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Chem. Eur. J. **2001**.

(η^3 -1,3-Dialkylallyl)(phosphino-oxazoline)palladium
Complexes: X-Ray Crystallographic Studies, NMR
Investigations and Quantum Chemical Calculations
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Prof. Dr. Michael Reggelin, Dr. Frank Rominger
Prof. Dr. Günter Helmchen*

Calculated geometries of the isomers of complex 6

66 exosynsyn

Pd	.703719	1.548737	-.513851
N	1.935920	-.213579	-.762888
P	-1.114057	-.008406	.000995
C	1.624340	-1.373698	-1.182935
O	2.664186	-2.236316	-1.313588
C	3.913392	-1.520084	-1.019226
C	3.408447	-.169083	-.444662
C	.324153	-1.942121	-1.589972
C	-.926805	-1.459924	-1.182218
C	-2.068229	-2.089674	-1.648199
C	-1.988094	-3.176450	-2.505772
C	.392642	-3.044759	-2.433088
C	-.756728	-3.655060	-2.897327
H	-3.029520	-1.731444	-1.346348
H	-2.887575	-3.641810	-2.854976
H	1.351626	-3.418289	-2.717234
H	-.683599	-4.497353	-3.554123
H	4.474317	-2.116007	-.325058
H	4.449050	-1.405346	-1.946831
H	3.835661	.657727	-.985619
C	1.116419	3.776572	-.306733
C	-.269230	3.476762	-.384718
C	1.963440	3.357874	-1.308874
H	1.530546	4.104149	.631134
C	-1.191844	3.831319	.765930
H	-.721898	3.527161	-1.363716
C	3.465064	3.500271	-1.227329
H	1.555100	3.228018	-2.299268
C	-1.006641	-.772716	1.700740
C	-1.193603	-2.130504	1.914062
C	-1.121069	-2.645427	3.197894
C	-.867868	-1.808426	4.269647
C	-.682272	-.451946	4.060365
C	-.746863	.064576	2.779602
H	-1.392770	-2.785542	1.090947
H	-1.264353	-3.695152	3.356998
H	-.814705	-2.209268	5.261753
H	-.486944	.198850	4.888766
H	-.596808	1.114801	2.621818
C	-2.894625	.511748	-.199293
C	-3.857890	.208117	.749383
C	-5.166973	.625286	.563546
C	-5.515441	1.339261	-.567266
C	-4.553929	1.643045	-1.518798
C	-3.247277	1.235397	-1.333807
H	-3.596095	-.346137	1.626926
H	-5.907461	.389651	1.301040
H	-6.527941	1.659407	-.708909
H	-4.821596	2.195610	-2.396864
H	-2.506470	1.474330	-2.072672
H	-2.095730	3.239253	.732093
H	-.708244	3.672818	1.722862
H	-1.480603	4.876975	.705823

H	3.960661	2.741993	-1.818862
H	3.763019	4.464508	-1.629082
H	3.818346	3.436330	-.205788
C	3.081480	-1.110669	1.922346
C	3.649727	.031106	1.063074
H	2.016835	-1.227947	1.774788
H	3.570509	-2.053506	1.705830
H	3.245825	-.891363	2.970819
C	5.157447	.221445	1.327643
H	3.139427	.948971	1.336696
H	5.561467	1.042963	.745260
H	5.325709	.439248	2.375228
H	5.715627	-.676680	1.085755

