28730600
 H -4.86122300 -1.42181400 -0.89919400
 H -3.10491500 -4.59380600 1.43530900
 H -0.94979200 -3.34256100 1.32454300
 C -2.61596700 0.11077800 -1.08522900
 C -3.08482300 1.29176900 -0.20949900
 P -3.03708900 2.93876900 -1.11518600
 C -3.49193300 4.04599800 0.31792300
 C -1.19437000 3.23787100 -1.15075000
 H -3.18908600 0.09885800 -2.02086600
 H -1.56100700 0.24028100 -1.34995300
 H -4.12631800 1.12905300 0.09863600
 H -2.47366600 1.34039300 0.69985500
 H -0.72571800 2.61118100 -1.91655900
 H -1.00664900 4.28263900 -1.42247800

H -0.71710500 3.02665500 -0.18637100
 H -2.86656600 3.87093600 1.20203100
 H -3.38437900 5.09327700 0.01528700
 H -4.54075900 3.88589600 0.59061900

TS8-1h'

C -1.45980500 2.59396300 -2.77750600
 C -2.84396500 3.14307400 -2.34565900
 H -1.42068900 2.33538400 -3.84169800
 H -0.67641800 3.34613900 -2.60244200
 C -2.96707400 2.77571300 -0.84414300
 H -2.95890600 4.21630800 -2.53090300
 H -3.63124300 2.62531200 -2.90719600
 H -2.44841700 3.52851600 -0.23200700
 H -4.00298200 2.73352600 -0.49615800
 C -1.26769600 1.39746200 -1.86034400
 C -0.35138600 0.41204700 -1.79046900
 C -2.24618100 1.43748100 -0.76688100
 C -2.31038000 0.39989200 0.11339500
 Si -2.96978400 0.45652000 1.88033300
 H 0.46881600 0.33785500 -2.51133900
 Ni -0.76167400 -0.82703700 -0.40978300
 C -2.73894400 -1.64355100 -0.38252700
 O -1.98419000 -2.27136500 0.37729500
 O -3.70473900 -1.69226500 -1.07224000
 C -4.52866600 -0.59847500 2.12973900
 H -4.33642200 -1.66444800 1.96551400
 H -4.90143900 -0.48359700 3.15583500
 H -5.33051700 -0.29706700 1.44576400
 C -1.60472100 -0.19305900 3.03295400
 H -1.93145200 -0.15083300 4.07994900
 H -1.35414400 -1.23378600 2.80104400
 H -0.68941900 0.40595300 2.94631600
 C -3.38020400 2.22880100 2.43630900
 H -2.53445500 2.91087500 2.29068000
 H -4.24281800 2.64677200 1.90592800
 H -3.62257300 2.22840200 3.50708100
 C 4.14679400 0.58061300 0.63427100
 C 4.18953700 1.97780300 0.55351300
 C 5.42729600 2.62032300 0.56845400
 C 6.58337000 1.84764200 0.66179200
 C 6.44111000 0.46052300 0.73507600
 N 5.26084700 -0.16699500 0.72244600
 H 5.48578800 3.70393700 0.50898400

H 3.26718400 2.54731900 0.48226600
 H 7.56955300 2.30161800 0.67817500
 H 7.31968300 -0.17900600 0.80977900
 C 2.83471100 -0.17619200 0.61532900
 C 2.71749400 -1.07954100 -0.62709800
 P 1.13302100 -2.04011200 -0.68399400
 C 1.24036700 -2.92286600 -2.30285500
 C 1.37092900 -3.39698300 0.54751700
 H 1.99308300 0.52472000 0.63960400
 H 2.77792100 -0.78994100 1.52344100
 H 2.74499900 -0.46163700 -1.53319200
 H 3.57278800 -1.76413700 -0.66869500
 H 1.46227200 -2.97593900 1.55332000
 H 0.48860000 -4.04417100 0.53597400
 H 2.26413900 -3.99237700 0.32797300
 H 2.18966100 -3.45975900 -2.40796100
 H 0.41441900 -3.63683600 -2.38002800
 H 1.14150600 -2.20169400 -3.11959800

INT5-1f

Ni 0.82145900 -0.61732400 -0.22044300
 O -0.21786300 0.76662700 -0.56293100
 O -1.76138500 2.32719600 -0.73493600
 C -1.46889800 1.15478600 -0.48069900
 C -2.57347400 0.23003200 -0.06033500
 C -2.63124700 -1.09286000 -0.37382600
 C -3.90990700 -1.92777800 -0.27815700
 H -4.81804300 -1.32563400 -0.30916500
 H -3.92466700 -2.49857900 0.66292000
 C -3.80256000 -2.89399600 -1.46943600
 C -2.30880000 -3.25021800 -1.50349800
 H -4.08482800 -2.37026300 -2.39113000
 H -4.45294000 -3.76954800 -1.37058400
 H -2.11019000 -4.11475100 -0.85442100
 H -1.94986600 -3.51165700 -2.50483700
 C -1.60175700 -2.00147000 -0.94732900
 C -0.26127300 -1.93857500 -0.89983100
 Si -3.95813000 1.23093500 0.81215000
 C -5.02150900 0.13714300 1.96094500
 H -4.40727200 -0.53840200 2.56918900
 H -5.56260400 0.79350400 2.65505300
 H -5.77013300 -0.46946400 1.44138700
 C -3.16849000 2.50068700 1.97864600
 H -2.49977200 2.01310100 2.69998700

H -2.59052500 3.24542200 1.42739800
 H -3.94911100 3.01449700 2.55454300
 C -5.09822200 2.07942100 -0.44048900
 H -5.61211600 1.35245300 -1.08163300
 H -5.86699100 2.67612000 0.06728600
 H -4.51006400 2.74221600 -1.08212000
 C 2.15428400 -2.88014900 0.94628400
 C 3.21136700 -3.61102100 1.47425600
 C 4.50375900 -3.10746300 1.33206700
 C 4.68518700 -1.89826500 0.66467600
 C 3.58340700 -1.20829000 0.15212600
 N 2.32922200 -1.70872900 0.30297100
 H 5.35715900 -3.64822700 1.73099800
 H 1.12762200 -3.22109700 1.02080700
 H 3.01813600 -4.54888800 1.98382100
 H 5.67818000 -1.48171300 0.52970700
 C 3.72866100 0.10237600 -0.58596300
 C 3.12322400 1.31508600 0.15475200
 P 3.18062900 2.88886300 -0.89257900
 C 4.66311600 3.72140500 -0.11454700
 H 5.57457300 3.16112400 -0.35237300
 H 4.77624300 4.72509500 -0.53882200
 H 4.57668700 3.81117600 0.97570700
 C 1.80263800 3.83894600 -0.07749200
 H 1.90056900 3.87571400 1.01496500
 H 1.80484600 4.86533800 -0.46099200
 H 0.84181000 3.38189100 -0.33952000
 H 4.79222000 0.28297700 -0.77863200
 H 3.24298900 0.00880800 -1.56626800
 H 3.61611800 1.46070900 1.12531900
 H 2.05691900 1.15457300 0.36965100
 H 0.32097000 -2.75573400 -1.33803700

INT7-1f

Ni -0.98291000 0.46023200 -0.60582300
 O 0.17372700 -0.71927200 -1.43374400
 O 1.97474100 -1.94296700 -1.84826200
 C 1.41819100 -1.04129300 -1.20984200
 C 2.24818600 -0.35283700 -0.15366800
 C 2.31306400 1.00102200 -0.07554500
 C 3.42557600 1.80608000 0.58848900
 H 4.31878400 1.22175600 0.81687300
 H 3.07040200 2.25261400 1.53044900
 C 3.69837800 2.91795300 -0.44702400

C 2.30478000 3.25911500 -1.01876800
 H 4.33839400 2.51544900 -1.24132700
 H 4.21088900 3.78585200 -0.01782300
 H 1.86721600 4.11588800 -0.48753300
 H 2.34609400 3.53356500 -2.07951900
 C 1.46489600 1.99369800 -0.78279500
 C 0.15071200 1.90277600 -1.05008200
 Si 3.38416000 -1.57364800 0.76521700
 C 3.71729500 -0.98051800 2.54790500
 H 2.77846000 -0.75241900 3.06863000
 H 4.21509500 -1.78143600 3.11043000
 H 4.35520900 -0.09298600 2.61184700
 C 2.50583500 -3.24367700 0.94779900
 H 1.55579500 -3.13621900 1.48751300
 H 2.29178400 -3.67724400 -0.03217300
 H 3.12937900 -3.94493700 1.51733700
 C 5.03548200 -1.80271900 -0.13714300
 H 5.60555600 -0.86716900 -0.19098000
 H 5.66514400 -2.54897900 0.36426600
 H 4.84340700 -2.14131300 -1.16037400
 P -2.30778400 1.92345500 0.37873200
 C -1.47779200 2.89271300 1.71248600
 H -0.59958700 3.38650900 1.28927100
 H -2.15019200 3.63679500 2.15412200
 H -1.12967800 2.21228400 2.49616800
 C -3.12460400 3.22486400 -0.64452900
 H -3.75942300 3.87646900 -0.03420400
 H -2.36032900 3.83426300 -1.13535400
 H -3.73430000 2.75253200 -1.42096000
 C -3.71677600 1.11195000 1.27682500
 C -3.28990800 -0.27318000 1.80925600
 C -3.19129300 -1.32277200 0.72367700
 C -4.03484500 -2.43709900 0.75903900
 C -3.95451900 -3.40302900 -0.24156600
 C -3.01711600 -3.23059500 -1.25504100
 C -2.20199300 -2.10243200 -1.22831600
 N -2.28599500 -1.15712300 -0.26882900
 H -4.60613300 -4.27221700 -0.22224800
 H -4.74417300 -2.54084700 1.57435800
 H -2.90073100 -3.95528100 -2.05407500
 H -1.41787600 -1.94047200 -1.95964600
 H -4.56331800 1.00208200 0.58843300
 H -4.04863900 1.75249800 2.10279900
 H -4.01629900 -0.61312400 2.55498200

H -2.32512000 -0.19376300 2.32845300
 H -0.30285700 2.75024600 -1.57976400

TS6-1f

Ni -0.96761600 0.59868800 -0.65990200
 O 0.32476400 -0.16431600 -1.81616600
 O 1.14955800 -2.18893800 -1.41366700
 C 1.18969900 -0.98795800 -1.12308900
 C 2.13808800 -0.42691600 -0.15987700
 C 2.39405200 0.94311700 -0.15247800
 C 3.62702200 1.63670600 0.41533400
 H 4.50361100 0.98836900 0.47560300
 H 3.42432100 2.00119000 1.43390300
 C 3.84302100 2.82344000 -0.55183200
 C 2.42549700 3.20873200 -1.03446400
 H 4.43550600 2.48002500 -1.40857500
 H 4.38349500 3.65780900 -0.09061300
 H 2.01331400 4.01558100 -0.40732500
 H 2.42167200 3.58765800 -2.06573700
 C 1.64384000 1.91317700 -0.87190600
 C 0.40173000 1.63005900 -1.40412000
 Si 3.04850600 -1.77301800 0.81303200
 C 4.05388200 -1.06529500 2.27257900
 H 4.33239500 -1.89291500 2.93852300
 H 4.98282100 -0.57042000 1.96936000
 H 3.47439400 -0.35038600 2.86968800
 C 4.23312500 -2.76808300 -0.28437400
 H 3.68362800 -3.19068800 -1.13118600
 H 5.03873100 -2.13764700 -0.68112500
 H 4.69832000 -3.59089900 0.27389700
 C 1.77608000 -2.93839300 1.60932100
 H 1.11531800 -3.35997500 0.84709800
 H 2.27647800 -3.76327300 2.13342200
 H 1.15951100 -2.40625400 2.34582100
 P -2.06000100 2.03286900 0.55293400
 C -1.13936000 2.67716000 2.02070900
 H -0.19988000 3.11973700 1.67604700
 H -1.71641500 3.42624700 2.57496200
 H -0.88631900 1.84949500 2.69053700
 C -2.71437700 3.57948400 -0.21882100
 H -3.27349700 4.18975300 0.49944000
 H -1.87709100 4.16747600 -0.60810100
 H -3.36823800 3.32480500 -1.05878200
 C -3.56884000 1.24429500 1.29694500

C -3.28010200 -0.20951900 1.73250100
 C -3.16193500 -1.21665400 0.60447200
 C -4.00409200 -2.33220100 0.58504700
 C -3.86305300 -3.29432900 -0.41355600
 C -2.86929600 -3.11929200 -1.37135100
 C -2.07113100 -1.98039700 -1.30339100
 N -2.21605100 -1.03891800 -0.34805000
 H -4.51087500 -4.16640900 -0.43238600
 H -4.75739800 -2.44454000 1.35892900
 H -2.69903400 -3.84683600 -2.15789400
 H -1.26276000 -1.81239600 -2.00712200
 H -4.36823300 1.25771400 0.54582800
 H -3.92067500 1.82829200 2.15681300
 H -4.08174500 -0.54328300 2.40031800
 H -2.35725000 -0.23911700 2.32863800
 H 0.04476800 2.18249900 -2.28006800

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C -3.78492300 -0.80614200 0.00631900
 H -3.97722300 -0.30959900 0.96625800
 H -4.00276700 -0.06659700 -0.77503600
 C -4.70471300 -2.02129000 -0.15022800
 H -4.48705900 -2.76101100 0.63099200
 H -4.51237500 -2.51750000 -1.11030300
 C -6.19934000 -1.63940800 -0.07561600
 H -6.42366100 -0.89438500 -0.85266900
 H -6.40132300 -1.14460400 0.88533600
 C -7.09251900 -2.78733600 -0.22981000
 C -7.81776500 -3.75781400 -0.36151300
 Si -8.91851500 -5.21598500 -0.56148800
 C -10.71733300 -4.65630200 -0.39014500
 H -10.97700400 -3.91126400 -1.15095800
 H -11.40304100 -5.50524500 -0.50492400
 H -10.90235400 -4.20757700 0.59259400
 C -8.63577200 -5.97009400 -2.27331200
 H -8.85879900 -5.24886500 -3.06795600
 H -7.59608000 -6.29360000 -2.39897800
 H -9.27928200 -6.84573000 -2.42572100
 C -8.50783600 -6.48660800 0.77868400
 H -7.46652300 -6.82096500 0.70570200
 H -8.65438800 -6.06914500 1.78149200
 H -9.15057900 -7.37122500 0.68714400
 C -2.29127700 -1.18894600 -0.06865200
 H -2.09035300 -1.68630900 -1.02811200

H -2.06606200 -1.93102800 0.71044600
 C -1.39704100 -0.03998700 0.08058600
 C -0.67553000 0.92043600 0.20585100
 H -0.03422400 1.76482600 0.31586100

INT1-4a

Ni -3.06702800 -0.26333900 -0.02151700
 C -1.90002300 -1.74664700 -0.04317500
 C -1.19581300 -0.67388200 -0.05360100
 H -1.88032600 -2.82755700 -0.04412700
 C 0.17750600 -0.09504700 -0.08030600
 H 0.31357300 0.47685100 -1.01096700
 H 0.28806400 0.63982100 0.73119800
 P -3.17716000 1.94509300 0.00936800
 P -5.09653200 -1.14353200 -0.00229700
 C -2.36397800 2.74023000 1.47810100
 H -1.32930300 2.39244800 1.55134500
 H -2.37256000 3.83507200 1.41195600
 H -2.88346400 2.43475000 2.39218700
 C -2.30597400 2.80487600 -1.38781700
 H -2.33056700 3.89609800 -1.27967300
 H -1.26492100 2.47098900 -1.42575200
 H -2.77910600 2.53021800 -2.33626600
 C -4.79121600 2.87467900 -0.00390200
 H -5.39794600 2.57585200 0.85763800
 H -4.63998300 3.96025200 0.03309500
 H -5.35129100 2.63034300 -0.91291200
 C -6.19613200 -0.78922900 1.45524000
 H -6.37814700 0.28778300 1.52924300
 H -7.16005400 -1.30706400 1.38002900
 H -5.69251800 -1.10831700 2.37361600
 C -6.24148800 -0.73078900 -1.40847300
 H -7.20019700 -1.25741300 -1.32819100
 H -6.43068000 0.34728500 -1.42794200
 H -5.76398600 -1.00500000 -2.35481600
 C -5.18524400 -2.99575700 -0.03835500
 H -4.65047000 -3.39880900 0.82750100
 H -6.21890500 -3.36217200 -0.02549800
 H -4.68522900 -3.36283600 -0.94024900
 C 1.29492500 -1.14764100 0.03428000
 H 1.17870900 -1.87568700 -0.78003500
 H 1.15826800 -1.70669500 0.97004300
 C 2.70108900 -0.53953800 -0.00831700
 H 2.81945700 0.19377500 0.80030500

H 2.84606000 0.00899000 -0.94829800
 C 3.80912600 -1.60833200 0.12203700
 H 3.69565200 -2.34915300 -0.68269300
 H 3.67105100 -2.16073700 1.06272200
 C 5.16059300 -1.05037600 0.08039100
 C 6.27829300 -0.56538700 0.04301200
 Si 7.96469000 0.15752800 -0.01266800
 C 9.23750800 -1.24248600 -0.02260700
 H 9.10390700 -1.89441600 -0.89354000
 H 10.25900300 -0.84309700 -0.05640100
 H 9.15073800 -1.86463500 0.87560000
 C 8.14045100 1.19877000 -1.58310600
 H 7.98617600 0.59186700 -2.48270400
 H 7.40865200 2.01459100 -1.60222100
 H 9.14108100 1.64463500 -1.64715100
 C 8.22040100 1.24990000 1.51143200
 H 7.48831400 2.06508300 1.54248400
 H 8.11560700 0.67271600 2.43733400
 H 9.22171700 1.69878300 1.50788600

INT2-4a

Ni 0.76584300 -0.23343800 -0.38773500
 C 2.63168500 0.09756400 -0.31220000
 C 2.02388300 1.13059500 0.11095000
 O 0.23214700 -2.21371900 1.62272600
 O 0.51046200 -2.36011100 -0.69882800
 C 0.42110300 -1.99960600 0.46364300
 C 1.98334500 2.50981000 0.66036200
 H 1.36911600 3.14708000 0.00851600
 H 1.47146400 2.49445800 1.63305800
 H 3.54657400 -0.42314300 -0.54567800
 P -1.40225600 0.41420200 -0.19860000
 C -1.89050500 0.99825200 1.48702200
 H -2.95122900 1.27001100 1.53545900
 H -1.68612700 0.20137900 2.20879000
 H -1.28572100 1.86745100 1.76360900
 C -1.92080200 1.82352500 -1.28204400
 H -2.96751900 2.10178200 -1.11369700
 H -1.28501900 2.69214900 -1.08406900
 H -1.79123000 1.54385500 -2.33242000
 C -2.70363200 -0.85307000 -0.55888500
 H -3.71297600 -0.43558400 -0.46991100
 H -2.56464500 -1.24586100 -1.57083900
 H -2.60227300 -1.68705100 0.14268600

C 3.38195300 3.13508500 0.82473300
 C 3.32821600 4.55801900 1.39136300
 H 3.88594700 3.13962900 -0.15088200
 H 3.98187200 2.49188100 1.48192700
 H 2.73206400 5.20324600 0.73292400
 H 2.82346500 4.55665700 2.36619300
 C 4.73410100 5.17630300 1.55729700
 H 5.24861500 5.17431600 0.58555900
 H 5.33590200 4.53753000 2.21968800
 C 4.70472600 6.53851800 2.08891700
 C 4.65876800 7.67321200 2.53125500
 Si 4.60507300 9.38671300 3.19264800
 C 3.09813200 10.27625500 2.47285600
 H 3.14651600 10.31906900 1.37865900
 H 2.16665300 9.76706900 2.74596600
 H 3.03776000 11.30650700 2.84571500
 C 6.18915000 10.28997100 2.68937700
 H 6.19095500 11.31773900 3.07374300
 H 7.07787800 9.78393200 3.08362400
 H 6.29029300 10.34015100 1.59915800
 C 4.47358400 9.31942500 5.07876300
 H 3.56374300 8.79773200 5.39726600
 H 5.32969600 8.79552700 5.51918000
 H 4.44581700 10.33077700 5.50358100

TS1-4a

Ni -3.82048100 0.27059200 0.00706600
 C -2.54091600 1.97825400 0.01421700
 C -2.06206000 0.73882700 0.02059700
 H -1.92056700 2.87073600 0.01683500
 C -0.69714600 0.13670600 0.03360900
 H -0.58936500 -0.48783700 0.93336000
 H -0.59950100 -0.55150000 -0.81948900
 O -4.11060500 3.80855000 0.00379700
 O -5.12703000 1.77846200 -0.00478800
 C -4.14711500 2.59377200 0.00275600
 P -3.90118100 -1.85827400 -0.00425300
 C -3.14125000 -2.69728900 -1.46215300
 H -2.07593100 -2.45408300 -1.51472100
 H -3.25775800 -3.78512000 -1.39966800
 H -3.61737000 -2.33711800 -2.37896700
 C -3.12761300 -2.72128700 1.43216500
 H -3.59499000 -2.37673100 2.35943400
 H -3.24451800 -3.80794900 1.35256400

H -2.06192900 -2.47853700 1.47835400
 C -5.63434300 -2.49647800 -0.00182400
 H -6.16416300 -2.11510000 -0.87999900
 H -5.65783400 -3.59225800 -0.01300800
 H -6.15504600 -2.13339800 0.88945300
 C 0.44805400 1.16582900 -0.01128400
 C 1.83224800 0.50810700 0.00594700
 H 0.34909600 1.84705900 0.84414300
 H 0.33825400 1.78046400 -0.91452300
 H 1.94972800 -0.09908100 0.91286500
 H 1.93393900 -0.17846900 -0.84459100
 C 2.97413700 1.54668800 -0.05143500
 H 2.87758800 2.24096900 0.79572800
 H 2.86345200 2.15881800 -0.95806500
 C 4.30472700 0.93989400 -0.03357700
 C 5.40573200 0.41770500 -0.01769200
 Si 7.07768500 -0.34585900 0.00508400
 C 7.24831600 -1.40899600 1.56072700
 H 6.49970600 -2.20944100 1.58011800
 H 8.23974000 -1.87693600 1.60651500
 H 7.11934700 -0.80948500 2.46918000
 C 8.37688800 1.02860500 0.01352800
 H 9.39068100 0.60911600 0.02792400
 H 8.28974100 1.66309900 -0.87589900
 H 8.26844400 1.67231500 0.89395300
 C 7.28338300 -1.42336500 -1.53640600
 H 6.53433300 -2.22307800 -1.56597500
 H 7.17638700 -0.83199200 -2.45301500
 H 8.27496900 -1.89282800 -1.55487300

INT3-4a

Ni 3.91047100 -0.06467500 -0.00204400
 O 4.81517300 -1.61674100 -0.00258700
 O 4.55091600 -3.85518100 0.00144500
 C 4.08053400 -2.73241600 0.00021000
 C 2.62577400 -2.40827800 0.00113000
 C 2.32591800 -1.10040100 -0.00037900
 H 1.89436500 -3.21523500 0.00258300
 C 0.95861100 -0.47712800 -0.00112400
 H 0.86178200 0.18216300 0.87508300
 H 0.86146400 0.17870500 -0.87988500
 P 3.32584000 2.12092800 0.00052600
 C 2.41386000 2.80838100 1.45233600
 H 2.32389600 3.89813300 1.38358000

H 1.41232000 2.37218600 1.50468300
 H 2.94534200 2.54923600 2.37305000
 C 4.88738500 3.11851200 -0.00246700
 H 5.48034100 2.87801100 -0.89074000
 H 4.67275100 4.19292000 -0.00052400
 H 5.48517700 2.87579000 0.88195400
 C 2.40620200 2.81161300 -1.44490100
 H 1.40420300 2.37595300 -1.49254700
 H 2.31709600 3.90126400 -1.37347400
 H 2.93249500 2.55409800 -2.36904800
 C -0.21517100 -1.47468400 0.00109000
 C -1.57728300 -0.77098300 0.00017800
 H -0.13462700 -2.12480100 0.88204000
 H -0.13515100 -2.12805900 -0.87749000
 H -1.66500200 -0.11838700 0.87870700
 H -1.66549300 -0.12163200 -0.88070200
 C -2.75608000 -1.76951400 0.00235600
 H -2.67602800 -2.42488400 0.88147000
 H -2.67652600 -2.42812300 -0.87438000
 C -4.06271700 -1.11234100 0.00151900
 C -5.14070400 -0.54371800 0.00074000
 Si -6.77545600 0.29569400 -0.00044900
 C -8.13976100 -1.01404200 -0.00321000
 H -9.13167600 -0.54487100 -0.00401100
 H -8.07280300 -1.65656900 -0.88863200
 H -8.07494300 -1.65806700 0.88128200
 C -6.91642900 1.37245900 1.54902800
 H -6.82849400 0.77085100 2.46100300
 H -6.13118000 2.13678000 1.57669100
 H -7.88513100 1.88697000 1.57975200
 C -6.91276900 1.37517000 -1.54837000
 H -6.12751200 2.13959500 -1.57279200
 H -6.82258900 0.77517300 -2.46118700
 H -7.88143200 1.88966700 -1.58052600

INT4-4a

Ni 0.51632600 0.30481100 -0.02085100
 O 2.14809300 0.55960300 0.80572000
 O 3.27635000 1.98053100 2.12992300
 C 2.27272200 1.70112200 1.49562000
 C 1.06448700 2.55626100 1.37102100
 C 0.06135800 2.06976400 0.62329000
 H 1.05549500 3.52973600 1.86476600
 C -1.18007700 2.87339600 0.32420800

H -1.22065200 3.71339800 1.03410700
 H -2.09123400 2.28190400 0.49018300
 P 1.69117700 -1.67140300 -0.72986300
 C -0.97065700 1.26176700 -2.48535800
 H -1.37979400 0.75581000 -3.37089000
 C -1.05476900 0.33551600 -1.34039600
 C -1.49013000 -0.40744300 -0.44995800
 C 1.01905000 -2.95380600 -1.88725000
 H 0.11983700 -3.41236500 -1.46527700
 H 0.74058100 -2.48027800 -2.83467300
 H 1.75459300 -3.74024700 -2.09140000
 C 2.30733900 -2.66322200 0.70069500
 H 2.78745000 -1.96800700 1.39467700
 H 1.46952700 -3.14586800 1.21523200
 H 3.02360600 -3.43226400 0.38942500
 C 3.25381700 -1.15516300 -1.56651400
 H 3.02282800 -0.68702500 -2.52927500
 H 3.73705700 -0.41398400 -0.92522800
 H 3.92607900 -2.00397300 -1.73528500
 Si -2.40010000 -1.38824300 0.84377900
 C -2.31176000 -3.22715000 0.41317900
 H -1.28739000 -3.61104400 0.47770200
 H -2.92395100 -3.80885000 1.11366100
 H -2.68543100 -3.42409500 -0.59818600
 C -1.61796200 -1.05845300 2.52605600
 H -0.57371000 -1.38909600 2.55421800
 H -1.62657300 0.01003500 2.76675300
 H -2.16361000 -1.59113000 3.31514200
 C -4.19606600 -0.79775100 0.79551200
 H -4.64506100 -0.95551100 -0.19181400
 H -4.80088000 -1.34417100 1.52992000
 H -4.26792900 0.26996400 1.03152900
 C -1.22352100 3.46970800 -1.10876200
 H -0.21702500 3.82002800 -1.37346500
 H -1.86286000 4.36223800 -1.08729400
 C -1.76635200 2.56153200 -2.22260400
 H -2.80668700 2.28921700 -2.00120400
 H -1.78373200 3.12975500 -3.16195400
 H 0.07564600 1.50002100 -2.71009200

TS2-4a

Ni 0.68718900 0.06330600 -0.03859100
 O 2.40765800 0.51515800 -0.71300900
 O 3.72870200 2.32655200 -0.95967500

C 2.71635300 1.78542600 -0.53836400
 C 1.70241800 2.50512400 0.29377000
 C 0.49774600 1.97534000 0.57568400
 H 2.01339300 3.44355200 0.75800300
 P 1.62480900 -1.98981000 0.24400000
 C -1.53165800 2.29584900 -1.19283100
 H -2.25208800 1.94838900 -1.94478200
 H -0.74478600 2.84547300 -1.72047000
 C -0.96051300 1.08304700 -0.52663200
 C -1.24332100 -0.11598400 -0.13325100
 Si -2.65058600 -1.33189500 -0.12675200
 C -4.26627200 -0.43529000 -0.55527000
 H -4.22413000 0.01586100 -1.55373700
 H -5.11271400 -1.13377600 -0.54508900
 H -4.48766500 0.36261400 0.16335800
 C -2.33835300 -2.66179800 -1.43946100
 H -1.38823600 -3.18569000 -1.28989700
 H -3.13825500 -3.41287900 -1.43185900
 H -2.31155900 -2.21451300 -2.44018500
 C -2.81876900 -2.09989800 1.59453900
 H -3.64324200 -2.82332300 1.62121000
 H -1.90581800 -2.61996700 1.90244800
 H -3.02971900 -1.32940600 2.34572500
 C 0.82550200 -3.48094000 0.99190600
 H 0.50435900 -3.25277500 2.01314400
 H -0.05349500 -3.78199500 0.41632300
 H 1.52954200 -4.32033900 1.02475600
 C 2.29703300 -2.60786700 -1.35729400
 H 2.84570500 -1.78198400 -1.81791000
 H 2.96345200 -3.46564500 -1.21185500
 H 1.47650000 -2.89780200 -2.02131200
 C 3.13482300 -1.79947400 1.28680100
 H 2.85000100 -1.53022800 2.30895800
 H 3.72196900 -2.72463500 1.31021800
 H 3.73065000 -0.98752700 0.86372200
 C -2.24284500 3.21578300 -0.17743300
 H -2.70798000 4.05175700 -0.71519300
 C -0.43718900 2.64932600 1.56199000
 H 0.17177500 3.10587300 2.35371900
 C -1.29628600 3.75075800 0.90196100
 H -1.87686600 4.27208400 1.67413600
 H -0.61761000 4.49335700 0.46159300
 H -1.08441300 1.90760800 2.04391500
 H -3.05689400 2.64693700 0.29092800

INT5-4a

C 3.77247700 -0.64758900 -1.95255700
C 3.07017500 0.66717800 -2.30566200
C 2.39133900 1.27994100 -1.06869700
C 1.43268600 0.30875000 -0.37005500
C 0.21075000 0.67631400 0.05641200
Si -0.52107200 2.40592000 0.28826900
C -1.07852800 3.14287300 -1.37720800
H -1.82791500 2.51317100 -1.87317400
H -1.52945600 4.13236300 -1.22811500
H -0.24123100 3.26481600 -2.07435500
C -2.02180700 2.31593400 1.44311100
H -2.39436400 3.32774300 1.65045400
H -2.85293700 1.73876000 1.02308500
H -1.74614800 1.85911200 2.40059500
C 0.73671900 3.56341800 1.10965700
H 1.08547600 3.13239400 2.05532000
H 1.61594700 3.75120800 0.48474000
H 0.27370800 4.53285400 1.33453200
C 2.77256800 -1.64119900 -1.33767700
C 2.01791200 -1.05119300 -0.15726200
C 1.98374100 -1.70490500 1.02273100
H 2.54001200 -2.63663300 1.11169700
Ni -0.83231400 -0.65268800 0.88898300
C 1.40092600 -1.26433200 2.34106800
O 2.00940200 -1.54052200 3.36558400
O 0.23861600 -0.63283300 2.34260900
H 1.86948200 2.19948200 -1.34888000
H 3.17501000 1.56532200 -0.34949400
H 3.78529800 1.38621500 -2.72525300
H 2.31462500 0.48118200 -3.08297700
H 4.23841000 -1.08901000 -2.84262600
H 4.57947600 -0.45199200 -1.23294100
H 2.04475100 -1.91626500 -2.11899600
H 3.27822000 -2.56546800 -1.03662900
P -2.23662700 -1.17651300 -0.77001900
C -3.77594200 -0.19523500 -1.07482600
H -3.51953200 0.84011800 -1.31695700
H -4.35706800 -0.62014100 -1.90095600
H -4.39369200 -0.18967500 -0.17134400
C -1.46304800 -1.24947100 -2.44292500
H -1.07556300 -0.26147400 -2.70565300
H -0.61899700 -1.94511200 -2.42091600

H -2.18187700 -1.57631800 -3.20233000
C -2.91091100 -2.88818900 -0.55049200
H -3.49357900 -2.93990500 0.37507100
H -3.55293100 -3.17830600 -1.38983300
H -2.08441000 -3.60127800 -0.47028400

TS3-4a

Ni 1.06934900 -0.01988400 0.79296700
O -0.32165500 0.61797400 1.85907800
O -0.95329200 -0.34973400 3.78712300
C -0.88405500 -0.42088500 2.57273000
C -1.39689000 -1.53880000 1.78041500
C -1.73503500 -1.48500200 0.45402300
H -1.66084700 -2.41341800 2.36863900
C -2.41654600 -2.68719700 -0.18209200
P 2.58933400 -0.91633200 -0.48652100
C -1.50017700 -0.30009300 -0.34712700
C -0.56741800 0.63544000 0.03905600
Si -0.43117600 2.48959800 -0.38336000
C 0.08751900 2.71873000 -2.19809500
H 0.22273700 3.78796400 -2.40692300
H 1.04197700 2.22229400 -2.40831200
H -0.65265400 2.33913200 -2.91085500
C -2.09863300 3.33859700 -0.08436100
H -2.02550400 4.41569700 -0.28152400
H -2.89183500 2.93623400 -0.72430200
H -2.41116700 3.20959700 0.95822000
C 0.87663800 3.29624200 0.71543400
H 0.92992200 4.37376400 0.51219900
H 0.63472000 3.15573500 1.77343000
H 1.87223900 2.87079900 0.54226800
C 3.48589900 0.15072700 -1.70715200
H 2.76917800 0.58465200 -2.41091200
H 3.98721400 0.97123200 -1.18453900
H 4.23143100 -0.42391400 -2.26876100
C 1.97785300 -2.29024900 -1.56540700
H 2.77851700 -2.70462300 -2.18876300
H 1.56183800 -3.08529300 -0.93902900
H 1.17647800 -1.91442400 -2.20871300
C 3.99592900 -1.72315800 0.41213200
H 3.60494300 -2.47819300 1.10116900
H 4.69826600 -2.20021300 -0.28146200
H 4.53211400 -0.97351300 1.00262200
C -2.40956400 -0.04194000 -1.54976000

H -3.30875800 0.49620300 -1.20776400
H -1.91619600 0.61551900 -2.27170000
C -2.86357300 -1.32912400 -2.25164900
H -2.00639900 -1.80057000 -2.75461700
C -3.46234700 -2.31020400 -1.24051100
H -3.82436700 -3.21602000 -1.74224300
H -4.33240200 -1.84694900 -0.75407900
H -1.64039000 -3.29823200 -0.67033100
H -3.59327500 -1.08217400 -3.03283400
H -2.86111900 -3.31834500 0.59550000

TS4-4a

Ni 2.72162400 -0.00547700 0.01604300
C 1.59369200 -1.61169900 -0.52322100
C 0.95811400 -0.46559500 -0.37554100
H 1.28596400 -2.62270900 -0.27468800
O 3.53480000 -2.89314600 -1.45428300
O 3.21278400 -0.80247500 -2.33895200
C 3.04195000 -1.78889500 -1.62405500
P 2.75678900 2.17725700 -0.23515700
P 4.64665900 -0.70592800 1.03192300
C -0.43537700 0.05083800 -0.31511600
H -0.61501200 0.63112500 -1.23504800
H -0.53444700 0.77066900 0.50954500
C -1.51540200 -1.04037200 -0.19173000
H -1.42076300 -1.73011600 -1.04048900
H -1.32314400 -1.63188800 0.71374400
C -2.93371300 -0.46170000 -0.13900900
H -3.13638900 0.12110300 -1.04694800
C -5.37096300 -1.01837900 0.07270400
C -6.49271700 -0.54538800 0.13039000
Si -8.18637400 0.16106400 0.22068900
C -8.35185100 1.15878700 1.82014900
H -9.35481400 1.59547500 1.90652700
H -8.18408200 0.52921700 2.70157500
H -7.62587400 1.97936400 1.85351000
C -9.44511000 -1.25067000 0.20699400
H -10.46963000 -0.86158300 0.26157500
H -9.36232000 -1.84857000 -0.70786400
H -9.29668300 -1.92346100 1.05941300
C -8.46334600 1.29094300 -1.27146700
H -8.36343300 0.73939900 -2.21334300
H -9.46784100 1.73186700 -1.24645900
H -7.73792600 2.11249900 -1.28766000

C 4.38971800 3.05381800 -0.21169100
H 5.05971000 2.58924300 -0.94202700
H 4.27582400 4.11526600 -0.46092300
H 4.84933300 2.97328300 0.77825500
C 1.76151200 3.22050600 0.92781300
H 0.72128100 2.88129500 0.92523300
H 2.14921700 3.11032600 1.94572500
H 1.79213500 4.28005100 0.64800000
C 2.10784000 2.67498700 -1.89251600
H 2.24727900 3.74597700 -2.08002100
H 2.62415600 2.09047200 -2.65938400
H 1.04235000 2.43541000 -1.95389700
C 6.12652200 -0.96308200 -0.04538300
H 6.42675300 -0.01692900 -0.50616200
H 6.97061600 -1.37143100 0.52261100
H 5.84778900 -1.66136800 -0.83972000
C 5.34540500 0.24441500 2.46314700
H 6.19206900 -0.28601600 2.91362800
H 5.68702100 1.23075300 2.13388000
H 4.57191300 0.38616700 3.22497300
C 4.40646400 -2.38487800 1.76321300
H 3.62278000 -2.34681100 2.52673400
H 4.08107300 -3.04935200 0.95727700
H 5.33011800 -2.76881600 2.21222200
C -4.01307600 -1.55755300 0.00341500
H -3.93810900 -2.25548600 -0.84283500
H -3.80942000 -2.15254900 0.90539500
H -3.02411800 0.23512400 0.70460800

INT6-4a

Ni 2.83664000 -0.12655800 -0.06746200
C 1.33686200 -2.34567000 -0.52406000
C 1.12161100 -1.03321800 -0.32848900
H 0.55895100 -3.09445100 -0.66642900
O 3.10653700 -3.96782100 -0.65262700
O 3.58686100 -1.82993300 -0.16170000
C 2.74299900 -2.81608000 -0.47054200
P 2.12187700 1.94669600 -0.56376100
P 5.03491900 0.24385600 0.75121000
C -0.26937100 -0.45611100 -0.18369500
H -0.42470500 0.36249200 -0.90163200
H -0.33884900 0.01872000 0.80832300
C -1.44763500 -1.43593600 -0.32652700
H -1.41116600 -1.91138300 -1.31608900

H -1.34036600 -2.24343000 0.40937900
 C -2.80281600 -0.74418500 -0.13690900
 H -2.92349500 0.05952000 -0.87553200
 C -5.28963800 -1.06888200 -0.08192300
 C -6.35621900 -0.50064600 0.07725700
 Si -7.96563600 0.35080300 0.31581500
 C -8.08116700 0.96579300 2.10167800
 H -9.03354900 1.48195200 2.27685200
 H -8.01564400 0.13446100 2.81303400
 H -7.27236100 1.66795300 2.33477300
 C -9.36988800 -0.86680200 -0.03647700
 H -10.34691100 -0.38403900 0.09183800
 H -9.31784100 -1.24981600 -1.06209700
 H -9.32946700 -1.72631200 0.64243400
 C -8.06908100 1.81700900 -0.87646100
 H -7.99692900 1.48674600 -1.91911600
 H -9.02062300 2.35089900 -0.75947100
 H -7.25938800 2.53374500 -0.69689400
 C 3.40609600 3.27966600 -0.65800900
 H 4.24118500 2.95020800 -1.28351200
 H 2.98202400 4.19329100 -1.08974000
 H 3.79014100 3.50813200 0.33933100
 C 0.82326500 2.82067700 0.42592100
 H -0.09669300 2.23513600 0.45920500
 H 1.18118900 2.95199500 1.45233300
 H 0.60612300 3.80564000 -0.00255600
 C 1.47817400 2.00912600 -2.29863200
 H 1.14172900 3.01885800 -2.55993900
 H 2.28303000 1.71452000 -2.97966500
 H 0.65489500 1.30508700 -2.43339200
 C 6.31617100 -0.44151400 -0.38570100
 H 6.44636500 0.22059000 -1.24838000
 H 7.28100200 -0.56312700 0.11955300
 H 5.94822400 -1.40919400 -0.73397200
 C 5.84429400 1.80124100 1.36337600
 H 6.81047100 1.57467900 1.82858000
 H 6.01406000 2.50090700 0.54001700
 H 5.20895300 2.29143700 2.10887600
 C 5.16489700 -0.83910200 2.24087800
 H 4.53500800 -0.44439500 3.04498400
 H 4.79724900 -1.82736800 1.95775000
 H 6.19898000 -0.90704700 2.59741000
 C -3.99315700 -1.72049900 -0.26691100
 H -3.96280800 -2.20323200 -1.25429300

H -3.88131100 -2.52968000 0.46890400
 H -2.84598100 -0.26656000 0.85088100
INT1-4b
 Ni 0.07996000 0.68913200 0.00594000
 C 0.24951300 2.63971800 0.19443900
 C -0.98094600 2.25759000 0.16159200
 C -2.41285000 2.67634700 0.21798200
 H -2.99594200 2.10470700 -0.51832900
 H -2.82331400 2.38939200 1.19833100
 P -1.46088000 -0.89361400 -0.19962800
 P 2.11983700 -0.22147900 -0.01192300
 C -2.80572400 -0.89883300 1.08360400
 H -3.28911000 0.08064800 1.11989500
 H -3.56328300 -1.66456700 0.87674800
 H -2.36568800 -1.09203900 2.06759500
 C -2.45668600 -0.77515000 -1.76508900
 H -3.26452000 -1.51644000 -1.79566100
 H -2.88653600 0.22658700 -1.85546200
 H -1.79723700 -0.93263000 -2.62489600
 C -1.07936800 -2.71672200 -0.22227600
 H -0.58977200 -3.00598400 0.71371400
 H -1.99110500 -3.31499000 -0.33885000
 H -0.39964200 -2.94873900 -1.04741000
 C 2.93995700 -0.29155100 1.65442900
 H 2.34233700 -0.91980100 2.32343600
 H 3.95564400 -0.70161500 1.59571100
 H 2.98020000 0.71167300 2.08655500
 C 2.39717000 -1.98000500 -0.56138400
 H 3.45810700 -2.25289200 -0.51026700
 H 1.82853500 -2.66697600 0.07171400
 H 2.05354800 -2.10533900 -1.59380000
 C 3.43896500 0.59413300 -1.03554400
 H 3.54970200 1.63968900 -0.74040100
 H 4.40615100 0.08732900 -0.93109600
 H 3.14008900 0.57416500 -2.08897700
 C -2.66655700 4.17720500 -0.00728900
 H -2.22737200 4.47274200 -0.97003500
 H -2.13776700 4.74945600 0.76427400
 C -4.15748800 4.53331400 0.01378700
 H -4.60117800 4.23909900 0.97411300
 H -4.69157700 3.96701600 -0.76065200
 C -4.40677100 6.04076100 -0.20962700
 H -3.96400800 6.34399600 -1.16903700
 H -3.87677700 6.61536800 0.56316900

C -5.82589100 6.39935000 -0.19452200
 C -7.00188400 6.67509100 -0.17870400
 H -8.03824000 6.92387100 -0.16520900
 Si 1.44538200 4.04312100 0.29026300
 C 0.62479800 5.64958600 0.89438300
 H -0.14301900 6.00218400 0.19702100
 H 0.15164400 5.51630800 1.87476500
 H 1.37351300 6.44646400 0.99427100
 C 2.84764800 3.67239200 1.51678500
 H 3.47731100 2.83385000 1.20132400
 H 3.49906400 4.54842100 1.63036800
 H 2.44275600 3.42990800 2.50704400
 C 2.17988400 4.38833200 -1.42669300
 H 2.92395600 5.19415800 -1.38370200
 H 2.66510000 3.50378200 -1.85329300
 H 1.39345500 4.69809600 -2.12559900