66 endosynsyn

Pd	.679861	1.655141	-.149428
N	1.975910	.019252	-.709642
P	-1.087642	-.055794	.048456
C	1.721445	-1.058476	-1.336954
O	2.803870	-1.830483	-1.613277
C	4.014804	-1.109629	-1.197231
C	3.441303	.058632	-.354333
C	.451539	-1.615569	-1.840833
C	-.820087	-1.284329	-1.354633
C	-1.926773	-1.902319	-1.912720
C	-1.793023	-2.825755	-2.938231
C	.574918	-2.555666	-2.857277
C	-.540906	-3.151824	-3.411943
H	-2.903930	-1.660431	-1.552527
H	-2.667385	-3.284462	-3.353773
H	1.550754	-2.816591	-3.202798
H	-.425812	-3.866595	-4.200626
H	4.630033	-1.795846	-.647713
H	4.516552	-.772713	-2.089361
H	3.837628	1.000728	-.689191
C	.701152	3.916256	-.279912
C	2.020652	3.481119	-.189905
C	-.235427	3.503712	.677550
H	.349504	4.340548	-1.204098
C	3.013896	3.759370	-1.298375
H	2.436346	3.333823	.795024
C	-1.700520	3.860957	.563023
H	.125921	3.350594	1.684226
C	-.970442	-1.082325	1.604095
C	-1.121739	-2.461200	1.595104
C	-1.042050	-3.173855	2.779963
C	-.818082	-2.514071	3.975056
C	-.668656	-1.137367	3.988520
C	-.739521	-.423646	2.806385
H	-1.298558	-2.980157	.675564
H	-1.157320	-4.238893	2.766885
H	-.759580	-3.067936	4.890248
H	-.496087	-.623404	4.912655
H	-.616980	.642195	2.821897
C	-2.891794	.398505	-.109744
C	-3.828200	.016538	.836469
C	-5.154392	.395737	.689687
C	-5.546171	1.146600	-.401724
C	-4.610936	1.526872	-1.352589

C	-3.288174	1.159662	-1.204905
H	-3.534694	-.572136	1.680844
H	-5.874163	.098657	1.425529
H	-6.571694	1.435166	-.514697
H	-4.912342	2.106984	-2.201534
H	-2.568200	1.458525	-1.942748
H	3.803571	3.021390	-1.314618
H	2.532635	3.763461	-2.268423
H	3.480947	4.727958	-1.145322
H	-2.320983	3.140737	1.077259
H	-1.876151	4.833451	1.014463
H	-2.019685	3.903723	-.469855
C	3.134657	-1.406383	1.734418
C	3.650456	-.073381	1.166214
H	2.077417	-1.536285	1.548277
H	3.669562	-2.251401	1.316642
H	3.282951	-1.423694	2.807713
C	5.141713	.129115	1.504955
H	3.087414	.731606	1.627031
H	5.507465	1.079994	1.131460
H	5.283262	.114988	2.578655
H	5.752131	-.662142	1.083269

66 exoansy

Pd	.705053	1.544035	-.340803
N	1.895259	-.197680	-.825589
P	-1.135117	-.004444	.063873
C	1.554578	-1.325349	-1.307639
O	2.585839	-2.168327	-1.575335
C	3.849955	-1.461421	-1.332924
C	3.385793	-.177523	-.597567
C	.232323	-1.886715	-1.652522
C	-.995816	-1.430464	-1.155019
C	-2.156807	-2.070999	-1.555822
C	-2.120455	-3.139329	-2.438322
C	.256682	-2.968540	-2.525931
C	-.911921	-3.587166	-2.925219
H	-3.100889	-1.733059	-1.184281
H	-3.034778	-3.613060	-2.733565
H	1.198613	-3.321122	-2.883049
H	-.870780	-4.413160	-3.605081
H	4.477378	-2.106899	-.748774
H	4.297510	-1.254801	-2.291060
H	3.781336	.701413	-1.077057
C	1.155667	3.685575	.277079
C	-.235236	3.424975	.071851
C	2.066112	3.483291	-.729588
H	1.517782	3.789819	1.285152
C	-1.002601	-.804667	1.746441
C	-1.285880	-2.147605	1.948789
C	-1.194371	-2.690033	3.219375
C	-.826697	-1.895109	4.290536
C	-.544097	-.554179	4.092854
C	-.626500	-.010795	2.823697
H	-1.573065	-2.770226	1.126663
H	-1.411809	-3.728222	3.369698
H	-.759365	-2.317370	5.272842
H	-.259090	.063913	4.920307
H	-.398617	1.026585	2.673390
C	-2.912169	.549293	-.084610
C	-3.781319	.486076	.991503