TS1-4b

Ni 1.44864500 1.15071700 -0.15026400
 C 1.21532500 -1.03246400 -0.03946400
 C 0.26260400 -0.16129200 0.29083600
 O 2.85656900 -1.73820700 -1.66472200
 O 3.10978500 0.41444800 -1.02400400
 C 2.56560900 -0.73166400 -1.03288800
 P 0.56070900 3.06103800 0.21822200
 Si 1.26052500 -2.90199900 0.41988500
 C 0.10757000 -3.24193900 1.89610700
 H 0.31218500 -4.25652400 2.26302400
 H 0.28053300 -2.55609200 2.73408300
 H -0.95685900 -3.20839300 1.63758900
 C 0.67117900 -3.96199900 -1.02924500
 H 1.30826700 -3.79437900 -1.90057800
 H 0.70591800 -5.02651200 -0.76293700
 H -0.36352000 -3.72344000 -1.30473500
 C 3.00439600 -3.34935000 0.99517000
 H 3.72812100 -3.23615300 0.18476700
 H 3.31992100 -2.71284900 1.83104200
 H 3.02809400 -4.38922800 1.34600500
 C -1.14159800 -0.21400800 0.79952300
 H -1.23631700 -1.01783600 1.53953700
 H -1.38716400 0.71633700 1.32752100
 C -0.99675300 3.48454500 -0.68167300
 H -1.79654100 2.79794700 -0.38885200
 H -1.31314700 4.51118800 -0.46494900

H -0.83514900 3.37941500 -1.75866500
 C -2.16905300 -0.44326500 -0.32973000
 H -2.04386500 0.33276300 -1.09737300
 H -1.94389800 -1.39752000 -0.82333200
 C 0.14343400 3.46367500 1.97349100
 H 1.04502400 3.38184300 2.58812800
 H -0.26248700 4.47759400 2.06520100
 H -0.59154400 2.74951200 2.35656300
 C 1.69400500 4.44335200 -0.25554900
 H 2.63322900 4.35213500 0.29875300
 H 1.92538500 4.37447100 -1.32282000
 H 1.24529200 5.42108800 -0.04488800
 C -3.61463200 -0.44389900 0.17996600
 H -3.74295700 -1.21914600 0.94616900
 H -3.84280100 0.51303600 0.66812700
 C -4.63698900 -0.68374200 -0.95174900
 H -4.50699500 0.08216300 -1.72970500
 H -4.42377100 -1.64646900 -1.43720100
 C -6.02319200 -0.67035600 -0.48268400
 C -7.16015400 -0.65396900 -0.07567900
 H -8.16634300 -0.64428000 0.27641600

TS4-4b

Ni 0.74582500 0.59823900 -0.05928400
 C 0.45395900 -1.46252500 -0.57038700
 C -0.52482000 -0.59400600 -0.71052500
 O 3.00691600 -1.68463500 -0.48663200
 O 2.18142400 -0.18434600 -2.00533800
 C 2.18640100 -1.00318300 -1.08892400
 P 0.10114100 2.48829700 -0.99284400
 P 2.40962200 1.06766600 1.45664500
 C -1.99727300 -0.57127700 -0.95994300
 H -2.33104200 -1.53351700 -1.36868400
 H -2.22123500 0.18255900 -1.72849500
 C -2.81174300 -0.24044000 0.30733800
 H -2.63125800 -1.02181200 1.05739600
 H -2.43119300 0.69315900 0.74237900
 C -4.31513300 -0.12148600 0.03407900
 H -4.69299000 -1.05271800 -0.40655800
 C -6.55711900 0.32851000 1.06946500
 C 1.31938100 3.88568600 -0.95212300
 H 2.28210100 3.53326900 -1.33502900
 H 0.97921700 4.72487700 -1.56992600
 H 1.46227400 4.23982200 0.07324000

C -1.46302400 3.36510000 -0.51966300
 H -2.31659800 2.68971100 -0.62893300
 H -1.41097700 3.67881400 0.52800400
 H -1.62913000 4.24872500 -1.14698000
 C -0.09679000 2.25782900 -2.81611200
 H -0.20422000 3.21619100 -3.33732900
 H 0.78024200 1.71961700 -3.18565500
 H -0.97596600 1.63996000 -3.02050500
 C 4.09538700 1.43734500 0.79114100
 H 4.06764600 2.33560400 0.16661300
 H 4.82423300 1.58286500 1.59707700
 H 4.40295700 0.59320700 0.16724800
 C 2.13218600 2.45483500 2.65756700
 H 2.95005600 2.52367400 3.38400300
 H 2.05334100 3.40952700 2.12860700
 H 1.19445600 2.28704100 3.19764400
 C 2.76244700 -0.33871400 2.60107400
 H 1.86059100 -0.59431900 3.16631400
 H 3.04734100 -1.19958900 1.99166400
 H 3.56934100 -0.09422700 3.30201400
 C -5.12071500 0.19084000 1.31371700
 H -4.94966300 -0.60361900 2.05379600
 H -4.73716400 1.11553300 1.76840100
 H -4.50256100 0.66850300 -0.70554800
 C -7.73900400 0.44001300 0.84701600
 H -8.78334400 0.53658000 0.65615700
 Si 0.42585000 -3.32164700 -0.20348800
 C 1.22669200 -3.69525100 1.46843800
 H 1.14478500 -4.76618000 1.69537400
 H 2.28593900 -3.42637000 1.45077600
 H 0.74164800 -3.14393600 2.28269600
 C 1.30856700 -4.25727500 -1.58981700
 H 0.82922400 -4.08018300 -2.56014700
 H 2.35353300 -3.94266800 -1.66265300
 H 1.28424700 -5.33801000 -1.39940900
 C -1.37213400 -3.94113700 -0.13477300
 H -1.96308500 -3.42994600 0.63451600
 H -1.89072000 -3.82455500 -1.09364800
 H -1.37875700 -5.01199400 0.10770400

INT8-4cd

C 0.56578800 -2.56841700 0.59469700
 C -0.70154900 -2.65914900 0.57755900
 C 1.48640500 -0.26095500 -0.81195000

C 1.00220300 0.76253400 -0.26239300
 Si 1.07548000 2.50331900 0.34679200
 H -1.56721000 -3.28003000 0.75212100
 Ni -0.21434100 -0.87616900 0.04031800
 C 0.43423700 3.70192300 -0.97456700
 H 0.48673100 4.73779500 -0.61553300
 H 1.03808300 3.63460200 -1.88719300
 H -0.60562200 3.49618000 -1.24908200
 C 0.07650400 2.69402800 1.94369400
 H 0.44051000 2.00019800 2.71064400
 H 0.16272600 3.71252000 2.34294800
 H -0.98823300 2.48447800 1.79118700
 C 2.88934400 2.91695100 0.71686500
 H 2.99232900 3.94358700 1.09109100
 H 3.30112200 2.24135100 1.47566000
 H 3.50961500 2.82520700 -0.18247900
 P -2.33862300 -0.11214600 -0.08098000
 C -2.84471500 1.55873000 -0.72306300
 H -2.43097800 1.70425000 -1.72631200
 H -3.93566500 1.65984000 -0.77131400
 H -2.44894500 2.34815100 -0.07759000
 C -3.29552900 -0.16645600 1.50860300
 H -4.35627100 0.06876100 1.35990500
 H -3.20499800 -1.16388700 1.94964000
 H -2.86825800 0.55085500 2.21697700
 C -3.38660800 -1.18841100 -1.17215600
 H -3.30660800 -2.22979600 -0.84816300
 H -4.44003100 -0.88419100 -1.15563300
 H -3.01647100 -1.12987000 -2.20100500
 C 1.90590900 -3.14829900 0.86641000
 C 2.46457900 -1.00648300 -1.63833300
 C 2.84581100 -3.25367000 -0.35107200
 C 3.43247000 -1.93300100 -0.86911700
 H 4.25213400 -2.17636600 -1.55829100
 H 3.88307500 -1.37431200 -0.03771600
 H 2.40785700 -2.54712200 1.63855000
 H 1.77462500 -4.15414200 1.29224400
 H 1.93111600 -1.60119000 -2.39172900
 H 3.06068000 -0.26531400 -2.19066900
 H 2.32636500 -3.77300900 -1.16810900
 H 3.68460100 -3.89955700 -0.05840900

TS7-4cd

C 0.56234500 -2.03521400 0.15531300

C -0.73953000 -2.06388700 -0.12477900
 C 1.40253400 -0.69095800 -0.03620500
 C 0.96713800 0.56191300 0.22525000
 Si 1.67831100 2.25917400 0.08634300
 H -1.40706300 -2.92059600 -0.10902300
 Ni -0.83624100 -0.22201500 -0.01719600
 C 0.70624900 3.20575600 -1.24870000
 H 1.04119100 4.24859800 -1.31906000
 H 0.83650300 2.74684200 -2.23678500
 H -0.36680000 3.21008100 -1.02358300
 C 1.41213600 3.12355200 1.75825100
 H 1.95146900 2.60491400 2.56061000
 H 1.76793300 4.16171000 1.73449100
 H 0.35012800 3.13300800 2.02955300
 C 3.53229100 2.45546800 -0.33615000
 H 3.81987000 3.51472800 -0.29595800
 H 4.17492600 1.91741100 0.37182700
 H 3.76987200 2.09282200 -1.34374100
 P -2.95332000 0.00033600 -0.03869300
 C -3.54203100 1.72220200 0.28756500
 H -3.13319900 2.39665600 -0.47084400
 H -4.63677000 1.78378700 0.27429100
 H -3.17171400 2.04912600 1.26373900
 C -3.88170300 -0.98872700 1.21548700
 H -4.96062000 -0.80913400 1.14775400
 H -3.68432700 -2.05379200 1.06364500
 H -3.53552700 -0.71938700 2.21787500
 C -3.79798500 -0.43179100 -1.62479100
 H -3.60084400 -1.48037800 -1.86608300
 H -4.88044600 -0.27036300 -1.56309000
 H -3.38959600 0.18298300 -2.43256400
 C 1.35163500 -3.21845000 0.69353100
 C 2.72513900 -1.03178700 -0.73870200
 C 2.66482600 -3.46744900 -0.06218100
 C 3.50756500 -2.19019300 -0.09988700
 H 4.43599300 -2.36061800 -0.66121900
 H 3.80162100 -1.91315800 0.92270700
 H 1.59367700 -3.00298500 1.74647200
 H 0.72003700 -4.11448100 0.68863200
 H 2.49891200 -1.30753000 -1.78190600
 H 3.34312900 -0.13259300 -0.77616500
 H 2.44000400 -3.78999900 -1.08886200
 H 3.21620500 -4.28729800 0.41636000

INT9-4cd

C 1.15559600 -1.84622300 0.03016600
 C -0.18529400 -1.70770700 0.00646100
 C 1.87137100 -0.54111500 0.00822800
 C 1.03534900 0.51980000 0.04325600
 Si 1.21870600 2.36095700 -0.00266900
 H -0.85526800 -2.57541900 0.03074100
 Ni -0.82794900 0.07564400 0.03945800
 C 1.76007500 3.02240800 -1.70161000
 H 1.73932500 4.11965900 -1.73299700
 H 2.78023900 2.70087600 -1.94395900
 H 1.10199000 2.65031800 -2.49614000
 C -0.56690200 2.97557200 0.32334000
 H -0.86865200 2.79239400 1.36294600
 H -0.68463800 4.04963200 0.13079400
 H -1.29872500 2.47077600 -0.33322700
 C 2.34385100 3.10594200 1.33680600
 H 2.29733700 4.20288600 1.32929100
 H 2.04569200 2.76354000 2.33482600
 H 3.39162700 2.81823000 1.18822900
 P -3.07974600 -0.42555000 -0.00753100
 C -4.38096300 0.89555000 -0.03540000
 H -4.24597000 1.52806100 -0.91894700
 H -5.39061400 0.46981400 -0.05672700
 H -4.28263800 1.52959000 0.85174500
 C -3.62414300 -1.47123500 1.41972600
 H -4.66055300 -1.80976600 1.30700700
 H -2.96686400 -2.34223100 1.50189100
 H -3.53476100 -0.89649700 2.34716400
 C -3.55245200 -1.46300400 -1.46537700
 H -2.88673600 -2.32933600 -1.52276500
 H -4.59134800 -1.80697000 -1.40359200
 H -3.42235900 -0.88120200 -2.38350400
 C 1.91482400 -3.15459700 0.15195300
 C 3.38247000 -0.51237000 -0.14234300
 C 3.36589400 -3.03561700 -0.34547200
 C 4.05763600 -1.82431300 0.29627400
 H 5.12147400 -1.80121500 0.02753800
 H 4.01031100 -1.92194200 1.39102200
 H 1.94867600 -3.44997900 1.21340200
 H 1.38306600 -3.95998000 -0.37145800
 H 3.62282700 -0.35105900 -1.20617400
 H 3.80622400 0.34410200 0.39740900
 H 3.37934900 -2.92271900 -1.43959000

H 3.91397500 -3.95828600 -0.11544900

TS8-4c

C 1.35906400 -1.51893600 -0.50709200
C -0.03770500 -1.50311900 -0.41319200
C 1.98546000 -0.25358100 -0.20196500
C 1.05930800 0.74605500 -0.05932800
Si 1.23805100 2.59610300 0.20533900
H -0.59582500 -2.23165200 -1.01105200
Ni -0.74804200 0.24694100 -0.15345500
C 2.18380100 3.44490000 -1.20424700
H 2.19447500 4.53433600 -1.07211200
H 3.22471500 3.10434300 -1.24956600
H 1.72186300 3.23026500 -2.17527300
C -0.54708800 3.26782000 0.22889700
H -1.14946500 2.78991400 1.01550700
H -0.56544500 4.34662000 0.42974700
H -1.05283800 3.11036300 -0.73352400
C 2.04604200 2.99991700 1.87469200
H 2.02565700 4.08062800 2.06575400
H 1.51887900 2.50352100 2.69764900
H 3.09258100 2.67607000 1.90714200
P -3.06180200 -0.06179000 -0.37998000
C -4.00833200 0.33277700 1.15859600
H -3.88529200 1.39170300 1.40983300
H -5.07705300 0.11674000 1.04701500
H -3.59317100 -0.26593900 1.97374700
C -3.60541800 -1.78810000 -0.74633300
H -4.69791600 -1.86023800 -0.78766000
H -3.19016400 -2.11538600 -1.70470700
H -3.22906700 -2.44733800 0.04020700
C -3.96261400 0.91750300 -1.67124300
H -3.56063000 0.67823000 -2.66113500
H -5.03826700 0.70708200 -1.66439400
H -3.81203500 1.98798900 -1.49595900
C 2.14985500 -2.76068000 -0.80876600
C 3.49963700 -0.13239000 -0.14139200
C 3.65027800 -2.49755100 -1.02322600
C 4.18688400 -1.50054400 0.01238500
H 5.27254700 -1.38464400 -0.09240400
H 4.00540000 -1.89414900 1.02254100
H 1.99395100 -3.42214200 0.05874700
H 1.70864700 -3.29477700 -1.66080100
H 3.86373700 0.34270600 -1.06580700

H 3.79174100 0.53540500 0.67882500

H 3.81876300 -2.09433800 -2.03227700

H 4.19906500 -3.44522600 -0.96889200

C -0.50482300 -2.27847500 1.31516600

O 0.03602100 -3.34665200 1.46232400

O -1.30745700 -1.51167400 1.82177700

TS8-4d

C 1.02961000 -1.99032900 0.00945300
C -0.30341500 -1.83053200 -0.14929500
C 1.77438000 -0.71611200 -0.00067000
C 1.03519900 0.42932500 0.13314800
Si 1.46039500 2.16620800 -0.48714700
H -0.95581800 -2.70705100 -0.23820900
Ni -0.90363700 -0.06007500 0.10357100
C 2.89172600 2.20694300 -1.74233000
H 2.94949200 3.21138400 -2.18214700
H 3.86646500 1.98999700 -1.29320600
H 2.73597400 1.49877800 -2.56490000
C -0.05990500 2.83474800 -1.41720900
H -0.92431800 2.94792300 -0.75518200
H 0.16497200 3.81860700 -1.84904100
H -0.34358600 2.16956100 -2.24299200
C 1.89504600 3.36148100 0.92247300
H 2.16354700 4.34636000 0.51902700
H 1.05481600 3.50222400 1.61103600
H 2.74687600 2.99640200 1.50831300
P -3.09757100 -0.46617200 -0.31474900
C -3.86940400 -1.71127700 0.81114000
H -3.81289100 -1.34948400 1.84257000
H -4.91825100 -1.89552200 0.55264700
H -3.31404000 -2.65224500 0.75296000
C -3.49202600 -1.12109100 -1.99613200
H -4.56123400 -1.33188300 -2.11062600
H -3.18957100 -0.38951000 -2.75202900
H -2.92244700 -2.03875500 -2.17039700
C -4.22121100 0.99215600 -0.15321100
H -3.93649900 1.75458300 -0.88537200
H -5.27127100 0.72071300 -0.31009700
H -4.10296600 1.42582300 0.84451000
C 1.74331000 -3.31953000 0.16382700
C 3.25945000 -0.76408500 -0.32767800
C 3.16612100 -3.29337000 -0.41778600
C 3.93149100 -2.07617500 0.11400600

H 4.97012300 -2.08673900 -0.23942700
H 3.97070100 -2.12275000 1.21173200
H 1.82098700 -3.55526200 1.23727100
H 1.14636900 -4.12308700 -0.28587200
H 3.38374400 -0.66798400 -1.41734100
H 3.77119100 0.09537000 0.11685700
H 3.12074300 -3.24403100 -1.51555500
H 3.69200300 -4.22188800 -0.16252100
C -0.08819300 0.88473000 1.89120400
O 0.53629900 0.60331200 2.86152000
O -1.05358500 1.51355400 1.43518500

INT5-4b

C 0.47614600 -0.24639100 1.96469000
C -0.59495700 -1.04651600 1.88562900
C 1.60774200 -0.26076100 0.98665800
C 1.43380900 -0.22176100 -0.35782800
Si 2.81986200 -0.22272500 -1.67758900
H -1.41215200 -0.96455200 2.60802900
Ni -0.94908500 -2.20608000 0.47914800
C 2.06802200 -0.49999400 -3.39043400
H 2.86219800 -0.56054100 -4.14551600
H 1.49944500 -1.43743700 -3.43305100
H 1.38603500 0.31081900 -3.65816600
C 3.75929100 1.42443200 -1.66241700
H 4.24515300 1.62343900 -0.70001200
H 4.53625600 1.43910500 -2.43746500
H 3.06618100 2.24895600 -1.86375700
C 4.02644200 -1.67067200 -1.39554300
H 4.73499800 -1.72346400 -2.23246900
H 4.61267500 -1.59849300 -0.47390600
H 3.48363500 -2.62417400 -1.36942600
P -1.11241700 -3.99267800 1.79032400
C -2.25557600 -3.85828300 3.23377500
H -3.27631700 -3.68130200 2.88078100
H -2.23863500 -4.76995800 3.84077600
H -1.95774900 -3.00959500 3.85621300
C 0.49139900 -4.47186700 2.56501000
H 0.37417700 -5.32412100 3.24336300
H 1.21311500 -4.73038800 1.78401800
H 0.88438800 -3.61357700 3.11733200
C -1.67133600 -5.55066400 0.96209100
H -1.00114000 -5.78765600 0.12961100
H -1.68101100 -6.39475500 1.66048400

H -2.67942200 -5.41279100 0.55817300
C 0.61762300 0.74326200 3.11908400
C 2.97561700 -0.27748500 1.65714200
C 1.99258600 0.65493000 3.79934900
C 3.11078400 0.78834700 2.76141200
H 4.09452700 0.69848100 3.23963000
H 3.06833000 1.78745600 2.30561600
H 0.49330600 1.75985100 2.71501000
H -0.18816800 0.59168500 3.84678800
H 3.13227500 -1.26771200 2.11614200
H 3.77214900 -0.14386000 0.92282800
H 2.08470100 -0.31203200 4.31549500
H 2.08142800 1.43493400 4.56648400
C 0.06736300 -0.01889900 -0.97333100
O -0.10969700 0.94524200 -1.71007700
O -0.87041500 -0.92560400 -0.76561100

TS3-4b

Ni -1.49347500 -0.66500600 -0.85911400
O -0.14057300 -0.53083500 -2.11316400
O 1.84207100 -1.54267900 -2.24071100
C 1.10248800 -0.80648500 -1.60332800
C 1.51134800 -0.18054600 -0.31977600
C 1.09402000 1.10174600 -0.01541000
C 1.73068200 1.91082500 1.10839200
P -3.11628300 -0.58515300 0.59363400
C 0.05067000 1.76182600 -0.78243900
C -0.87093800 1.00990200 -1.45011700
C -4.62992200 0.32336600 0.03974700
H -4.35757100 1.34428100 -0.24536400
H -5.05421200 -0.17144200 -0.83940900
H -5.38848700 0.36255000 0.82985100
C -2.70171000 0.27176700 2.17968400
H -3.56771800 0.32622500 2.84943600
H -1.89226600 -0.26500100 2.68382700
H -2.34991200 1.28480800 1.96226500
C -3.81715000 -2.19444900 1.18549800
H -3.02454400 -2.79434700 1.64370400
H -4.61654100 -2.04043100 1.91929900
H -4.21732200 -2.75672400 0.33585700
C 0.03676800 3.27979200 -0.92842900
H 0.71169100 3.56673600 -1.75161800
H -0.96293500 3.62404600 -1.21844400
C 0.50396400 3.99302000 0.34570300

H -0.24331200 3.86212600 1.14208600
 C 1.84536400 3.41348400 0.80125800
 H 2.21436000 3.93691500 1.69197400
 H 2.59317700 3.57018700 0.01084800
 H 1.11486000 1.79068900 2.01375000
 H 0.58901200 5.07131300 0.16139100
 H 2.71810900 1.51595300 1.35325100
 H -1.48892400 1.41194000 -2.25299400
 Si 2.80162800 -1.25098700 0.59826800
 C 2.84183200 -0.89440200 2.47226700
 H 3.31642500 -1.74598100 2.97702100
 H 3.41070600 0.00014200 2.74601100
 H 1.83370200 -0.79031700 2.89218300
 C 4.53486700 -0.99188800 -0.11999800
 H 4.87235700 0.04566600 -0.00672400
 H 5.27023400 -1.63795100 0.37631400
 H 4.53094000 -1.23141600 -1.18816300
 C 2.29212300 -3.07112000 0.45549700
 H 2.22625200 -3.38648900 -0.58859800
 H 3.02447600 -3.70894800 0.96688300
 H 1.31776600 -3.24618600 0.92998800