C	-5.082703	.946876	.858042
C	-5.518239	1.461848	-.347416
C	-4.651959	1.519703	-1.428740
C	-3.352892	1.069259	-1.298075
H	-3.455730	.080537	1.926938
H	-5.749959	.896121	1.694672
H	-6.524801	1.814264	-.448804
H	-4.988073	1.912685	-2.367180
H	-2.689760	1.111721	-2.140747
C	3.177432	-1.354806	1.674806
C	3.715469	-.135592	.906628
H	2.100885	-1.427112	1.600424
H	3.615438	-2.278589	1.314663
H	3.428509	-1.261084	2.724811
C	5.238431	.011144	1.103613
H	3.235625	.753009	1.302859
H	5.624632	.879341	.580026
H	5.466069	.126777	2.156256
H	5.768035	-.866341	.748809
H	1.739147	3.539842	-1.753117
C	3.557901	3.585608	-.513503
H	3.832020	3.357300	.508624
H	4.096281	2.922279	-1.177335
H	3.888739	4.596298	-.735043
H	-.842325	3.451802	.960048
C	-.970410	3.903127	-1.176065
H	-.410262	3.742840	-2.087677
H	-1.920871	3.397530	-1.263039
H	-1.168357	4.968040	-1.091009

66 endoansy

Pd	.696780	1.590945	-.310192
N	1.922206	-.142113	-.706586
P	-1.135367	.011012	.020709
C	1.605120	-1.229176	-1.287201
O	2.638340	-2.078312	-1.519010
C	3.889913	-1.420635	-1.115785
C	3.387994	-.160778	-.359902
C	.304844	-1.716532	-1.789473
C	-.947623	-1.271019	-1.344312
C	-2.088362	-1.811704	-1.911536
C	-2.006827	-2.775629	-2.905520
C	.373818	-2.697690	-2.770920
C	-.775094	-3.219958	-3.334011
H	-3.050138	-1.479305	-1.582325
H	-2.905749	-3.173678	-3.331052
H	1.332689	-3.047037	-3.084829
H	-.701068	-3.968329	-4.096007
H	4.440546	-2.113277	-.508716
H	4.434414	-1.179284	-2.013477
H	3.832799	.730811	-.768626
C	.790342	3.802812	-.773054
C	2.100311	3.474177	-.498828
C	-.256347	3.471927	.133121
H	.526745	4.041592	-1.788553
C	3.194863	3.611418	-1.533411
H	2.426304	3.421163	.525534
C	-1.050764	-.981534	1.599918
C	-1.287919	-2.348390	1.623441
C	-1.234139	-3.039746	2.822252
C	-.949161	-2.370523	3.998981

C	-.712842	-1.006203	3.979604	H	1.301412	3.945004	1.278562
C	-.759215	-.313971	2.783543	C	-1.406450	3.744527	1.156961
H	-1.511259	-2.874627	.718228	H	-.784821	3.676516	-.950259
H	-1.416479	-4.095382	2.834156	C	-.946410	-.998089	1.647872
H	-.910535	-2.907635	4.925146	C	-1.029713	-2.380401	1.726003
H	-.492344	-.484850	4.889298	C	-.944537	-3.010041	2.956894
H	-.568293	.740988	2.774227	C	-.781453	-2.263866	4.110045
C	-2.905233	.583881	-.116187	C	-.699168	-.883249	4.035777
C	-3.875510	.187017	.789379	C	-.776934	-.251667	2.808505
C	-5.174174	.655438	.660519	H	-1.158561	-2.966076	.839117
C	-5.505232	1.512206	-.371865	H	-1.007858	-4.078122	3.011533
C	-4.536724	1.907872	-1.281745	H	-.718167	-2.753563	5.060814
C	-3.240182	1.450005	-1.151934	H	-.573758	-.302664	4.927485
H	-3.627654	-.478515	1.590251	H	-.707775	.817492	2.755546
H	-5.920223	.347870	1.365185	C	-2.881458	.343069	-.163776
H	-6.509675	1.871699	-.469684	C	-3.843803	-.137991	.709792
H	-4.791381	2.569970	-2.084734	C	-5.173619	.211956	.534262
H	-2.493374	1.759693	-1.857831	C	-5.543654	1.036169	-.511805
H	3.954779	2.852733	-1.402318	C	-4.583259	1.518215	-1.387564
H	2.802103	3.532852	-2.539276	C	-3.256137	1.177203	-1.211859
H	3.682091	4.576693	-1.431732	H	-3.564855	-.777353	1.521794
C	3.017488	-1.437976	1.837508	H	-5.913442	-.160943	1.213488
C	3.603166	-.185103	1.164894	H	-6.572223	1.304217	-.645637
H	1.956043	-1.529290	1.653405	H	-4.867569	2.156751	-2.199603
H	3.510773	-2.340678	1.496060	H	-2.516015	1.554282	-1.891519
H	3.160675	-1.373745	2.909750	H	-2.274234	3.118363	1.001570
C	5.106278	-.042241	1.480287	H	-.979487	3.512830	2.125500
H	3.090298	.684768	1.562743	H	-1.744296	4.776754	1.177158
H	5.521383	.855710	1.034440	C	3.238420	-1.039411	1.886916
H	5.256879	.015912	2.551273	C	3.720513	.208646	1.128854
H	5.667208	-.896272	1.116021	H	2.179447	-1.206181	1.744003
H	-1.254531	3.587805	-.248326	H	3.777089	-1.927617	1.577101
C	-.146705	3.700027	1.636680	H	3.410854	-.907436	2.948630
H	-.904370	3.128844	2.157091	C	5.216516	.473918	1.395078
H	.821547	3.434412	2.039855	H	3.156652	1.062844	1.488599
H	-.320067	4.749768	1.856265	H	5.558200	1.367427	.882740
				H	5.385336	.611923	2.455992
				H	5.828412	-.361283	1.071599
				H	2.949164	3.424635	-.348015
				C	1.769679	3.618578	-2.190067
				H	2.311447	2.851305	-2.729290
				H	.738842	3.599281	-2.512889
				H	2.189177	4.578956	-2.477031