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O -0.44585600 2.61537300 -0.02741300
 O 1.75306700 2.30929600 0.05728700
 C 0.66829400 1.76059500 0.02963400
 C 0.41606400 0.32164300 0.03192300
 C -0.88839100 -0.13321400 0.03928500
 C -1.21912000 -1.61830300 -0.02064700
 C -1.99379900 0.80826800 0.03660700
 C -1.69487900 2.12686500 -0.01510600
 C -3.44827300 0.37457100 0.11181100
 H -3.78741500 0.42540300 1.15753600
 H -4.07476900 1.08041300 -0.44716400
 C -3.65815600 -1.05849400 -0.38615500
 H -3.49816000 -1.11014100 -1.47233800
 C -2.66985300 -1.98303800 0.32783400
 H -2.84688400 -3.03159700 0.06123100
 H -2.82512500 -1.90515300 1.41339200
 H -1.01095000 -1.95918800 -1.04547600
 H -4.69240100 -1.37009100 -0.19909000
 H -0.53418200 -2.17352300 0.62247600
 Si 2.07913500 -0.64426400 -0.01337700
 C 3.06461100 -0.23158000 1.54850800

H 2.54222400 -0.57161900 2.45137300
 H 4.04253500 -0.72922400 1.52687000
 H 3.22758200 0.84617500 1.63108400
 C 1.91006100 -2.53771800 -0.07419800
 H 2.92259900 -2.94835600 -0.18567200
 H 1.49205800 -2.96943500 0.84221100
 H 1.32055800 -2.89968900 -0.92327900
 C 3.00967700 -0.13910800 -1.58268700
 H 2.46100200 -0.43612700 -2.48514700
 H 3.16490200 0.94239400 -1.61467200
 H 3.99053900 -0.63015800 -1.61776000
 H -2.43712000 2.91933900 -0.04815700

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O -0.67686800 1.53879800 -0.03795600
 O 0.00903300 3.67268000 -0.00130800
 C 0.33879300 2.50739400 -0.00934000
 C 1.67246100 1.95990600 -0.00283100
 C 1.91702600 0.61822400 -0.01762400
 H 2.48091700 2.68431900 0.00037000
 C 3.35187100 0.12419400 -0.08946200
 C 0.80991300 -0.32037800 -0.01223800
 C -0.46188300 0.18350500 -0.02498400
 Si -2.21396300 -0.60272800 0.00878700
 C -2.23906500 -2.49474300 -0.04391400
 H -3.28363100 -2.82661000 0.02026500
 H -1.82998200 -2.89808800 -0.97702900
 H -1.70018900 -2.95331900 0.79200100
 C -3.02319200 -0.00957700 1.61116700
 H -4.07304700 -0.32483900 1.65578900
 H -2.51635600 -0.41547800 2.49473600
 H -2.99488400 1.08299800 1.67999400
 C -3.13037600 0.07945400 -1.49614900
 H -4.17978100 -0.24010300 -1.49027100
 H -3.10873800 1.17412500 -1.50109600
 H -2.68141300 -0.27011900 -2.43345400
 C 1.07580700 -1.81843400 0.07381000
 H 0.92415000 -2.14923500 1.11243100
 H 0.34872900 -2.36779200 -0.52903100
 C 2.49822100 -2.21541400 -0.34631400
 H 2.61109500 -2.11149800 -1.43499200
 C 3.53123300 -1.33095300 0.35595100
 H 4.55165800 -1.66156100 0.12955900
 H 3.40509200 -1.41159200 1.44483600

H 3.68037900 0.21078800 -1.13634300
H 2.66271100 -3.27351700 -0.11094600
H 3.99659000 0.79881900 0.48583700

INT1-4e

C -1.65251400 -1.18169400 -0.19025900
H -1.53032300 -1.63994300 -1.18123700
H -1.53410300 -1.99303200 0.54096400
C -3.05334600 -0.57202300 -0.06831400
H -3.17882600 0.23390800 -0.80332400
H -3.17940400 -0.11204100 0.92068300
C -4.17161700 -1.61738100 -0.27845100
H -4.05534100 -2.42577300 0.45782800
C -5.51811900 -1.05563400 -0.17415000
C -6.63147700 -0.56732700 -0.08457800
Si -8.31081900 0.16100600 0.04525900
C -9.17516400 0.02710700 -1.63295500
H -9.26168900 -1.01781200 -1.95254400
H -10.18753400 0.44825800 -1.58816300
H -8.62170200 0.56779900 -2.40936100
C -9.29860800 -0.78443800 1.35358400
H -9.39418000 -1.84431400 1.09096800
H -8.81449300 -0.72706200 2.33532800
H -10.31035700 -0.37159100 1.45425400
C -8.15974200 1.97956000 0.54679600
H -7.65099600 2.08482200 1.51197800
H -7.58879700 2.55039000 -0.19458700
H -9.14966200 2.44433500 0.63755600
C -0.52567700 -0.15506600 0.02355500
H -0.63986900 0.66574600 -0.70078600
C 0.84327600 -0.73442100 -0.09291300
C 1.55080700 -1.79048900 -0.30124800
H 1.49233600 -2.84775600 -0.53159900
C 4.86449000 -2.07480400 0.55102300
C 6.14442900 -2.59608600 0.70015300
C 7.22550800 -1.85493900 0.22555600
C 6.96913100 -0.62498800 -0.37413900
C 5.65551200 -0.15622200 -0.48956100
N 4.60667100 -0.88028100 -0.02505900
H 8.24266700 -2.22571000 0.31596000
H 3.98987900 -2.61720300 0.89062000
H 6.28046000 -3.56355200 1.17290700
H 7.78277400 -0.01867200 -0.76092200
Ni 2.67942600 -0.30649800 -0.01285900

C 5.38396200 1.18614800 -1.13287000
H 6.32452100 1.56459200 -1.54962600
H 4.69588400 1.04447800 -1.97702100
C 4.79688200 2.23634500 -0.15958200
H 4.88979600 3.23964900 -0.59383200
H 5.37173300 2.23532500 0.77485900
P 3.00822500 1.85163800 0.23381200
C 2.11757100 2.97733800 -0.94455600
H 2.31849900 2.66154400 -1.97339000
H 1.03934100 2.88940200 -0.77777400
H 2.41416500 4.02669200 -0.82586400
C 2.76535900 2.76400300 1.83276400
H 3.07817500 3.81321400 1.76874300
H 1.70674200 2.72736600 2.10949200
H 3.33507600 2.26794300 2.62514000
H -0.64311500 0.31154700 1.01324100
H -4.04815700 -2.08722500 -1.26495300

TS4-4e

C 1.84721700 -1.04333400 0.28069600
H 1.75812600 -1.53443900 1.25869900
H 1.68419700 -1.82479900 -0.47399300
C 3.25196500 -0.45312600 0.11605600
H 3.42039000 0.33340400 0.86334200
H 3.34631700 0.02660700 -0.86695700
C 4.35820800 -1.52202100 0.25842300
H 4.18702800 -2.32214800 -0.47623300
C 5.70698700 -0.98403400 0.08333800
C 6.82250400 -0.51703000 -0.06862000
Si 8.50829400 0.17391100 -0.29968800
C 8.58640000 1.06496900 -1.96743100
H 7.86050600 1.88490600 -2.01498200
H 9.58361600 1.49036000 -2.13691200
H 8.36997100 0.37974800 -2.79513100
C 8.87325900 1.39594600 1.09807300
H 8.15055800 2.22005300 1.10412300
H 8.82772600 0.90570700 2.07733000
H 9.87498000 1.82990200 0.98688000
C 9.76428000 -1.24040600 -0.26683900
H 9.72973500 -1.78136800 0.68578300
H 9.56909500 -1.96300100 -1.06752200
H 10.78503600 -0.86032400 -0.39973300
C 0.73481700 0.01283000 0.15501900
H 0.88839400 0.79057900 0.92087500

C -0.64482800 -0.52734000 0.31600600
 C -1.24955500 -1.66480100 0.58768900
 H -0.90719900 -2.69126800 0.49551300
 C -4.36436600 -1.58882900 -1.49454100
 C -5.57750500 -2.04050200 -2.00069300
 C -6.73592400 -1.34523100 -1.66009700
 C -6.62912600 -0.23583000 -0.82549800
 C -5.37703400 0.16310400 -0.34635700
 N -4.25611900 -0.50992400 -0.69506800
 H -7.70618700 -1.66422000 -2.03027900
 H -3.43494700 -2.10237300 -1.71476700
 H -5.60505800 -2.91975400 -2.63546800
 H -7.51246300 0.32160600 -0.53004700
 Ni -2.39838400 -0.09081000 -0.04362300
 C -5.24713600 1.34349700 0.59009200
 H -6.25146100 1.72314100 0.80765600
 H -4.82452300 0.98090600 1.53631800
 C -4.38285900 2.49855100 0.02975700
 H -4.55726700 3.41043200 0.61396400
 H -4.67410900 2.71668400 -1.00535000
 P -2.56873000 2.07205300 0.05838100
 C -2.00534900 2.73269100 1.68803700
 H -2.44251400 2.12068100 2.48207500
 H -0.91755200 2.63339500 1.75713000
 H -2.28002100 3.78478700 1.82761700
 C -1.83436600 3.26810900 -1.14777000
 H -2.10964000 4.30325300 -0.91417600
 H -0.74346800 3.17966100 -1.12694600
 H -2.17403700 3.02637200 -2.15975200
 H 0.81766500 0.53464600 -0.80946400
 H 4.27872200 -1.99723800 1.24668400
 C -2.76814500 -1.79657100 1.68697000
 O -3.18195800 -2.93262300 1.60731500
 O -2.99377400 -0.75027000 2.29602400

INT6-4e

C -1.71230700 -1.54672100 -0.23315700
 H -1.69819600 -2.01844500 -1.22487700
 H -1.63915700 -2.36193700 0.49844400
 C -3.03597200 -0.79744200 -0.04034200
 H -3.12201300 0.01137100 -0.77828100
 H -3.05920100 -0.31937200 0.94798000
 C -4.26683900 -1.72183200 -0.17329800
 H -4.20133300 -2.52471100 0.57479600

C -5.53597900 -1.01126300 -0.01833100
 C -6.57942400 -0.39452800 0.11112500
 Si -8.15543200 0.52843800 0.29968200
 C -8.25706200 1.22925200 2.05460200
 H -7.42166200 1.90805100 2.26171400
 H -9.18857500 1.79147400 2.19736200
 H -8.23054000 0.42993400 2.80411500
 C -8.19608800 1.94310900 -0.95710500
 H -7.36044200 2.63560100 -0.80318900
 H -8.13123600 1.56522600 -1.98394300
 H -9.12711100 2.51723500 -0.86952300
 C -9.60405200 -0.64871700 -0.00756700
 H -9.56238600 -1.07670600 -1.01574100
 H -9.59879900 -1.47949000 0.70732600
 H -10.56267000 -0.12461100 0.09475700
 C -0.49086100 -0.62198700 -0.08971100
 H -0.62247600 0.21692100 -0.78913000
 C 0.86937500 -1.25740600 -0.27902700
 C 1.02693400 -2.57529400 -0.49207000
 H 0.21830200 -3.29620300 -0.60555500
 C 5.10280200 -0.72367100 1.25090800
 C 6.39589300 -0.57698200 1.74335000
 C 7.15212000 0.51277900 1.32212000
 C 6.57838900 1.41339800 0.42806100
 C 5.26900300 1.21310900 -0.01866100
 N 4.53873400 0.15397300 0.39508400
 H 8.16908500 0.65856500 1.67544400
 H 4.49347900 -1.58312600 1.49872600
 H 6.79384700 -1.31589800 2.43078400
 H 7.13742900 2.27151500 0.06807200
 Ni 2.60134800 -0.40444300 -0.09991700
 C 4.63058600 2.19968400 -0.96824600
 H 5.36737400 2.96908600 -1.22186500
 H 4.37471700 1.69054100 -1.90744500
 C 3.37775300 2.86863600 -0.36781100
 H 3.11489700 3.76786200 -0.93845600
 H 3.58294600 3.18554900 0.66179300
 P 1.91975500 1.71450800 -0.35925800
 C 1.21912800 2.03369400 -2.04392900
 H 1.96406500 1.76100600 -2.79821700
 H 0.33507300 1.41583100 -2.21577900
 H 0.95196000 3.08907100 -2.17005800
 C 0.74938500 2.59773500 0.76828900
 H 0.65198400 3.65194300 0.48543900

H -0.23583800 2.12798300 0.73272200
H 1.12031300 2.53653500 1.79631400
H -0.52207400 -0.16591500 0.91306000
H -4.24392400 -2.21928200 -1.15357500
C 2.42299300 -3.08246600 -0.50440400
O 2.74038300 -4.24906300 -0.68524000
O 3.30065900 -2.11385000 -0.25933100

INT4-4e

C 0.97572800 -3.34424700 -1.68734900
H 1.22961000 -4.38205500 -1.93981700
H -0.11999500 -3.28346100 -1.72470600
C 1.58537000 -2.46482700 -2.79192100
H 2.67802000 -2.57213200 -2.78226700
H 1.24274800 -2.83772300 -3.76602700
C 1.24444700 -0.95676700 -2.73498700
H 0.15869300 -0.81363700 -2.78931100
C 1.78460600 -0.33586200 -1.51626200
C 2.48643800 0.04530000 -0.56940700
Si 3.86548300 0.39873900 0.64008000
C 4.81832600 1.90486900 0.00339800
H 4.19081400 2.80210700 -0.04669700
H 5.66271300 2.12746300 0.66771000
H 5.22138900 1.72466900 -0.99980200
C 3.15307200 0.71247200 2.35663500
H 2.51663200 1.60330100 2.39518100
H 2.54462400 -0.13597500 2.68793200
H 3.96620900 0.85255500 3.08024700
C 4.99367500 -1.11660800 0.66061300
H 4.46610100 -1.99996800 1.03678000
H 5.37369700 -1.34949000 -0.34054000
H 5.85692200 -0.93993700 1.31451600
C 1.44622300 -3.08103600 -0.22793300
H 1.37979300 -4.03399600 0.31799000
C 0.62117900 -2.06492300 0.52507500
C -0.24480200 -2.41717500 1.49000400
H -0.38630900 -3.43536000 1.85656300
Ni 0.49868800 -0.18778000 0.16504000
H 2.50880400 -2.80617100 -0.24406900
H 1.67270800 -0.45018800 -3.61092000
C -1.11741600 -1.32958800 2.00261800
O -2.03332500 -1.47901700 2.80247100
O -0.83460000 -0.15769700 1.43962800
P -4.80816500 -0.32921000 -0.58690100

C -5.87506600 -0.23896000 0.94324700
C -3.46466600 0.86704900 -0.04330100
C -3.97697800 -1.96879100 -0.25889100
H -6.35657700 0.74335600 1.00483600
H -5.29454300 -0.41065400 1.85730000
H -6.66667400 -0.99378800 0.88034400
H -3.95325000 1.84639100 0.05256700
H -3.06178700 0.59081600 0.93632200
H -3.55884800 -2.02880600 0.75191400
H -3.17639300 -2.13816900 -0.98748100
H -4.71317100 -2.76999500 -0.39092600
C -2.30307600 0.96555600 -1.05563900
H -2.70854600 1.14561600 -2.06147800
H -1.76057400 0.01669400 -1.08311600
C -1.33636700 2.08125100 -0.72690100
C -1.74284500 3.41417500 -0.89613200
C 0.73923200 2.80981900 0.00976800
C -0.88039300 4.45742400 -0.58729300
H -2.74186500 3.61383800 -1.27152900
C 0.39651500 4.14901400 -0.11706100
H 1.72507000 2.52621300 0.35836200
H -1.19365900 5.48999900 -0.71416800
H 1.11297700 4.92176700 0.14159700
N -0.09267100 1.79360200 -0.28178800

INT4-4e'

C 1.93510900 3.50098400 1.41721000
H 2.47139100 4.44736900 1.56661400
H 0.86589600 3.74087100 1.48682500
C 2.33614300 2.57801000 2.57774200
H 3.42201700 2.41665900 2.56198500
H 2.10853600 3.08514800 3.52445600
C 1.64081100 1.19729000 2.61765000
H 0.55148800 1.32188200 2.63343800
C 2.04331500 0.35428100 1.48191700
C 2.64202800 -0.29076500 0.61129600
Si 3.89701200 -1.13722000 -0.47745000
C 4.09796000 -2.92172100 0.11546100
H 3.16542800 -3.49166400 0.03557500
H 4.85397600 -3.43997100 -0.48761000
H 4.42411700 -2.95892200 1.16131200
C 3.32749100 -1.06795000 -2.27223700
H 2.38091100 -1.59731200 -2.42478700
H 3.17835800 -0.03230300 -2.59665500

H	4.07910800	-1.52477700	-2.92841800	O	-1.06675700	0.58083700	1.90909100
C	5.52140700	-0.19648000	-0.25346200	O	-1.83619600	2.40155900	3.00676800
H	5.42280000	0.84801400	-0.57038400	C	-1.18779300	1.87162300	2.11345500
H	5.84686400	-0.20175800	0.79305100	C	-0.48697000	2.68162000	1.05997500
H	6.31704500	-0.65427000	-0.85447500	C	0.44185500	2.16343800	0.23100700
C	2.23825400	2.99803100	-0.02140500	H	-0.85627800	3.69692300	0.89581000
H	2.35223800	3.88442000	-0.66336300	C	2.99546500	2.12246500	0.99971300
C	1.15411300	2.13102200	-0.61559500	H	3.90796500	1.59921300	1.31304200
C	0.25614600	2.61986500	-1.48735400	H	2.56893600	2.60291800	1.88666800
H	0.25522600	3.64063100	-1.87365800	C	2.04593300	1.09140100	0.46238300
Ni	0.74986300	0.28084700	-0.21321800	C	2.01747600	-0.03903300	-0.16695900
H	3.20990800	2.48585800	-0.02284600	Si	3.06347000	-1.32524500	-1.00867700
H	1.91233100	0.67726800	3.54703300	C	4.56726500	-0.48019300	-1.79723500
C	-0.84025200	1.70123100	-1.88049900	H	5.19277300	0.01435400	-1.04450400
O	-1.80506700	1.99984700	-2.57153100	H	5.19528600	-1.21271000	-2.32014200
O	-0.68989900	0.48471800	-1.35129300	H	4.26280000	0.27736200	-2.52899100
P	-0.31111600	-1.85065400	0.16829600	C	3.66339500	-2.60800600	0.25114400
C	-0.00267800	-3.17407600	-1.09097400	H	2.82967900	-3.16502800	0.69248300
C	-2.15347200	-1.67269200	0.05073700	H	4.32966700	-3.33354200	-0.23259200
C	-0.04181800	-2.74764100	1.76694500	H	4.22227400	-2.13461700	1.06691800
H	-0.21928800	-2.76887800	-2.08443900	C	2.05009400	-2.18101100	-2.35720100
H	-0.63994500	-4.04860100	-0.91695700	H	2.65445000	-2.92965200	-2.88447000
H	1.04425200	-3.49218900	-1.06879200	H	1.17702100	-2.69188300	-1.93581300
H	-2.34222200	-1.43128600	-0.99924700	H	1.68825200	-1.46142700	-3.10124400
H	-2.63650200	-2.63253000	0.27588500	C	3.33740100	3.17789700	-0.07314900
H	-0.60776400	-3.68510100	1.80653800	H	4.06591200	3.88829100	0.33802100
H	-0.35946900	-2.11300700	2.60068100	C	0.93618400	2.98079900	-0.95365100
H	1.02252500	-2.96721000	1.89812800	H	0.09933800	3.58219400	-1.33160700
C	-2.73523800	-0.54905300	0.93223500	C	2.09691500	3.92562700	-0.57336400
H	-2.13239500	0.35320200	0.78562200	H	2.36331600	4.54639400	-1.43861000
H	-2.69942200	-0.83105800	1.98985500	H	1.73827100	4.60955800	0.20768600
C	-4.17562700	-0.25349700	0.56761500	H	1.24755000	2.31570900	-1.76765800
C	-4.47754900	0.51449700	-0.56909100	H	3.82802500	2.66884500	-0.91306200
C	-6.40392200	-0.54744800	1.04389800	P	-4.20135200	0.29500800	-1.79482300
C	-5.81504500	0.74432900	-0.88190500	C	-5.50571000	0.99407800	-0.65682400
H	-3.68102200	0.91793400	-1.19149700	C	-3.23913400	-0.69660000	-0.52155500
C	-6.80544700	0.20403400	-0.05931800	C	-3.10580500	1.79970900	-1.94840300
H	-7.14527500	-0.98633900	1.71101100	H	-6.18420200	0.19538400	-0.33798100
H	-6.07791200	1.33910400	-1.75285300	H	-6.10022200	1.73788400	-1.19857800
H	-7.86065900	0.36043200	-0.26419900	H	-5.07478400	1.46669500	0.23398500
N	-5.12297100	-0.77920800	1.36136200	H	-2.96772000	-0.07821200	0.34291900
				H	-3.91873400	-1.48084400	-0.16212000
				H	-3.64517400	2.57920200	-2.49818100
				H	-2.20727900	1.55430300	-2.52468700
TS2-4e							
Ni	0.24819000	0.17577100	0.58722300				

H -2.80110500 2.19771900 -0.97350300
 C -1.96810000 -1.35618900 -1.10253500
 H -1.25722400 -0.58545700 -1.42269400
 H -2.22941700 -1.95160000 -1.98618800
 C -1.29859100 -2.24097900 -0.08085800
 C -1.72254700 -3.56238500 0.11507400
 C 0.22052100 -2.46010200 1.67181200
 C -1.15636200 -4.33516100 1.12257700
 H -2.50276500 -3.96499900 -0.52353500
 C -0.16756700 -3.76881300 1.92800300
 H 0.98699600 -1.97255400 2.26408200
 H -1.48323700 -5.35886400 1.28157100
 H 0.29717000 -4.32317600 2.73633400
 N -0.31787000 -1.71742200 0.68584500

TS2-4e'

Ni -0.63878100 0.22198400 -0.14568200
 O 0.92309500 1.04010400 -0.84300700
 O 1.99386600 3.02138800 -0.83852100
 C 1.04176900 2.30968200 -0.53223600
 C -0.09068500 2.79966300 0.30965300
 C -1.17915300 2.04637800 0.55589500
 H 0.04272800 3.75520100 0.82087400
 P 0.56358600 -1.69760600 0.16094100
 C -3.25841100 2.01618900 -1.18840400
 H -3.90743400 1.55242400 -1.94220000
 H -2.60026600 2.71964700 -1.70942800
 C -2.45429900 0.92244000 -0.55651400
 C -2.50517500 -0.31460100 -0.17385100
 Si -3.76956000 -1.67538600 -0.03087300
 C -5.38304000 -1.12399200 -0.86158600
 H -5.23864600 -0.92707100 -1.93057600
 H -6.14870200 -1.90490900 -0.77055800
 H -5.78540900 -0.21282400 -0.40402300
 C -3.19117300 -3.27085500 -0.86989300
 H -2.34608100 -3.73544800 -0.35081800
 H -4.00857000 -4.00282900 -0.88077300
 H -2.89440400 -3.09157100 -1.90988300
 C -4.09137900 -2.00028100 1.80772800
 H -4.82537000 -2.80519500 1.93946600
 H -3.17638700 -2.29160600 2.33598400
 H -4.48712600 -1.10615300 2.30374000
 C 0.07064700 -2.75541800 1.59626800
 H 0.15051700 -2.17072200 2.51847100

H -0.96779400 -3.07981700 1.48970100
 H 0.71661000 -3.63664100 1.68082700
 C 0.63925300 -2.89954500 -1.24123600
 H 0.99979900 -2.38626000 -2.13693800
 H 1.31270300 -3.73322300 -1.01292100
 H -0.35934100 -3.29075100 -1.45010100
 C 2.34966000 -1.33353700 0.53586000
 H 2.34606000 -0.46489900 1.20349400
 H 2.78125200 -2.17692400 1.08970100
 C -4.11922800 2.75886400 -0.14472200
 H -4.74137100 3.50399200 -0.65660600
 C -2.21742900 2.50104500 1.56497400
 H -1.69862600 3.04344700 2.36656800
 C -3.27799700 3.43634100 0.94173700
 H -3.93651600 3.81688600 1.73328000
 H -2.75873800 4.30611800 0.51761100
 H -2.70579900 1.63616100 2.02804700
 H -4.80485700 2.03550500 0.31591300
 C 3.21795800 -1.02422700 -0.70494100
 H 3.38513000 -1.94684900 -1.27154600
 H 2.69445000 -0.30264700 -1.33468800
 C 4.56129800 -0.46043600 -0.29518100
 C 4.79501800 0.92262300 -0.32789500
 C 6.67486400 -0.86982100 0.50753700
 C 6.04054300 1.39750600 0.08051900
 H 4.01368300 1.60262400 -0.66153900
 C 7.00642600 0.48541100 0.50698200
 H 7.40160300 -1.61383700 0.83301500
 H 6.25190700 2.46365300 0.06236800
 H 7.99119100 0.81062500 0.83019900
 N 5.48531700 -1.34494800 0.11979900

INT7-4e

C -4.48967700 -1.79484600 1.50874000
 H -5.12649600 -1.96095300 2.38720800
 H -4.77990400 -2.54268600 0.75768100
 C -4.70732400 -0.38895300 0.93904900
 C -3.79654900 -0.13901100 -0.27585400
 H -3.94917700 0.87607400 -0.65207100
 C -2.31496500 -0.38440000 0.02740600
 C -1.31402600 0.41402200 -0.39833600
 Si -1.42814300 1.73355400 -1.75253300
 C -2.49471100 3.25604000 -1.31929800
 H -2.10906700 3.79691100 -0.44691900

H -2.49091300 3.95708800 -2.16457600
 H -3.54005100 3.00023300 -1.11379300
 C 0.30693300 2.39921000 -2.16324300
 H 0.25107700 3.07245100 -3.02896700
 H 0.74965100 2.96934200 -1.33722300
 H 0.99586900 1.58593500 -2.41946500
 C -2.10191700 0.92692200 -3.33117100
 H -1.50569300 0.03928900 -3.57141600
 H -3.14304600 0.60477000 -3.21628000
 H -2.05590500 1.61488200 -4.18520800
 C -3.01177700 -2.00233900 1.88475000
 H -2.78353900 -1.33640200 2.73323100
 C -2.07757700 -1.67807700 0.73014500
 C -1.17854600 -2.59454000 0.31042000
 H -1.15378900 -3.55912300 0.81559300
 Ni 0.51083900 -0.06820800 -0.12577200
 H -2.84099500 -3.02719600 2.23403600
 H -4.10444300 -0.82480400 -1.08149500
 C -0.28711700 -2.58195700 -0.90350100
 O -0.01679900 -3.67217300 -1.41159500
 O 0.20424400 -1.45351300 -1.36073300
 P 0.63605600 1.18455000 1.68174000
 C -0.04608400 0.36024200 3.18559000
 C 2.40214700 1.54425600 2.14640000
 C -0.15158300 2.85333600 1.77027400
 H 0.41676600 -0.62331200 3.30731200
 H -1.12099300 0.21365000 3.05187500
 H 0.12782700 0.95952200 4.08651900
 H 2.45139600 2.46322800 2.74280900
 H 2.77740300 0.72846900 2.77568500
 H -1.21938300 2.75330800 1.56036200
 H 0.28188800 3.51781300 1.01702500
 H -0.01625300 3.30017000 2.76149400
 C 3.27690000 1.67791300 0.88273100
 H 4.21445800 2.18085400 1.14300800
 H 2.77508600 2.32176200 0.14732400
 C 3.61803800 0.35136500 0.23616000
 C 4.96167900 -0.00862700 0.09427800
 C 2.95779700 -1.62430700 -0.78738600
 C 5.30185000 -1.21966100 -0.50379900
 H 5.73209400 0.66773300 0.45166200
 C 4.27570800 -2.04200900 -0.95531200
 H 2.13033400 -2.21649000 -1.15935600
 H 6.34380100 -1.50665200 -0.61624900

H 4.47420400 -2.99339400 -1.43767900
 N 2.62025000 -0.45872800 -0.19547200
 H -4.49177000 0.35839100 1.71727100
 H -5.75725200 -0.24993600 0.65024500

TS6-4e

C 4.73370600 -0.28830200 2.02547500
 H 5.42670900 -0.80145800 2.70433800
 H 5.14809400 0.71402400 1.84590600
 C 4.61995300 -1.03376100 0.69382200
 C 3.70849900 -0.26960600 -0.27618200
 H 3.56271000 -0.87416300 -1.17779700
 C 2.36312900 0.11663100 0.34357300
 C 1.25716400 0.39080400 -0.47383800
 Si 1.31841600 0.91659700 -2.31503100
 C 1.84881300 -0.51508300 -3.45184700
 H 1.16819500 -1.37044300 -3.37195300
 H 1.81970500 -0.17307700 -4.49482100
 H 2.86495000 -0.87317800 -3.25509800
 C -0.39947300 1.47236700 -2.89125400
 H -0.35036200 1.81954700 -3.93198700
 H -1.13403000 0.65918600 -2.84468600
 H -0.77164300 2.29544800 -2.27330700
 C 2.51348100 2.37130500 -2.53602700
 H 2.22751700 3.19653500 -1.87406700
 H 3.54857000 2.09831900 -2.30317800
 H 2.48942700 2.74235700 -3.56870600
 C 3.35275100 -0.16575900 2.68083400
 H 3.04120800 -1.16703700 3.02040800
 C 2.28405900 0.37737500 1.74094000
 C 1.28949900 1.17411500 2.28553900
 H 1.30672900 1.39278400 3.34957400
 Ni -0.55229800 0.00118100 -0.04745500
 H 3.40803000 0.45770300 3.58073500
 H 4.24670700 0.63603800 -0.60290800
 C 0.35498900 1.98208800 1.54235600
 O -0.32875700 2.88965900 2.02045500
 O 0.23943600 1.74158000 0.18507100
 P -0.66082500 -2.16601400 0.07279200
 C 0.25107500 -2.92686400 1.48657100
 C -2.42502500 -2.69264500 0.33167100
 C -0.12918700 -3.23623400 -1.34197300
 H -0.12474400 -2.51191500 2.42644000
 H 1.30761100 -2.65412400 1.40097200

H 0.15557800 -4.01855200 1.50335600
 H -2.54615100 -3.75744400 0.09592700
 H -2.67220900 -2.56289500 1.39213800
 H 0.92947800 -3.05533600 -1.55020700
 H -0.69669000 -2.98038700 -2.24249600
 H -0.27271900 -4.30018800 -1.11993400
 C -3.37952800 -1.84526000 -0.53869800
 H -4.33860600 -2.36687300 -0.62932100
 H -2.97807400 -1.76812600 -1.55934100
 C -3.65446100 -0.45158100 -0.00752200
 C -4.97541300 -0.05739600 0.22528200
 C -2.88684800 1.63468700 0.67431100
 C -5.24812800 1.22654100 0.69336800
 H -5.78192800 -0.75891100 0.03424100
 C -4.18078100 2.08839700 0.92203300
 H -2.03186600 2.27774600 0.86444500
 H -6.27234300 1.54058900 0.87551200
 H -4.32929700 3.09796100 1.29086400
 N -2.61806500 0.39158900 0.21913000
 H 4.21099200 -2.03910100 0.87567100
 H 5.60875500 -1.17220600 0.23783100

INT2-4e

C 2.03852700 -1.23716500 -0.86167800
 H 1.83194400 -2.17715200 -0.33251300
 H 2.08280700 -1.48491100 -1.93048200
 C 3.38316400 -0.66269600 -0.40275200
 H 3.34080100 -0.41037100 0.66481000
 H 3.59250700 0.27394400 -0.93553200
 C 4.55409500 -1.64244300 -0.63814900
 H 4.59472600 -1.91097100 -1.70365700
 C 5.84752000 -1.09906200 -0.22450100
 C 6.91413900 -0.62346900 0.12410100
 Si 8.52576500 0.09208400 0.64014000
 C 8.83943000 1.67590200 -0.34627400
 H 8.05020800 2.41635100 -0.17222600
 H 9.79542900 2.13197600 -0.05964900
 H 8.87500100 1.47332300 -1.42287500
 C 8.46187800 0.48697200 2.48951900
 H 7.66578500 1.20544000 2.71648700
 H 8.27535400 -0.41570100 3.08262800
 H 9.41082400 0.92063500 2.82943300
 C 9.89710100 -1.16483400 0.29663200
 H 9.73404500 -2.09363300 0.85530000

H 9.94585400 -1.42047000 -0.76807900
 H 10.87582000 -0.76483600 0.59017200
 C 0.86845600 -0.26302000 -0.62557100
 H 0.80706500 -0.00819300 0.44161800
 C -0.43911300 -0.79661600 -1.08517400
 C -1.17819500 -1.67215100 -1.64429900
 H -1.27736400 -2.61613300 -2.15804700
 C -2.27155100 2.66429200 -0.72387600
 C -2.40494800 3.90888200 -0.12012400
 C -2.92756900 3.96690200 1.17196800
 C -3.30040100 2.78074100 1.79640900
 C -3.14548400 1.55953700 1.12950500
 N -2.62538600 1.51135800 -0.11919800
 H -3.04230600 4.91869800 1.68305400
 H -1.87517100 2.56603300 -1.72920300
 H -2.10310200 4.80406200 -0.65360700
 H -3.71307400 2.78634100 2.80073800
 Ni -2.25928100 -0.24029000 -1.08341400

C -3.59205600 0.26287600 1.75985300
 H -2.93310300 -0.54094100 1.40861700
 H -3.47782100 0.32525300 2.84858600
 C -5.06037800 -0.06868000 1.41318300
 H -5.19042200 -0.09424700 0.32445500
 H -5.71188000 0.72430500 1.80388600
 P -5.64046700 -1.68535100 2.17742200
 C -4.84195300 -2.90007100 1.00498200
 H -3.76001600 -2.93094100 1.17187800
 H -5.23381300 -3.90334700 1.20626300
 H -5.02576700 -2.64956200 -0.04660600
 C -7.37607000 -1.70372400 1.48980400
 H -7.40111000 -1.54243500 0.40522900
 H -7.84269800 -2.66985600 1.71085800
 H -7.97553600 -0.92688100 1.97682500
 H 1.06923200 0.68470800 -1.14531200
 H 4.35960800 -2.57953100 -0.09680700
 C -3.28953000 0.21796300 -2.68927300
 O -4.18274700 -0.35886000 -2.08179100
 O -2.90754200 0.84734900 -3.63136900

TS1-4e

C -1.97840400 1.23490800 -0.45861500
 H -1.79649900 2.01116600 0.29655300
 H -1.98371200 1.74272300 -1.43240100
 C -3.33947500 0.57672800 -0.20700100

H -3.34078500 0.07738200 0.77045600
 H -3.52504100 -0.20404400 -0.95608800
 C -4.49880000 1.59653600 -0.24948300
 H -4.51022900 2.09376300 -1.23011600
 C -5.80666500 0.99397800 0.00616900
 C -6.88855600 0.47698200 0.22394900
 Si -8.53101000 -0.27685200 0.55744800
 C -8.68674800 -1.88338400 -0.43013000
 H -7.90846100 -2.60216700 -0.14878700
 H -9.66004900 -2.35732800 -0.25101400
 H -8.59767600 -1.69931600 -1.50696900
 C -8.67784300 -0.64267900 2.40778500
 H -7.89768500 -1.33707800 2.74039600
 H -8.58513900 0.27283300 3.00324600
 H -9.65003900 -1.09571300 2.63938800
 C -9.88167100 0.93741700 0.02926200
 H -9.80195800 1.88419200 0.57567800
 H -9.81633500 1.16405300 -1.04112800
 H -10.87834800 0.52147800 0.22342200
 C -0.81596300 0.22526500 -0.42700100
 H -0.80482300 -0.29664400 0.54132200
 C 0.52636100 0.83111200 -0.65885300
 C 1.01429000 2.04775400 -0.84437900
 H 0.44463000 2.97170100 -0.86199900
 C 1.74734700 -2.31233900 -1.54396100
 C 1.85945800 -3.69449600 -1.58374400
 C 2.68152900 -4.32236300 -0.64709200
 C 3.35515200 -3.53781400 0.28290400
 C 3.21100800 -2.14541900 0.27293900
 N 2.40509900 -1.54843200 -0.64269800
 H 2.79153300 -5.40284800 -0.63971200
 H 1.11655400 -1.77585500 -2.24293400
 H 1.31018600 -4.25814600 -2.33014100
 H 4.00032800 -3.99080800 1.02891100
 Ni 2.27163400 0.33772200 -0.76997800
 C 3.96919100 -1.27558600 1.24439200
 H 3.32758100 -0.43900800 1.54571600
 H 4.18849000 -1.85991000 2.14594300
 C 5.28676400 -0.73145400 0.64758300
 H 5.07520200 -0.09331900 -0.21896200
 H 5.90602500 -1.57083500 0.30469000
 P 6.30402900 0.22809100 1.90806700
 C 5.26031900 1.76852600 2.06031900
 H 4.39329400 1.57539800 2.70172100

H 5.85395500 2.55144100 2.54541400
 H 4.91119800 2.13041500 1.08660700
 C 7.61592800 0.87067300 0.74587500
 H 7.18641300 1.38286800 -0.12327500
 H 8.26205300 1.57296500 1.28365000
 H 8.24287000 0.04211300 0.39829500
 H -0.99386200 -0.55901700 -1.17812200
 H -4.31230800 2.38952000 0.48910000
 C 2.65475200 2.62881700 -1.11496800
 O 3.62780100 1.81156500 -1.11153900
 O 2.60183000 3.83048700 -1.27115800

INT3-4e

C 1.60841400 -1.61371200 -0.32726900
 H 1.41882100 -2.22639100 0.56403100
 H 1.67371900 -2.30946100 -1.17432200
 C 2.94037700 -0.87079700 -0.17035100
 H 2.88598000 -0.17376400 0.67599300
 H 3.14053100 -0.26254200 -1.06217600
 C 4.12713700 -1.83456900 0.05245900
 H 4.18669000 -2.53863500 -0.78992600
 C 5.40841600 -1.14518300 0.20164600
 C 6.46637800 -0.55229600 0.32314400
 Si 8.07309700 0.31911700 0.50696300
 C 8.32479800 1.46939300 -0.97432300
 H 7.52598400 2.21735100 -1.03761700
 H 9.27922800 2.00491600 -0.89490100
 H 8.33304300 0.90925800 -1.91641200
 C 8.05082300 1.32864500 2.10709400
 H 7.25049000 2.07759900 2.09557400
 H 7.89318200 0.68584800 2.98076700
 H 9.00191100 1.85749200 2.24792600
 C 9.46287700 -0.96257600 0.57345000
 H 9.33041200 -1.64787300 1.41850600
 H 9.49366800 -1.56461600 -0.34191800
 H 10.43946900 -0.47531500 0.68719100
 C 0.42289500 -0.65613100 -0.54399400
 H 0.37991300 0.05711400 0.29289700
 C -0.91922200 -1.32373300 -0.68832200
 C -1.16267300 -2.64383000 -0.72639900
 H -0.40308300 -3.42292900 -0.67933400
 C -1.27798100 2.03959400 -1.75603900
 C -1.01557600 3.40031100 -1.85425200
 C -1.57259100 4.25394600 -0.90260300

C -2.37802000 3.71350500 0.09725800
 C -2.60802700 2.33589100 0.14062000
 N -2.04400500 1.51251600 -0.77988900
 H -1.38768600 5.32353400 -0.94112300
 H -0.87152800 1.33243700 -2.46955100
 H -0.39072800 3.77344600 -2.65847100
 H -2.83477900 4.34970300 0.84839400
 Ni -2.55050300 -0.36344700 -0.77117000
 C -3.51370100 1.70430400 1.17071000
 H -2.95603900 0.91831200 1.69581300
 H -3.79307700 2.45723000 1.91555000
 C -4.79240100 1.10244700 0.54795200
 H -4.55000600 0.30685700 -0.18035800
 H -5.33242400 1.88026600 -0.00707400
 P -5.97584800 0.38920800 1.82670400
 C -5.04198200 -1.15059000 2.31336100
 H -4.20707200 -0.89329500 2.97435200
 H -5.71548900 -1.80129300 2.88215100
 H -4.65940700 -1.70146500 1.44628900
 C -7.21130400 -0.35790400 0.64575800
 H -6.73780300 -1.01832100 -0.09019600
 H -7.94515000 -0.93819600 1.21512400
 H -7.75206400 0.43756900 0.12133400
 H 0.62970100 -0.04114700 -1.43301400
 H 3.93491400 -2.44680900 0.94523800
 C -2.59741800 -3.03309900 -0.80882900
 O -3.39157300 -1.95631100 -0.81307900
 O -3.01494600 -4.17687100 -0.84982300

TS5-4e

C 4.16608700 0.26205300 -0.27246000
 H 5.16969600 0.04578500 -0.65746100
 H 3.92920400 1.28864600 -0.57692100
 C 4.15122200 0.17612000 1.25892300
 H 4.33165000 -0.85902100 1.56764600
 H 4.95711400 0.78188000 1.68942700
 C 2.78569400 0.66000500 1.82379300
 H 2.84429200 1.72335100 2.08750500
 C 1.66897300 0.51788400 0.82682400
 C 0.86601000 1.25122100 0.11910800
 Si 0.49821000 3.01345800 -0.32203000
 C 0.29263500 3.17447000 -2.20061800
 H -0.56011400 2.59248300 -2.56903700
 H 0.12492900 4.22125600 -2.48381400

H 1.18673700 2.82568500 -2.73089100
 C -1.07903100 3.61259000 0.53960900
 H -1.27415300 4.66310800 0.28887600
 H -1.95949900 3.02959100 0.25022700
 H -0.98108700 3.54296700 1.62930200
 C 1.93844700 4.12649200 0.21897900
 H 2.07544100 4.10750600 1.30669000
 H 2.88427400 3.81804200 -0.24177400
 H 1.75200300 5.16840700 -0.07177100
 C 3.14348900 -0.73117800 -0.90464600
 H 2.72163800 -0.29038200 -1.81594500
 C 2.01760200 -1.14935400 0.02859500
 C 2.03934300 -2.36655500 0.62499200
 H 2.87655500 -3.04856400 0.46902200
 Ni 0.09460800 -0.57033600 0.13175100
 H 3.67110600 -1.64634900 -1.20494900
 H 2.53803300 0.10724800 2.73777000
 C 0.86539700 -2.87867200 1.38875900
 O 0.93027500 -3.86506700 2.11698900
 O -0.22721000 -2.18363200 1.15196400
 P -0.73554800 -1.33404700 -1.96394100
 C -0.67344200 -3.17118800 -2.15304300
 C -2.56766900 -0.97622400 -2.01290700
 C -0.18991600 -0.74894500 -3.64024100
 H -1.04492800 -3.62404500 -1.22907100
 H 0.36866600 -3.48360800 -2.27730300
 H -1.25773700 -3.52945400 -3.00837800
 H -2.93048800 -0.99293200 -3.04842700
 H -3.08308500 -1.78104700 -1.47590600
 H 0.87248200 -0.97832300 -3.77447500
 H -0.30638000 0.33737100 -3.71110100
 H -0.75702400 -1.22255100 -4.45068600
 C -2.90155200 0.38622700 -1.35817900
 H -3.87379500 0.73437800 -1.72433400
 H -2.16478300 1.13846900 -1.66781000
 C -2.96114800 0.33479700 0.15403100
 C -4.17042200 0.59114600 0.81238100
 C -1.91922700 -0.07420500 2.18576600
 C -4.23590100 0.51796600 2.20139600
 H -5.05112700 0.84217700 0.22910500
 C -3.08472600 0.17431900 2.90509500
 H -1.00823000 -0.38306600 2.68361400
 H -5.16947500 0.71751500 2.72024400
 H -3.08065000 0.08896000 3.98676400

N -1.84681600 0.01600000 0.84625900

INT1-4f

C 3.33513200 0.08023900 -0.12307800

H 2.94981400 -0.59604300 -0.89875300

H 3.32545300 1.08730100 -0.56022800

C 4.76993400 -0.31454900 0.24449600

H 4.78479100 -1.32409800 0.67619400

H 5.15858000 0.35882800 1.01937000

C 5.72004800 -0.27739400 -0.97235600

H 5.71351300 0.73223800 -1.40684100

H 5.33465900 -0.94595000 -1.75545000

C 7.09523700 -0.65649900 -0.64378700

C 8.22430100 -0.97273100 -0.35298600

Si -0.00400900 3.19298600 -0.02075900

C -0.85688000 4.09825400 1.41840200

H -0.28613500 3.98759200 2.34811700

H -0.94866300 5.17165600 1.20746400

H -1.86656400 3.71213000 1.60368200

C 1.67370400 4.03626700 -0.32562900

H 2.31437500 3.97677300 0.56260600

H 2.21137800 3.56068900 -1.15496100

H 1.54860200 5.09789900 -0.57586500

C -1.06870500 3.39237400 -1.57859000

H -0.59830800 2.89769600 -2.43698200

H -2.05791900 2.93998400 -1.44095900

H -1.21300300 4.44932800 -1.83683200

C 2.37631800 0.05512700 1.08490400

H 2.75160000 0.75334600 1.84847200

H 2.40375900 -0.94397900 1.54044700

C 0.97748900 0.42726600 0.71164500

C 0.20465300 1.40801300 0.37238700

C -3.33407800 0.88002900 0.57947900

C -4.70067300 1.09794500 0.44630500

C -5.42821300 0.26630500 -0.40394800

C -4.75032800 -0.75073500 -1.07099600

C -3.37355000 -0.91959000 -0.88554500

N -2.66739000 -0.10130900 -0.06625400

H -6.49615400 0.40592300 -0.54581400

H -2.72399900 1.50774300 1.21825900

H -5.17329000 1.90779000 0.99282900

H -5.28003700 -1.42130900 -1.74113200

Ni -0.70946800 -0.29809500 0.36247800

C -2.64230100 -2.04928900 -1.57519300

H -3.32269400 -2.51471900 -2.29771000

H -1.79880500 -1.63755400 -2.14460400

C -2.12422000 -3.12725000 -0.59190800

H -1.84563600 -4.03252100 -1.14545500

H -2.92655300 -3.40863100 0.10139900

P -0.66141600 -2.49398600 0.39618600

C 0.75514000 -3.32341500 -0.47403300

H 0.84478300 -2.92150000 -1.48832300

H 1.68622800 -3.09773900 0.05557500

H 0.63094400 -4.41195200 -0.52808100

C -0.76575300 -3.53196100 1.93450600

H -0.83196100 -4.60430900 1.71367900

H 0.12201300 -3.35294700 2.55015100

H -1.64227900 -3.23120300 2.51755500

H 9.22216300 -1.24909300 -0.10004600

TS1-4f

C 3.29250900 -0.07331700 0.13699000

H 3.36893100 0.83692100 0.74516600

H 2.95845500 -0.86608900 0.82015200

C 4.66274400 -0.43243300 -0.44893700

H 4.99862500 0.35834500 -1.13189100

H 4.58855900 -1.34867100 -1.04964500

C 5.73192400 -0.63643800 0.64619500

H 5.39697100 -1.41899100 1.34191600

H 5.81919000 0.28151800 1.24409400

C 7.04459300 -0.99453200 0.10679100

C 8.11910300 -1.29085700 -0.35860400

Si 0.14022300 3.29369900 -0.53232400

C -1.65535700 3.79158100 -0.86657700

H -2.23637800 3.75449100 0.05896800

H -1.70567500 4.81189300 -1.26804400

H -2.12356300 3.12115100 -1.59780200

C 0.93485700 4.45758600 0.73200500

H 0.41983700 4.38220500 1.69408600

H 1.99271800 4.21392100 0.88983200

H 0.88213000 5.49966800 0.39111600

C 1.09887300 3.44549400 -2.16959000

H 2.17436300 3.27476500 -2.03927700

H 0.73441300 2.73539800 -2.92189700

H 0.98070700 4.45510500 -2.58432200

C 2.22068400 0.14635200 -0.95459800

H 2.15917100 -0.74805100 -1.58668200

H 2.54125200 0.97582000 -1.60102400

C 0.89363700 0.46507200 -0.35539800
 C 0.20570000 1.50968000 0.07177400
 C -3.45089400 0.53670600 0.52457300
 C -4.83967000 0.62022700 0.49561500
 C -5.55542000 -0.35637600 -0.18985100
 C -4.84523200 -1.37811800 -0.81489000
 C -3.44877100 -1.40878000 -0.74775600
 N -2.75531500 -0.45252300 -0.07926100
 H -6.64030900 -0.32673600 -0.23979600
 H -2.86530300 1.28754200 1.04287000
 H -5.33437300 1.44219200 1.00234900
 H -5.36564600 -2.15929500 -1.36033200
 Ni -0.71223400 -0.35953000 -0.00243200
 C -2.69540500 -2.53592300 -1.42250100
 H -3.42188900 -3.16323500 -1.95093100
 H -2.02506400 -2.11886300 -2.18619200
 C -1.88292600 -3.41206900 -0.44254700
 H -1.60616900 -4.35621300 -0.92678500
 H -2.49722200 -3.66333800 0.43014700
 P -0.35032700 -2.51286700 0.13051200
 C 0.98332300 -3.38023500 -0.82057400
 H 0.85701300 -3.19652600 -1.89243700
 H 1.96149200 -2.99045100 -0.52373300
 H 0.96455200 -4.46149500 -0.63997900
 C -0.07779200 -3.14580500 1.84393000
 H -0.04282900 -4.24079000 1.88070200
 H 0.86052000 -2.73647800 2.22897100
 H -0.87955900 -2.77805800 2.49040000
 H 9.07091600 -1.54949900 -0.76286400
 C -0.52366900 1.36505600 1.81412300
 O -1.22786200 2.34181000 2.02477300
 O -0.11478500 0.37698200 2.40517700

TS4-4f

C 3.44541100 -0.41016700 0.23221900
 H 3.73003200 0.61135800 0.51560700
 H 3.14182500 -0.90971600 1.16325600
 C 4.64778900 -1.13825800 -0.37931700
 H 4.95379100 -0.64023800 -1.30827400
 H 4.36640100 -2.16279100 -0.65594900
 C 5.85504800 -1.19236100 0.58147500
 H 5.55367700 -1.67985100 1.51969900
 H 6.14991600 -0.16918800 0.85379900
 C 7.00573800 -1.89719500 0.01487400

C 7.94319300 -2.48384000 -0.47060900
 Si 1.49208000 3.20532000 -0.35185000
 C 0.16761700 4.45072600 -0.86997900
 H -0.47678800 4.71459100 -0.02748200
 H 0.63900900 5.36746600 -1.24678700
 H -0.46188000 4.04925600 -1.67349000
 C 2.58645100 3.86604300 1.04009900
 H 1.98662800 4.04611500 1.93523700
 H 3.38245700 3.15598500 1.29530800
 H 3.06519000 4.80654700 0.73751200
 C 2.59062400 2.89052000 -1.87199100
 H 3.47012100 2.27652500 -1.64680800
 H 2.04041000 2.41242700 -2.69131200
 H 2.96050400 3.85361000 -2.24763300
 C 2.24208700 -0.34770400 -0.73195600
 H 1.97026000 -1.36707000 -1.03537900
 H 2.54245000 0.17376600 -1.65049600
 C 1.04726100 0.33243300 -0.14604700
 C 0.64776300 1.56271000 0.16592300
 C 0.05003000 -2.89599500 0.70549800
 C -0.08989000 -4.27653700 0.68203800
 C -1.20908600 -4.82194400 0.05265400
 C -2.13851300 -3.95890700 -0.51936900
 C -1.94988500 -2.57393300 -0.45900000
 N -0.85180300 -2.05481800 0.15080700
 H -1.35299600 -5.89744100 0.00639900
 H 0.90347500 -2.42372900 1.17729700
 H 0.66557400 -4.90214500 1.14535500
 H -3.02123100 -4.34488500 -1.01940300
 Ni -0.62687900 -0.17573900 0.32453300
 C -2.97295500 -1.62039500 -1.02564200
 H -2.45044200 -0.77572400 -1.49098700
 H -3.53587200 -2.13085300 -1.81620200
 C -3.94977000 -1.09704700 0.05132600
 H -3.40486000 -0.52467700 0.81170500
 H -4.42969600 -1.94854500 0.55171800
 P -5.32875600 -0.03869700 -0.67287400
 C -4.35469200 1.46840100 -1.18979100
 H -3.82312600 1.26906200 -2.12692500
 H -5.05439100 2.28952800 -1.38241100
 H -3.63223000 1.77927700 -0.42680400
 C -6.03403000 0.59643600 0.93425000
 H -5.26602500 1.04915400 1.57251700
 H -6.80368400 1.34640200 0.72188400

H -6.51215700 -0.22498300 1.47922200
H 8.77564500 -2.99775800 -0.89411600
C -0.66420800 1.98649600 1.22552700
O -1.74272100 1.32442900 1.18499700
O -0.34608300 2.95957400 1.88966300

INT8-4gh

C 2.35194000 2.76611100 -1.23774300
C 4.19007500 1.37445800 -0.01567600
H 2.02975500 3.11648800 -0.24674900
H 2.27633900 3.63185400 -1.91223000
C 3.76000700 -0.09240100 -0.22212900
H 5.28272400 1.37492900 0.09520900
H 4.06751800 -0.40416900 -1.23076100
H 4.32278800 -0.72129200 0.48311500
C 1.40722500 1.72797900 -1.71700100
C 0.55732900 1.25542900 -2.51947600
C 2.31519900 -0.39336400 -0.04443700
C 1.39014500 -1.03179800 0.55017700
Si 0.90989800 -2.25236000 1.84786800
H -0.02681000 1.31121200 -3.42300000
Ni 0.68796600 0.02682300 -1.01130500
C 2.20782800 -2.23797900 3.23353700
H 1.95809900 -2.96453500 4.01751700
H 3.20327300 -2.49135800 2.84955300
H 2.27547900 -1.24960300 3.70332200
C -0.78214500 -1.85128800 2.59667700
H -1.56557100 -1.85008300 1.83073900
H -1.05595300 -2.59384600 3.35694100
H -0.78553700 -0.86623200 3.07781500
C 0.83995400 -3.99535800 1.09813800
H 0.62813800 -4.74332900 1.87303300
H 0.05441300 -4.07326800 0.33773500
H 1.79238200 -4.26397900 0.62598900
C 3.83292900 2.34799500 -1.14712600
H 4.41656900 3.26673800 -1.00034700
H 4.15263400 1.92871700 -2.11092100
H 3.78352300 1.74422800 0.93561300
C -0.93653300 -2.24636400 -1.80249000
C -2.32598200 -0.46519000 -1.26816400
C -2.00672600 -3.06143300 -2.15435400
H 0.08445000 -2.60865200 -1.86304900
C -3.45005500 -1.23601400 -1.59616000
C -3.29715700 -2.54429300 -2.04333600

H -1.82520400 -4.07305200 -2.50294000
H -4.43743300 -0.79394100 -1.50201300
H -4.16422600 -3.14489600 -2.30405600
C -2.48682600 0.95896300 -0.79009200
H -1.71111700 1.56927200 -1.26339300
H -3.46055000 1.33587700 -1.12538600
C -2.38307500 1.10050600 0.74246000
H -3.12000400 0.44475000 1.22513100
H -1.38855200 0.77944500 1.07531300
P -2.74520800 2.84785400 1.32731000
C -2.44904900 2.60070800 3.15470200
H -1.48903300 2.11242800 3.36335600
H -2.46489100 3.57217600 3.66088000
H -3.25359900 1.99133500 3.58057100
C -1.13809500 3.68520600 0.87635800
H -0.26436500 3.13497300 1.24669100
H -1.05371200 3.77498300 -0.21150500
H -1.12636800 4.69698600 1.29676400
N -1.07722800 -0.97874600 -1.36648600

INT8-4gh'

C 4.37925400 1.26633600 -1.14811300
C 3.48481100 -0.50649500 -2.84155900
H 4.86395000 0.43099200 -0.62214100
H 5.09151800 2.10443300 -1.12412700
C 1.97344000 -0.57552500 -2.53052100
H 3.60376900 -0.77290800 -3.90035900
H 1.47507900 0.27275700 -3.01899400
H 1.56589600 -1.48538500 -2.99485200
C 3.15612500 1.66418400 -0.40560100
C 2.46770200 2.51904300 0.23216000
C 1.60252800 -0.60921300 -1.09553000
C 1.16340200 -1.16576300 -0.05281600
Si 0.75828200 -2.70617200 0.88579600
H 2.37387700 3.52818900 0.60079300
Ni 1.51976000 0.84651800 0.26150500
C 1.05647600 -4.18606600 -0.26449100
H 0.87387100 -5.13406400 0.25777500
H 0.38922300 -4.15058500 -1.13386400
H 2.08792200 -4.20164500 -0.63543300
C 1.90982300 -2.83480400 2.38434900
H 1.79743200 -1.96862100 3.04694500
H 1.70095300 -3.73838500 2.97119200
H 2.95968200 -2.87293500 2.07065300

C -1.04329600 -2.75848400 1.46861500
 H -1.29700900 -3.77787200 1.78781000
 H -1.21938900 -2.10014400 2.32721400
 H -1.74214500 -2.46760300 0.67580700
 C 4.16413100 0.85186500 -2.61769500
 H 5.15358900 0.81423800 -3.09302700
 H 3.60004200 1.63785600 -3.13851900
 H 4.00808400 -1.28243400 -2.26651600
 C -4.83596600 -1.28659400 -1.04264100
 C -3.51699300 0.58613700 -0.80493000
 C -5.90748200 -0.55224900 -1.55405500
 H -4.91661800 -2.36616700 -0.92298600
 C -4.53885200 1.40301000 -1.30654800
 C -5.74986300 0.82614000 -1.68681200
 H -6.83092500 -1.04865800 -1.83664700
 H -4.38121700 2.47406600 -1.39794100
 H -6.55436400 1.44268500 -2.07946700
 C -2.17989000 1.15445000 -0.37726200
 H -1.38700600 0.67390200 -0.96316700
 H -2.14687400 2.22637800 -0.60658200
 C -1.89576900 0.90964600 1.11649500
 H -2.64348900 1.41719300 1.74182600
 H -1.98102900 -0.16315600 1.30992400
 P -0.18113200 1.43404000 1.63299300
 C -0.42563100 3.26138000 1.85871100
 H -1.29446900 3.48234300 2.48998800
 H 0.46693300 3.69373100 2.32169000
 H -0.56078100 3.73997800 0.88367200
 C -0.16152700 0.89072800 3.40912200
 H -1.04773900 1.23689900 3.95430700
 H -0.11323600 -0.20058200 3.46527000
 H 0.73334400 1.29191300 3.89648000
 N -3.67081000 -0.74421100 -0.67574000

TS7-4gh

C -1.21794200 1.95972300 -1.04682900
 C -0.13161400 1.78523500 -1.84203200
 C -2.20653000 0.85047200 -0.49724600
 C -1.68607300 -0.20775600 0.12771000
 Si -2.32213500 -1.59760300 1.19195700
 H 0.41553700 2.69770800 -2.09918000
 Ni -0.04973800 0.14317800 -0.81217100
 C -3.88861000 -1.09859700 2.14877700
 H -4.75332400 -0.95588000 1.49073300

H -4.15456900 -1.87728200 2.87556800
 H -3.73578000 -0.16568700 2.70425500
 C -2.71963500 -3.13914700 0.15395000
 H -3.46528800 -2.92015200 -0.61975000
 H -1.82607500 -3.53283200 -0.34345400
 H -3.12392900 -3.93733600 0.78981300
 C -0.99676500 -2.05081700 2.46994000
 H -1.35584500 -2.83993900 3.14264400
 H -0.08079400 -2.41326800 1.98971200
 H -0.72974700 -1.18430700 3.08694600
 C 1.96493400 -1.76306600 -0.04344200
 C 2.65589000 -2.97530100 -0.14714300
 C 2.23229600 -3.95325800 -1.04217800
 C 1.10928000 -3.69443100 -1.82938800
 C 0.45991200 -2.47685300 -1.68029100
 N 0.86687000 -1.52823900 -0.80706300
 H 2.76597600 -4.89556700 -1.12490000
 H 3.52645900 -3.13650800 0.48120300
 H 0.73636000 -4.41829800 -2.54635500
 H -0.41704300 -2.22750500 -2.26677100
 C 2.44224200 -0.66441700 0.87230600
 C 3.32780100 0.35838800 0.12639900
 P 3.98248900 1.71581600 1.24865400
 C 4.82869400 2.75216400 -0.05386000
 C 2.42871600 2.72726900 1.47401400
 H 3.00676000 -1.10418000 1.70306900
 H 1.56570900 -0.15969800 1.29424700
 H 4.20038400 -0.15595400 -0.29810500
 H 2.76179500 0.79497500 -0.70735200
 H 1.76169100 2.23702200 2.19065900
 H 2.69499600 3.70539600 1.89008500
 H 1.88368400 2.87329400 0.53362400
 H 4.17176900 2.97802100 -0.90284600
 H 5.16403600 3.69493800 0.39192000
 H 5.71522500 2.22645500 -0.42495600
 C -3.66558000 1.21119000 -0.71767400
 C -4.01987400 2.59486300 -0.14256800
 C -3.07357500 3.67584900 -0.67809700
 C -1.60271600 3.30652000 -0.42090800
 H -3.84507400 1.22521600 -1.80412000
 H -0.93858900 4.08438400 -0.81462700
 H -1.43751500 3.25813500 0.66658100
 H -4.31435400 0.43951300 -0.29248200
 H -3.22953600 3.79879800 -1.75915300

H -3.30059900 4.64426500 -0.21252700
H -5.06239600 2.84047600 -0.38365700
H -3.94790200 2.55549300 0.95354700

TS7-4gh*

C -1.98532200 2.07095700 0.27146600
C -0.68686600 1.94731900 0.54174300
C -2.80704900 0.84161700 -0.33110200
C -2.64957000 -0.45944700 0.00118200
Si -3.41577100 -2.05469700 -0.52092100
H -0.00167900 2.71802600 0.88314700
Ni -0.83088100 0.10526700 0.55256900
C -2.10028300 -3.07955000 -1.43725800
H -2.48709500 -4.06940400 -1.71143000
H -1.77841300 -2.58022600 -2.35966000
H -1.21132000 -3.22568700 -0.81252500
C -3.91752500 -2.98244600 1.06072400
H -4.67626600 -2.42306500 1.62212200
H -4.33432900 -3.97161400 0.83115900
H -3.05503000 -3.12061100 1.72296800
C -4.96914800 -2.01456800 -1.63511800
H -5.37003800 -3.02927100 -1.76190300
H -5.76890900 -1.40122900 -1.20148600
H -4.75414700 -1.62189600 -2.63651600
P 1.06070800 -0.37043200 1.41178800
C 1.24936500 -2.15641200 1.85343000
H 1.16629700 -2.76299300 0.94653600
H 2.20642800 -2.36853500 2.34291500
H 0.43272300 -2.43907200 2.52432100
C 1.41986300 0.48939600 3.00876900
H 2.36649200 0.16342500 3.45254100
H 1.45210800 1.57058200 2.84434500
H 0.60827400 0.27970400 3.71206000
C 2.52373500 -0.00484400 0.32620100
H 2.42316600 1.04151000 0.01431600
H 2.39661300 -0.60970900 -0.57899700
C -2.80178700 3.32871900 0.52331200
C -3.68286000 1.35245200 -1.48524900
C -3.65662600 3.74985700 -0.68037800
C -4.53546000 2.58470100 -1.14285400
H -5.12856500 2.87688400 -2.01985200
H -5.25045500 2.32541100 -0.34886700
H -3.47523100 3.12201500 1.37038100
H -2.13678100 4.14247200 0.83557000

H -3.02131800 1.61855500 -2.32609500
H -4.31960800 0.53525300 -1.82998400
H -2.99917100 4.06355900 -1.50373000
H -4.26929400 4.62048300 -0.41194400
C 3.92677400 -0.26185200 0.91262300
H 3.99235200 -1.29411900 1.27567800
H 4.11349000 0.40053500 1.76512100
C 5.00506600 -0.06282800 -0.13353100
C 5.91927400 0.99498200 -0.06038900
C 6.88176300 1.12980500 -1.06072100
H 5.87752100 1.69661500 0.76812800
C 5.94624000 -0.81491500 -2.09217000
C 6.90015300 0.20507800 -2.10300200
H 7.60359500 1.94146800 -1.02454400
H 5.92644300 -1.55839500 -2.88772300
H 7.63048700 0.26730000 -2.90394300
N 5.01972500 -0.95447700 -1.13915100

INT9-4gh

C -1.51438300 0.52710200 -1.88180600
C -0.24376800 0.08075300 -1.82210300
C -2.33905700 0.07740300 -0.72671300
C -1.63833700 -0.63247000 0.19181700
Si -2.17592800 -1.51340500 1.74034400
H 0.51090400 0.30580300 -2.58385600
Ni 0.19155400 -0.88468000 -0.26848600
C -2.87900600 -0.36222900 3.08331400
H -3.80645200 0.12301700 2.75660300
H -3.10223600 -0.91775100 4.00365000
H -2.16425000 0.43049000 3.33499000
C -3.43074800 -2.90553100 1.40817900
H -4.37816200 -2.50870700 1.02436600
H -3.04417600 -3.61069000 0.66221000
H -3.65233800 -3.47237900 2.32198100
C -0.60542300 -2.32950500 2.46273000
H -0.83548600 -2.91355800 3.36301700
H -0.13932100 -3.02058100 1.74549100
H 0.14776100 -1.58260500 2.75044100
C 3.17598500 -0.66851700 -0.01443500
C 4.49643000 -1.00132600 -0.33721700
C 4.75368300 -1.97864300 -1.29499000
C 3.67761800 -2.60836700 -1.92028200
C 2.39094000 -2.23078100 -1.55383700
N 2.13800400 -1.29004400 -0.62258800

H	5.77614700	-2.24406800	-1.54893000	C	4.93055700	-1.87355800	0.71405200
H	5.31041700	-0.48985100	0.16715100	H	5.65832800	-1.05505600	0.65802400
H	3.82523700	-3.37389800	-2.67478300	H	5.35506600	-2.65345200	1.35970800
H	1.51624500	-2.68100900	-2.01290100	H	4.82753400	-2.29030400	-0.29502300
C	2.86089800	0.41738700	0.98713300	C	3.48186700	-0.62490200	3.14832500
C	2.46401700	1.74314600	0.30328800	H	3.89546800	-1.40315000	3.80315600
P	2.12838800	3.12790100	1.52954500	H	4.16325900	0.23365500	3.17963500
C	1.46193200	4.38815800	0.32362900	H	2.52494300	-0.30129100	3.57550600
C	0.51483700	2.53270700	2.25886800	C	-4.13753400	0.72935100	0.38498800
H	3.73285700	0.57662600	1.63228200	C	-4.04600100	1.58200300	1.49222400
H	2.04037200	0.07852800	1.63106700	C	-5.21093300	1.94639200	2.16670900
H	3.28425300	2.07746800	-0.34603700	C	-6.43156100	1.44707500	1.71577800
H	1.58204800	1.57782500	-0.32930700	C	-6.42352700	0.60140800	0.60478700
H	0.70326700	1.74953500	3.00106100	N	-5.31428600	0.24536200	-0.05070900
H	0.03429200	3.36679400	2.78263700	H	-5.16448200	2.60858400	3.02731000
H	-0.17495200	2.14086000	1.50134600	H	-3.07680300	1.95288800	1.81350200
H	0.66614800	3.97786200	-0.30969800	H	-7.36576800	1.70266300	2.20667700
H	1.06487000	5.24600400	0.87719400	H	-7.35640300	0.19091700	0.22004500
H	2.27206500	4.75247800	-0.31749500	C	-2.90747900	0.29439000	-0.38405500
C	-3.83681400	0.33865100	-0.73237000	C	-2.69587200	-1.23000800	-0.30289800
C	-4.24518300	1.50933700	-1.64410700	P	-1.17062500	-1.82264500	-1.18805000
C	-3.61583400	1.36251000	-3.03660100	C	-1.33281100	-3.66084100	-0.99394700
C	-2.08243400	1.44967200	-2.94498700	C	-1.59689100	-1.59732000	-2.97527800
H	-4.34873400	-0.56595800	-1.09995500	H	-2.01981700	0.81665200	-0.01169300
H	-1.61672800	1.24883200	-3.91856700	H	-3.03840500	0.58682400	-1.43366400
H	-1.82258600	2.49068900	-2.69143800	H	-2.58363000	-1.53042400	0.74707500
H	-4.20460100	0.49938900	0.28899600	H	-3.58145200	-1.74371300	-0.69627600
H	-3.91184800	0.39479000	-3.46749100	H	-1.58738600	-0.53429100	-3.23159800
H	-3.99249300	2.13964800	-3.71403000	H	-0.83875100	-2.09392700	-3.58925800
H	-5.33920200	1.55662200	-1.71856600	H	-2.58185300	-2.01510400	-3.21295200
H	-3.91779400	2.46154500	-1.20074900	H	-2.31331000	-4.01629300	-1.33025200
INT9-4gh'				H	-0.55458100	-4.16336600	-1.57765500
C	1.65214300	1.74308300	-1.09864600	H	-1.19782200	-3.93633200	0.05690400
C	0.65738000	0.86993700	-1.35411500	C	3.74261400	2.12345500	0.39961600
C	2.65336900	1.20962700	-0.13523000	C	4.03466800	3.32005400	-0.52399100
C	2.41179400	-0.07125100	0.22502900	C	2.73437400	4.03198700	-0.92457600
Si	3.25333600	-1.26411300	1.37093400	C	1.84162200	3.09618700	-1.75843500
H	-0.15049800	1.09208200	-2.05984000	H	3.41509400	2.52395500	1.37323900
Ni	0.80022200	-0.81151000	-0.50014600	H	0.87086100	3.56266100	-1.97145700
C	2.07648000	-2.77107700	1.44751500	H	2.33142100	2.94999400	-2.73497700
H	2.49798900	-3.59065400	2.04349500	H	4.65994400	1.55493400	0.59959600
H	1.11224000	-2.50454200	1.90285900	H	2.20072200	4.34974700	-0.01662300
H	1.87813600	-3.18186000	0.44533800	H	2.95494800	4.94209100	-1.49699500
				H	4.71669700	4.01775100	-0.02139800

H 4.54921800 2.97439300 -1.43279500

TS8-4g

C -3.48190400 1.35283300 -1.40089800
C -4.64482900 0.41803400 0.61868000
H -4.10702600 0.83333400 -2.14333400
H -3.12336900 2.26356600 -1.89847800
C -3.34993400 -0.14898900 1.22444300
H -5.36534400 0.61890000 1.42123200
H -3.04962800 0.50353400 2.05788700
H -3.54548600 -1.13036400 1.66978000
C -2.31451900 0.44159600 -1.06762600
C -1.29992500 0.18796600 -1.94095400
C -2.19262400 -0.22985700 0.23071100
C -0.99086300 -0.84836000 0.44615900
Si -0.65970400 -2.00612600 1.90819500
H -1.18750500 0.78948800 -2.84705700
Ni 0.20099700 -0.63009600 -1.07249400
C -1.89820800 -3.45289900 1.88196700
H -2.94084200 -3.14457700 2.00829200
H -1.82947200 -3.99587600 0.93161000
H -1.66394600 -4.16121100 2.68741500
C 1.04535800 -2.84029000 1.86437300
H 1.87486300 -2.14097800 2.00885000
H 1.09175500 -3.57661200 2.67727100
H 1.21682500 -3.37954300 0.92594300
C -0.76828300 -1.09891600 3.58063700
H -0.54981800 -1.79086800 4.40446700
H -0.03925000 -0.28086100 3.63698200
H -1.75975200 -0.67041700 3.76297800
C -4.35411100 1.69111700 -0.18344000
H -5.28508800 2.16648400 -0.51557900
H -3.83951800 2.41821400 0.46141000
H -5.10887100 -0.32745800 -0.04302500
C 2.81619800 -1.80384200 -1.01679800
C 2.71015200 0.02301800 0.42700600
C 4.16510800 -2.00936800 -0.75859800
H 2.27571300 -2.42557700 -1.72260200
C 4.06850800 -0.13382300 0.73192200
C 4.80341000 -1.15749300 0.14279300
H 4.69355900 -2.81794300 -1.25227300
H 4.53489200 0.55455500 1.43006700
H 5.85588500 -1.28629300 0.37944800
C 1.91883600 1.16824300 1.00872800

H 0.87263200 0.86094600 1.11116900

H 2.30586000 1.39741700 2.00910800

C 2.00614200 2.43375900 0.12579500

H 3.06008600 2.67868900 -0.06249900

H 1.53768300 2.23951400 -0.84870400

P 1.24561100 3.94397300 0.94533300

C 1.48673200 5.16682600 -0.44428000

H 1.11427900 4.79393300 -1.40635400

H 0.96087700 6.09700000 -0.20288900

H 2.55102200 5.40495200 -0.54690500

C -0.56878700 3.57538100 0.71652200

H -0.81756500 3.31378400 -0.31887700

H -0.86684700 2.74408400 1.36333600

H -1.15283500 4.45394200 1.01242700

N 2.09685900 -0.82397300 -0.43202100

C -0.67100200 -1.51967800 -2.87923100

O -1.57779600 -2.22910500 -3.18106200

O 0.53020400 -1.26572800 -3.04884900

TS8-4g'

C 0.96955800 3.41422900 0.08863300
C 3.48254700 3.70547300 -0.04176200
H 0.81057800 3.66500500 1.14955800
H 0.01602600 3.64442000 -0.40545500
C 3.69965200 2.27397600 -0.56206900
H 4.29266800 4.35592100 -0.39334800
H 3.86429000 2.31553600 -1.65027400
H 4.61422500 1.84593000 -0.13317000
C 1.22465700 1.93250000 0.06000700
C 0.26371400 0.97971200 0.42534800
C 2.51257300 1.37153600 -0.26698300
C 2.46615600 0.00205400 -0.32500800
Si 3.76442800 -1.26322300 -0.82238200
H -0.78908900 1.24007500 0.27421400
Ni 0.85025100 -0.81879500 0.15798700
C 5.23353000 -1.27129100 0.37950000
H 5.80588000 -0.33798000 0.32961900
H 4.89321000 -1.39784800 1.41378200
H 5.91996800 -2.09594500 0.14803700
C 2.89556900 -2.95644000 -0.71061400
H 2.06682500 -3.03612900 -1.42664500
H 3.59207400 -3.77566300 -0.93037400
H 2.49735900 -3.14220800 0.29768000
C 4.36971900 -1.00998100 -2.60320100

H 5.06058500 -1.80827700 -2.90300700
 H 3.53043600 -1.01190400 -3.30888200
 H 4.89526600 -0.05456400 -2.71529100
 C 2.12177000 4.24760700 -0.49876800
 H 2.00301000 5.29646700 -0.20213500
 H 2.07686400 4.22443700 -1.59719200
 H 3.52520100 3.71038700 1.05665700
 C -6.62695800 0.02657400 -0.73046100
 C -4.33705000 0.18691000 -0.86529700
 C -6.79102400 1.41308000 -0.73372900
 H -7.49479100 -0.62952400 -0.67624800
 C -4.40181200 1.58571800 -0.87354200
 C -5.64816300 2.20749200 -0.80643200
 H -7.78348100 1.85030900 -0.68086600
 H -3.48976900 2.17321000 -0.93119400
 H -5.72349100 3.29164700 -0.81136200
 C -3.01438700 -0.54952000 -0.90874200
 H -3.08099100 -1.32657800 -1.67906500
 H -2.20868200 0.13382100 -1.19860500
 C -2.69326400 -1.20030300 0.45136600
 H -2.63717900 -0.43155100 1.23193600
 H -3.50572800 -1.88459900 0.72442700
 P -1.07967800 -2.11976100 0.49517300
 C -1.16203300 -2.95827500 2.14072700
 H -2.11723200 -3.47526400 2.28581600
 H -0.34760000 -3.68617200 2.22060900
 H -1.01751500 -2.20479100 2.91897200
 C -1.37346400 -3.52874700 -0.67602700
 H -2.30183900 -4.06150100 -0.44093800
 H -1.42553600 -3.16226800 -1.70567600
 H -0.53708700 -4.23271800 -0.61234800
 N -5.43803100 -0.58150100 -0.79373600
 C 0.19521100 0.98379600 2.35465000
 O -0.09854200 2.08305100 2.76044900
 O 0.40215400 -0.16429900 2.71248700

TS8-4h

C -1.28834800 -2.15823000 2.77258800
 C -3.54971400 -2.59951000 1.75081400
 H -1.70123900 -1.63569200 3.65001100
 H -0.34011400 -2.60376900 3.09937900
 C -3.20837600 -1.80648400 0.47651700
 H -4.29972900 -3.36380100 1.51200700
 H -2.91124800 -2.52509700 -0.30307700

H -4.09663300 -1.29048300 0.09529900
 C -1.03852700 -1.14310000 1.67344900
 C 0.10646900 -0.44525700 1.47915600
 C -2.07115900 -0.82001400 0.67831600
 C -1.84167200 0.29811900 -0.09210800
 Si -2.55999400 0.64233100 -1.81143200
 H 0.98648800 -0.61572200 2.11005300
 Ni -0.05858200 1.01566300 0.31052700
 C -4.15039100 1.67889700 -1.73662200
 H -4.93105000 1.17281500 -1.15617100
 H -3.97941400 2.65676200 -1.27233400
 H -4.54447200 1.85316800 -2.74617800
 C -1.27019400 1.57885000 -2.84750900
 H -0.32305400 1.02733200 -2.91179500
 H -1.64122100 1.70873600 -3.87236000
 H -1.05644900 2.56963000 -2.43542400
 C -2.94042200 -0.95766000 -2.77235600
 H -3.15460600 -0.71257700 -3.82093000
 H -2.08625300 -1.64607500 -2.76543700
 H -3.80772200 -1.49851400 -2.37978400
 C -2.29376400 -3.24304600 2.35159400
 H -2.55635400 -3.86616300 3.21565800
 H -1.83535100 -3.90968000 1.60631200
 H -4.00594300 -1.93002600 2.49369800
 C 1.93922900 2.88422200 1.17520400
 C 2.88116800 1.22744500 -0.16627700
 C 3.16074800 3.51843700 1.35824000
 H 1.02657100 3.27986700 1.60809200
 C 4.14108900 1.82433700 -0.02687000
 C 4.28817800 2.97297900 0.74255900
 H 3.21902000 4.41869500 1.96074100
 H 4.99401700 1.38200300 -0.53283300
 H 5.26230800 3.44117900 0.85263900
 C 2.70938300 -0.02424000 -0.99567200
 H 1.64304800 -0.16169800 -1.20203300
 H 3.21793500 0.11678000 -1.95858500
 C 3.27079600 -1.28095300 -0.29957900
 H 4.32633200 -1.12164000 -0.04179300
 H 2.72715600 -1.45779400 0.63674400
 P 3.20760500 -2.80930400 -1.39242900
 C 3.77174200 -4.06685400 -0.13275700
 H 3.19603700 -4.02018900 0.79991400
 H 3.67171100 -5.07257900 -0.55516100
 H 4.83080100 -3.90882800 0.09871000

C 1.37412900 -3.15965300 -1.37045200
H 0.93837900 -3.07369100 -0.36801000
H 0.85150900 -2.46499300 -2.03601600
H 1.20072400 -4.17225800 -1.75156900
N 1.79734700 1.76237400 0.43965400
C -1.89490000 2.20858000 0.79986900
O -2.75294900 2.27256200 1.61917800
O -1.07321200 2.83679300 0.12279000

TS8-4h'

C -1.41003600 2.88616900 -2.25891600
C -3.39360900 3.60558100 -0.88848200
H -2.02221400 2.63075800 -3.13865400
H -0.42182800 3.16916900 -2.64316700
C -3.12919000 2.54076300 0.19044200
H -3.92163300 4.45450500 -0.43644200
H -2.60594000 3.02738600 1.02808100
H -4.07521600 2.16685700 0.59521700
C -1.29384400 1.65921900 -1.37475300
C -0.31082900 0.73373100 -1.44856900
C -2.27955300 1.38221100 -0.31148500
C -2.24823100 0.13025100 0.24481700
Si -2.82434400 -0.38500400 1.97231300
H 0.51904400 0.86908400 -2.15194700
Ni -0.67444400 -0.85666600 -0.50285100
C -4.43594500 -1.38846400 1.93433300
H -5.24831000 -0.82266100 1.46301000
H -4.32010400 -2.32566900 1.37903800
H -4.75225600 -1.64231400 2.95433000
C -1.45272400 -1.44899500 2.75086900
H -0.49815200 -0.90802000 2.78167300
H -1.71772900 -1.70863300 3.78396500
H -1.30034100 -2.38094100 2.19767600
C -3.08203300 1.07775800 3.16447000
H -3.22825100 0.68586100 4.17973700
H -2.21084300 1.74319200 3.19395600
H -3.95935200 1.68504200 2.91895900
C -2.08496100 4.06587000 -1.54101100
H -2.27305400 4.87953900 -2.25255100
H -1.41392500 4.46725100 -0.76736700
H -4.05905000 3.19427200 -1.66091500
C 6.55250000 0.41883100 0.73601200
C 4.25396100 0.49111800 0.71231600
C 6.66036800 1.79812800 0.92477400

H 7.44749000 -0.19829200 0.66764600
C 4.26206000 1.87903700 0.89793200
C 5.48443700 2.54164200 1.00638800
H 7.63578500 2.26836200 1.00479300
H 3.32493400 2.42534300 0.95719200
H 5.51602900 3.61810400 1.15277000
C 2.96017300 -0.28528700 0.57928600
H 2.94790700 -1.06671200 1.34982500
H 2.10278800 0.37126200 0.76336100
C 2.82530300 -0.93210200 -0.81224700
H 2.80656300 -0.14945400 -1.58075800
H 3.69793300 -1.56550400 -1.01056300
P 1.26906600 -1.91983200 -1.01308600
C 1.37489600 -2.48863000 -2.76878400
H 2.33563600 -2.97086400 -2.98097900
H 0.56570200 -3.19818600 -2.96787400
H 1.24695600 -1.63269700 -3.43846300
C 1.59514900 -3.47165500 -0.06203800
H 2.52300800 -3.95668500 -0.38528900
H 1.66399000 -3.24792600 1.00683500
H 0.75641100 -4.15961700 -0.20728800
N 5.38733400 -0.22786800 0.63126700
C -2.67684900 -1.62840900 -0.86839300
O -3.60468400 -1.44474800 -1.58771400
O -1.94660600 -2.47439700 -0.33137600

INT7-4e

C 4.26147300 1.94030100 2.10842300
C 4.69325000 0.80030000 1.18187300
C 3.85428800 0.79488900 -0.10681600
C 2.34357000 0.75136300 0.15187900
C 1.51841300 -0.07729600 -0.51704000
Si 1.87190800 -1.16251700 -2.02765400
C 2.96705700 -2.65167500 -1.57110600
H 2.48711900 -3.27763800 -0.80856300
H 3.13983600 -3.28253300 -2.45251000
H 3.94679100 -2.34924600 -1.18395500
C 0.24945700 -1.84375400 -2.73594100
H 0.44998200 -2.40869600 -3.65566700
H -0.25780700 -2.51826700 -2.03685700
H -0.44245200 -1.03179700 -2.98906100
C 2.69465700 -0.14209100 -3.40007000
H 2.06812000 0.72043300 -3.65614900
H 3.67988200 0.23921800 -3.11108200

H 2.82254500 -0.74498400 -4.30832900
 C 2.76009000 1.83538400 2.42267600
 C 1.89624400 1.74994100 1.17357300
 C 0.84991300 2.59136400 1.03279100
 H 0.69148700 3.34345800 1.80366400
 Ni -0.31405700 0.02387400 -0.10911500
 C -0.12990000 2.73951600 -0.09470700
 O -0.65807000 3.83164200 -0.27736800
 O -0.42988400 1.67835400 -0.82424900
 P -4.62721800 0.92235500 -0.23226400
 C -4.37917600 2.59590300 0.55565800
 C -3.23185300 0.00519000 0.64118200
 C -3.83050300 1.24977300 -1.88814100
 H -4.59533200 2.53671300 1.62831900
 H -5.08959700 3.30383200 0.11506700
 H -3.36419700 2.98478700 0.40906800
 H -2.32805000 0.63648700 0.61711200
 H -3.51377600 -0.09412200 1.69745200
 H -4.44541700 1.97885400 -2.42765700
 H -3.81296700 0.33403100 -2.48963400
 H -2.81313900 1.64515700 -1.79146300
 C -2.95281000 -1.39378400 0.05052100
 H -2.63340700 -1.29505500 -0.99522600
 H -3.87947900 -1.97836000 0.04588900
 C -1.89219600 -2.15903400 0.80902500
 C -2.19454600 -3.31277100 1.53713900
 C 0.34617000 -2.31881000 1.45862400
 C -1.19161100 -3.97825600 2.23866500
 H -3.21606200 -3.67924100 1.54509100
 C 0.10598900 -3.47004600 2.19926700
 H 1.33350600 -1.87698300 1.38479500
 H -1.42013900 -4.87632300 2.80534700
 H 0.92171700 -3.94996600 2.72955100
 N -0.62266800 -1.67626900 0.77632300
 H 4.15582000 -0.04043400 -0.74431900
 H 4.07654800 1.71620500 -0.66821900
 H 5.75725700 0.88949700 0.92795000
 H 4.57089900 -0.16129700 1.70188800
 H 4.83934000 1.92330500 3.04113000
 H 4.46596700 2.90527400 1.62398000
 H 2.59927000 0.91966000 3.01532000
 H 2.43534000 2.67494200 3.04722900

INT7-4f

C 4.36908100 -2.22722600 1.15934700
 H 5.15791200 -2.88370200 0.77026400
 H 4.86251200 -1.48074400 1.79750500
 C 3.36414500 -3.02619800 1.99413900
 H 2.93018700 -3.82699900 1.37741300
 H 3.86374400 -3.51264700 2.84187600
 C 2.24366500 -2.10696600 2.50302000
 H 2.67928400 -1.39176200 3.21812700
 C 1.58183200 -1.30993000 1.38043500
 C 0.24679100 -1.28262300 1.26833200
 Si 3.50281900 1.60962900 -1.18380600
 C 5.15308000 2.03702400 -0.35453000
 H 5.71210500 1.14447200 -0.04948300
 H 5.79399800 2.61831700 -1.02970600
 H 4.97032700 2.63965100 0.54215900
 C 3.80501100 0.61008900 -2.77761900
 H 4.30002800 1.25146100 -3.51847100
 H 4.43071100 -0.27809600 -2.64336100
 H 2.85412800 0.28114200 -3.21564100
 C 2.64292900 3.20284600 -1.73433300
 H 1.67739900 2.99144200 -2.21106800
 H 2.45553600 3.86772900 -0.88737200
 H 3.26427800 3.73121600 -2.46865300
 C 3.67106400 -1.51185600 -0.01229500
 H 4.40677000 -0.93657700 -0.57703200
 C 2.51577000 -0.62479400 0.43512400
 C 2.36655700 0.66020200 0.02857200
 Ni -0.73233900 -0.29808100 0.03953700
 H 3.27821400 -2.28105700 -0.69751600
 H 1.48768400 -2.68055900 3.05177300
 C 1.31250800 1.56142100 0.62336100
 O 1.65799400 2.60554500 1.16632800
 O 0.03692400 1.25136600 0.46679600
 P -4.51906600 2.34612200 0.44448200
 C -4.53357700 2.56723100 2.29762300
 C -3.88974900 0.57159100 0.39783900
 C -2.95176400 3.27238200 0.03463800
 H -5.30989200 1.93448500 2.74175400
 H -4.77891200 3.60822800 2.53372900
 H -3.56800500 2.32291200 2.75673500
 H -3.03640400 0.45530400 1.08043900
 H -4.69876100 -0.06922100 0.77220800
 H -3.08534900 4.32253300 0.31781200
 H -2.77507400 3.25224900 -1.04636400

H -2.06437200 2.87778200 0.54321200
 C -3.49231800 0.11278000 -1.02230600
 H -2.65194900 0.72306600 -1.38620700
 H -4.32218100 0.29448800 -1.71496600
 C -3.11047800 -1.34869000 -1.08959100
 C -3.97916800 -2.31286400 -1.60678300
 C -1.51663100 -2.99855300 -0.64564500
 C -3.59435400 -3.65124400 -1.63843000
 H -4.94890300 -2.00269000 -1.98299700
 C -2.33620100 -4.00097400 -1.14934600
 H -0.52991600 -3.20571600 -0.24706800
 H -4.26315000 -4.40610900 -2.04182800
 H -1.98813300 -5.02837700 -1.15707300
 N -1.89058400 -1.70365900 -0.61126500
 H -0.38619500 -1.80415000 1.99336400

TS6-4e

C 1.01239100 1.66685900 -0.12998000
 C 1.56866700 0.48549700 0.31812700
 Si 2.31449200 0.06871800 2.02041500
 C 0.89164500 -0.23685400 3.24376000
 H 0.23938600 -1.04366800 2.88855900
 H 1.28963900 -0.53786500 4.22130000
 H 0.27013300 0.65205400 3.40319300
 C 3.36344800 -1.50089300 1.90694300
 H 3.86737600 -1.68495900 2.86483600
 H 2.75564600 -2.38201400 1.67208300
 H 4.12680100 -1.40587100 1.12828900
 C 3.42705200 1.46450000 2.66465600
 H 2.87382400 2.38759600 2.86635600
 H 3.91612400 1.15883100 3.59857200
 H 4.21536000 1.69728600 1.93904300
 C 0.88352500 1.93042200 -1.54558800
 C 1.62980400 1.25551000 -2.47843600
 H 1.55913500 1.53160500 -3.52677300
 Ni 1.19612100 -1.17766500 -0.59395600
 C 2.71085300 0.32654300 -2.17964900
 O 3.60731800 0.02462000 -2.94838600
 O 2.71805200 -0.19919900 -0.89530900
 P -3.93796300 1.32759900 0.00179300
 C -5.79363600 1.16920300 0.12037500
 C -3.50944000 -0.49782900 -0.13405800
 C -3.54928800 1.60082100 1.80827900
 H -6.20343500 0.88197700 -0.85395700

H -6.22322900 2.14118500 0.38594000
 H -6.11068300 0.43199400 0.86871600
 H -3.87508500 -1.02077700 0.76085800
 H -4.07290400 -0.89054200 -0.99077300
 H -3.86987300 2.60650600 2.10085000
 H -2.46863500 1.53981100 1.97447300
 H -4.04692600 0.87085600 2.45913800
 C -2.00766500 -0.74511900 -0.33467200
 H -1.41961000 -0.22693300 0.43327200
 H -1.67958200 -0.29821700 -1.28237100
 C -1.57907200 -2.19594500 -0.32386100
 C -2.48662100 -3.25935000 -0.27824400
 C 0.19230200 -3.71841000 -0.34637200
 C -2.03309000 -4.57606300 -0.27328700
 H -3.54940500 -3.05195700 -0.25099500
 C -0.66034500 -4.81299900 -0.30598200
 H 1.26925600 -3.85096600 -0.36914200
 H -2.74022200 -5.40006400 -0.24270500
 H -0.25106900 -5.81756100 -0.29890400
 N -0.24135500 -2.43607800 -0.36340200
 C -0.05684100 3.02858200 -2.01655400
 C -0.09819500 4.23130200 -1.06492700
 C -0.40332900 3.75575300 0.35716000
 C 0.68241600 2.79199500 0.85625000
 H -0.47651000 4.60673400 1.04641500
 H 0.86821200 4.75505000 -1.08246000
 H -0.85626200 4.94738800 -1.40510300
 H -1.07385500 2.61095600 -2.08050300
 H 0.21699800 3.34285900 -3.02990800
 H 1.59787500 3.37676100 1.04019200
 H 0.38721800 2.38237600 1.82881600
 H -1.38146500 3.25618700 0.36050600

TS6-4f

C -3.86699500 2.93469000 -0.09486400
 C -2.76246300 3.87074500 -0.58667500
 C -1.88063300 3.13061500 -1.59642600
 H -1.03168600 3.76143800 -1.88844700
 C -1.38440500 1.78801800 -1.06203700
 C -0.21080100 1.26674000 -1.56612600
 Si -2.96561300 -1.58679900 1.05059000
 C -1.82042800 -3.00267200 1.59650500
 H -0.93126000 -2.61347600 2.11163400
 H -2.34369000 -3.65873600 2.30444000

H -1.49580000 -3.59783500 0.74094000
 C -3.46350400 -0.76998200 2.70603700
 H -3.67006000 -1.56655500 3.43309700
 H -2.65378700 -0.15651900 3.12065800
 H -4.35941300 -0.14346900 2.65108700
 C -4.52482700 -2.30919100 0.24672800
 H -5.25808600 -1.52765900 0.01187800
 H -4.25652500 -2.81347800 -0.68708100
 H -5.01425400 -3.03811800 0.90564100
 C -3.28187000 1.69658800 0.60331400
 H -2.85996400 2.01005700 1.57083600
 C -2.19011300 0.98717200 -0.19327800
 C -2.04695000 -0.40352900 -0.12635300
 Ni 1.04913200 0.06997000 -0.84873600
 H -4.09513400 1.00559900 0.83374700
 H -2.46888400 2.96954800 -2.51621500
 C -1.30986700 -1.15206700 -1.15781700
 O -1.53705100 -2.34253900 -1.39996500
 O -0.36642100 -0.52865700 -1.93558800
 P 2.37919300 -1.84684800 -0.66116300
 C 3.63324800 -2.27352900 -1.95535500
 C 3.38720600 -1.67811500 0.89991000
 C 1.48975000 -3.44872000 -0.42468700
 H 4.30089800 -1.42234500 -2.12383300
 H 3.11163000 -2.48601700 -2.89421800
 H 4.23066100 -3.14978800 -1.67848100
 H 3.50230600 -2.65080100 1.39226200
 H 4.39305300 -1.31869800 0.65182100
 H 0.72492800 -3.54715100 -1.20064700
 H 0.96466900 -3.43341000 0.53492200
 H 2.17563800 -4.30356300 -0.44612500
 C 2.69424000 -0.68016100 1.86234000
 H 3.12880800 -0.78013900 2.86310900
 H 1.63010300 -0.93310800 1.95302200
 C 2.83305400 0.76334000 1.43055300
 C 3.65284800 1.62861500 2.16332300
 C 2.32736500 2.48896800 -0.04574800
 C 3.81322900 2.95390200 1.76882700
 H 4.15827700 1.25131900 3.04673900
 C 3.13370400 3.39270400 0.63505600
 H 1.75989100 2.79457100 -0.91602100
 H 4.44869500 3.62699800 2.33707400
 H 3.21178700 4.41570700 0.28188700
 N 2.17339700 1.19880300 0.32459500

H -2.15437600 4.20286300 0.26760200
 H -3.19013900 4.77115100 -1.04657300
 H -4.47567200 2.61724600 -0.95389700
 H -4.54416000 3.45357100 0.59552900
 H 0.19978600 1.69271600 -2.48968800

L2=PN

P 2.80811000 -0.48289500 0.24492200
 C 3.16132100 1.25590600 0.83014800
 C 1.02071400 -0.29035000 -0.29433500
 C 3.61782400 -0.39984100 -1.43651500
 H 2.64066600 1.44648200 1.77442900
 H 2.85533700 2.01660700 0.10106400
 H 4.23503500 1.36269000 1.02022100
 H 0.89458900 0.61256200 -0.90586600
 H 0.78516500 -1.15107500 -0.93471300
 H 3.28466500 0.46524400 -2.02326200
 H 3.39252800 -1.31277600 -1.99849400
 H 4.70533100 -0.34403300 -1.31668900
 C 0.03014500 -0.24639200 0.88686500
 H 0.27066900 0.60619600 1.53307200
 H 0.13135600 -1.15545800 1.49139400
 C -1.40038700 -0.09265600 0.41666600
 C -2.30944700 -1.15812300 0.46272800
 C -2.98818700 1.28566200 -0.51746800
 C -3.60764500 -0.96663100 -0.00796200
 H -1.99985700 -2.11902700 0.86441400
 C -3.96099500 0.28422600 -0.51150900
 H -3.22433500 2.27825900 -0.89954600
 H -4.32958800 -1.77877000 0.02075400
 H -4.96001900 0.48358800 -0.88749000
 N -1.74046300 1.11459200 -0.06926200

NiL2

Ni 0.35894800 1.26094000 -0.20760400
 C -2.49661900 1.21560300 -0.00525100
 C -1.39507900 -0.81900000 -0.34946400
 C -3.65421500 0.57912900 0.42935500
 H -2.44893600 2.29705000 -0.07703500
 C -2.53372200 -1.50678100 0.06797800
 C -3.67970800 -0.81326200 0.46774900
 H -4.51838600 1.17097600 0.71551700
 H -2.51996100 -2.59285200 0.07371900
 H -4.56708000 -1.34977900 0.79056100

C -0.15832800 -1.57857600 -0.79386900
 H -0.45383300 -2.62203600 -0.96313300
 H 0.16530000 -1.17732600 -1.76322400
 C 1.04462000 -1.57295700 0.19196200
 H 0.68082700 -1.73723900 1.21406000
 H 1.71332300 -2.41194200 -0.05006700
 P 2.01398500 0.05440300 0.18440800
 C 3.30763400 -0.31386000 -1.10870500
 H 3.85583600 -1.24085700 -0.89748600
 H 2.83181900 -0.39736500 -2.09097700
 H 4.02037900 0.51616900 -1.15430800
 C 3.03954800 -0.16599900 1.72599200
 H 3.79739500 0.62326800 1.77210000
 H 2.39865500 -0.06846500 2.60804800
 H 3.54318500 -1.14079900 1.75606300
 N -1.37194500 0.55186200 -0.37736000

Ni(L2)₂

P 1.68676200 -1.85538100 -1.39296600
 C 2.69309500 -3.37606800 -1.76468100
 C 3.03948500 -0.69504600 -0.83524600
 C 1.35978900 -1.24662800 -3.12207200
 H 3.07995600 -3.79409300 -0.82995100
 H 3.53467500 -3.15991000 -2.43436800
 H 2.05250600 -4.13141900 -2.23122500
 H 3.50647100 -1.14357400 0.04875400
 H 3.81274200 -0.61914700 -1.61290400
 H 2.28353000 -1.15499000 -3.70729300
 H 0.86155400 -0.27298300 -3.08557600
 H 0.68601100 -1.94493300 -3.62906700
 C 2.51679100 0.70023600 -0.44946700
 H 1.69444300 0.57155700 0.26713700
 H 2.09825800 1.21121700 -1.32473900
 C 3.58866800 1.56775700 0.17644000
 C 3.95456000 2.80171400 -0.37800500
 C 5.11417800 1.82895300 1.88013800
 C 4.94381300 3.56257000 0.24333300
 H 3.46611900 3.15698800 -1.28107100
 C 5.54168700 3.06899900 1.40163500
 H 5.55458800 1.40711400 2.78295800
 H 5.24119000 4.52285200 -0.17029200
 H 6.31629000 3.62399700 1.92236800
 N 4.16710000 1.09121500 1.29331300
 Ni -0.00724800 -2.00599900 -0.07851200

P -1.69427900 -1.95636800 1.24218000
 C -3.08873400 -0.81790900 0.72960400
 H -3.86263800 -0.80752300 1.51025200
 H -3.53415700 -1.27097900 -0.16557200
 C -2.59931000 0.59985000 0.41497500
 H -2.13591800 1.04895700 1.30285600
 H -1.79239800 0.53908200 -0.32821300
 C -3.64004200 1.58225700 -0.09155500
 C -4.97068200 1.23392100 -0.35684400
 C -4.03730400 3.75960600 -0.73154100
 C -5.84994100 2.20905000 -0.82925300
 H -5.31689300 0.21853500 -0.19632400
 C -5.37907200 3.50492000 -1.02414500
 H -3.62596400 4.75948500 -0.86744300
 H -6.88617500 1.95651800 -1.03971000
 H -6.02570600 4.29724700 -1.38920800
 N -3.18586900 2.83633500 -0.27866200
 C -1.38448500 -1.39623300 2.99027700
 H -0.91481700 -0.40808500 2.98774700
 H -2.30895900 -1.35311600 3.57986400
 H -0.68845200 -2.09153100 3.47053700
 C -2.65640600 -3.51717100 1.56489600
 H -3.50122900 -3.34952200 2.24453600
 H -3.03307600 -3.91753200 0.61820900
 H -1.99138800 -4.26752100 2.00440600

Ni(L2)₂-1

Ni 0.05510800 1.49766000 -0.20517200
 C 2.54594200 2.23583600 0.73850700
 C 2.70525100 0.87311400 -1.14570200
 C 3.92454300 2.35816600 0.83783100
 H 1.88703000 2.73120700 1.44156100
 C 4.09898200 0.96211700 -1.09590100
 C 4.72700900 1.70799100 -0.10106300
 H 4.35321000 2.95679100 1.63543000
 H 4.68317200 0.44190800 -1.84956300
 H 5.80985600 1.78301500 -0.06236800
 C -2.39395500 2.13563400 -1.31499000
 C -2.62213400 1.25203000 0.82964500
 C -3.76436700 2.30332000 -1.45444200
 H -1.71087600 2.42159300 -2.10587300
 C -4.00921200 1.39941800 0.74586400
 C -4.59854200 1.92868800 -0.39999100
 H -4.16194700 2.72407800 -2.37267700

H -4.61893800 1.09676000 1.59227000
 H -5.67597300 2.04887800 -0.46620800
 C -1.98178800 0.65110900 2.05697300
 H -1.03703900 1.17767400 2.23844700
 H -2.63686200 0.81555900 2.92159900
 C 2.02080900 0.04272000 -2.20415400
 H 1.08473900 0.54657000 -2.47376900
 H 2.65704200 0.00006800 -3.09703100
 C -1.70264000 -0.85784600 1.89723900
 H -2.62811700 -1.37400900 1.60803700
 H -0.97605600 -0.99991100 1.08525300
 P -1.10127400 -1.67234600 3.47730800
 C 1.71003300 -1.38904200 -1.72090700
 H 2.63235600 -1.86479900 -1.36114600
 H 1.01279300 -1.33511800 -0.87373300
 P 1.02308500 -2.49410600 -3.07382800
 C 0.62232300 -3.99228100 -2.03191500
 H 0.02595900 -3.74232800 -1.14533800
 H 0.06569000 -4.71845500 -2.63444700
 H 1.55073700 -4.47405300 -1.70618800
 C -0.69531800 -1.78394800 -3.24641500
 H -1.18582800 -1.63125900 -2.27759200
 H -0.65125400 -0.82283000 -3.76885400
 H -1.30634400 -2.46203300 -3.85272600
 C 0.63148000 -0.98162700 3.57514700
 H 1.16294400 -1.03799500 2.61726600
 H 0.59852800 0.06558400 3.89325600
 H 1.19813000 -1.53781200 4.33038200
 C -0.71028700 -3.36239600 2.78485500
 H -0.19854500 -3.96119200 3.54624000
 H -1.64133900 -3.87904800 2.52723500
 H -0.07559700 -3.31484300 1.89099500
 N -1.80824000 1.62232100 -0.20068600
 N 1.92264200 1.51232000 -0.22920200

Ni(L2)₂-2

Ni -0.51381900 0.70761300 0.51129600
 C -1.35753200 1.02973200 -2.19661400
 C -2.43571400 -0.79006700 -1.23550300
 C -2.30546500 1.13648700 -3.20801800
 H -0.50090700 1.69732300 -2.16609400
 C -3.41487500 -0.74666200 -2.23190900
 C -3.36374300 0.22765700 -3.22927700
 H -2.19964200 1.90365100 -3.96939400

H -4.21216000 -1.48479200 -2.22223700
 H -4.12156500 0.26631100 -4.00662700
 C -2.50368500 -1.83055900 -0.14005300
 H -3.16389100 -2.64125700 -0.47190600
 H -1.50619400 -2.26475000 0.00513500
 C -3.02180300 -1.27073100 1.20774400
 H -3.92621100 -0.67392800 1.03158600
 H -3.30503200 -2.09775500 1.87227300
 P -1.73039400 -0.16675000 2.01873100
 C -0.95232900 -1.38418900 3.19956400
 H -1.69871200 -1.89980200 3.81803800
 H -0.37864100 -2.12866700 2.63755000
 H -0.25509600 -0.85244700 3.85552700
 C -2.81191100 0.77682600 3.20694400
 H -2.17980200 1.35708600 3.88711100
 H -3.43825900 1.48087600 2.64904000
 H -3.45864800 0.11727400 3.79987800
 N -1.41367300 0.10913100 -1.20443000
 P 2.30852600 -2.77476200 -0.13762700
 C 4.14296100 -3.06097100 0.07724200
 H 4.73188800 -2.66989200 -0.76254600
 H 4.49003300 -2.58601300 1.00108000
 H 4.33564800 -4.13569400 0.16853700
 C 2.09842300 -3.49308700 -1.84906600
 H 1.08744500 -3.28036900 -2.21329700
 H 2.82155700 -3.08925800 -2.56888300
 H 2.21641600 -4.58155500 -1.80788400
 C 2.29814300 -0.95575500 -0.58482400
 H 1.30212600 -0.74135300 -0.99185700
 H 3.03596100 -0.74942400 -1.37369500
 C 2.53839300 -0.03053600 0.62754000
 H 3.55629300 -0.17429800 1.01108500
 H 1.83404500 -0.29974300 1.42703800
 C 2.33045600 1.42716300 0.30190500
 C 3.40773800 2.28158700 0.06578200
 C 3.19618100 3.62507200 -0.24465700
 H 4.41635000 1.88200500 0.13067100
 C 0.84557200 3.18155700 -0.05404000
 C 1.87470200 4.07656300 -0.30532600
 H 4.03064500 4.29532500 -0.42788600
 H -0.18991500 3.50770700 -0.07414500
 H 1.63899800 5.11131300 -0.53640800
 N 1.03640700 1.86817100 0.25026600

Ni(L2)₂-3

Ni	-1.20833100	-0.45179300	0.10206300
C	0.17858400	2.00633700	0.56029700
C	-1.81400400	2.37860200	-0.57761400
C	0.29730300	3.34883100	0.90823500
H	0.95631500	1.29951600	0.82717200
C	-1.73879500	3.74238000	-0.28385200
C	-0.68141700	4.24162300	0.47714400
H	1.15836700	3.67917000	1.48082300
H	-2.51371600	4.40737100	-0.65487400
H	-0.61755400	5.30110300	0.70943600
C	-2.98345200	1.83619500	-1.37007800
H	-3.47067400	2.67368600	-1.88419100
H	-2.60433000	1.15864800	-2.14625900
C	-4.03119900	1.09228400	-0.50289500
H	-4.25878300	1.69278600	0.38739700
H	-4.96774900	0.98018200	-1.06571800
P	-3.36630400	-0.57707200	0.05594000
C	-4.13542700	-1.67488400	-1.24310900
H	-5.22175300	-1.53632100	-1.31945900
H	-3.68239600	-1.46327600	-2.21747800
H	-3.92698200	-2.72219800	-1.00140300
C	-4.51825600	-0.93094900	1.47898500
H	-4.37619300	-1.96536200	1.80953000
H	-4.26997200	-0.27466000	2.31972900
H	-5.57381200	-0.78691500	1.21426000
N	-0.86434100	1.50431300	-0.14485300
P	0.17820300	-2.09282100	0.29448200
C	0.01595300	-3.21642800	1.77505200
H	0.75505800	-4.02794200	1.76914500
H	0.14161700	-2.63074800	2.69195500
H	-0.99027700	-3.64702300	1.78953900
C	0.15214500	-3.36796500	-1.06859400
H	0.36142100	-2.88924900	-2.03067600
H	0.88712100	-4.16598600	-0.90118000
H	-0.84631600	-3.81263700	-1.12872300
C	2.03129400	-1.77474000	0.40477800
H	2.59583400	-2.71440700	0.49232500
H	2.18663200	-1.21247000	1.33375000
C	2.55866700	-0.93209300	-0.77230000
H	1.81645700	-0.15587500	-1.00507700
H	2.66286800	-1.55462800	-1.66893700
C	3.87612900	-0.25872100	-0.46015200
C	5.06292200	-0.59901200	-1.12321700

C	6.24714100	0.05328300	-0.78376700
H	5.05162600	-1.36429100	-1.89429300
C	4.98775100	1.30396900	0.81677900
C	6.21494300	1.02991200	0.21041600
H	7.17757700	-0.19674100	-1.28726400
H	4.91823300	2.06158200	1.59664400
H	7.11022500	1.56639600	0.50999400
N	3.84637700	0.68527700	0.49958000

Ni(L2)₂-4

Ni	0.19397800	-0.65508500	0.21422000
C	1.35077100	2.05558400	-0.05686100
C	2.84169000	0.47858800	-0.86667700
C	2.20067700	3.11296700	-0.35744500
H	0.38639400	2.23526900	0.40778600
C	3.74263200	1.49614200	-1.20313900
C	3.43110300	2.83028500	-0.95140800
H	1.89979900	4.13040200	-0.12566500
H	4.69269400	1.22945900	-1.65748600
H	4.12977400	3.62254500	-1.20522700
C	-1.60775200	1.13518700	-1.32033300
C	-2.77589400	0.15198400	0.42122100
C	-2.72483600	1.82977800	-1.76817400
H	-0.65613400	1.22768900	-1.83438000
C	-3.93751500	0.82999700	0.03132800
C	-3.92497600	1.67906600	-1.07279600
H	-2.64867000	2.46994600	-2.64215100
H	-4.85160600	0.67865500	0.59848800
H	-4.82537800	2.20183700	-1.38309600
C	-2.82582400	-0.80669700	1.59070300
H	-3.85185600	-0.81142600	1.97843300
H	-2.62490000	-1.81953300	1.21195000
C	3.22223600	-0.96605200	-1.10449100
H	4.23574800	-0.98303200	-1.52342700
H	3.27209200	-1.47269200	-0.12966700
C	-1.84616800	-0.49796500	2.74500800
H	-1.84384100	0.58022200	2.95159300
H	-2.19171300	-0.99867300	3.65974200
P	-0.08863100	-1.01702700	2.33046200
C	2.27239600	-1.75477100	-2.03405900
H	1.99370500	-1.13224000	-2.89437300
H	2.79633100	-2.63523400	-2.43023500
P	0.69809600	-2.26481400	-1.14505300
C	-0.32860100	-2.78074200	-2.62120400

H 0.20607800 -3.45529200 -3.30309900
H -1.23522200 -3.28618300 -2.27018100
H -0.63987200 -1.88871500 -3.17552700
C 1.20376800 -3.96915100 -0.56326800
H 1.58773500 -4.59870500 -1.37721500
H 1.97495500 -3.87732300 0.20864200
H 0.34084800 -4.46852400 -0.10953500
C -0.08825800 -2.74364100 3.04774400
H -0.39990300 -2.76762300 4.10058900
H -0.75958800 -3.38104900 2.46282700
H 0.91929600 -3.16621100 2.96857600
C 0.80909400 -0.15218800 3.72671700
H 1.85092700 -0.49057400 3.75122800
H 0.81513400 0.92769300 3.54293800
H 0.35651400 -0.34317000 4.70894600
N -1.60483000 0.30915400 -0.24971400
N 1.63739800 0.75604500 -0.30001700