66 exosyan

Pd	.663520	1.624226	-.254938
N	1.998840	-.004653	-.694618
P	-1.074892	-.081133	.026465
C	1.772266	-1.132213	-1.240055
O	2.874570	-1.890834	-1.466085
C	4.068893	-1.121860	-1.089184
C	3.468853	.127471	-.387933
C	.516985	-1.751335	-1.711839
C	-.769681	-1.397170	-1.282802
C	-1.858948	-2.057205	-1.825369
C	-1.694198	-3.051626	-2.777492
C	.670434	-2.763432	-2.652465
C	-.428178	-3.406135	-3.189766
H	-2.846131	-1.794602	-1.508942
H	-2.555161	-3.542825	-3.183732
H	1.655731	-3.041053	-2.955308
H	-.288913	-4.176691	-3.919855
H	4.667443	-1.743443	-.451152
H	4.598767	-.879030	-1.994918
H	3.820273	1.032731	-.856980
C	.972485	3.788947	.265922
C	-.395129	3.549533	.045170
C	1.928965	3.440195	-.687496

66 endosyan

Pd	.570095	1.674845	-.551164
N	1.890704	-.005128	-.857244
P	-1.099012	-.044005	.071139
C	1.639263	-1.142864	-1.371239
O	2.734895	-1.884704	-1.678815
C	3.931768	-1.059819	-1.460523
C	3.375760	.112689	-.616342
C	.361877	-1.801026	-1.703507
C	-.884268	-1.452779	-1.163222
C	-1.999220	-2.180484	-1.542070
C	-1.900704	-3.228074	-2.445785
C	.450423	-2.861907	-2.596946
C	-.675425	-3.567600	-2.975596
H	-2.956266	-1.929112	-1.137682
H	-2.781734	-3.770602	-2.723431
H	1.407999	-3.130464	-2.984901

H	-.587603	-4.376239	-3.671667
H	4.659901	-1.667162	-.958690
H	4.291669	-.744082	-2.426323
H	3.705250	1.061140	-1.006430
C	.566960	3.819291	-1.219227
C	1.887323	3.431102	-.951781
C	-.430249	3.676943	-.251561
H	.266202	3.937371	-2.245331
C	-.719107	-.814856	1.729601
C	-.796415	-2.183669	1.942612
C	-.520098	-2.706043	3.195080
C	-.172356	-1.865845	4.237969
C	-.097216	-.498945	4.030145
C	-.365660	.025157	2.778704
H	-1.067912	-2.841074	1.142199
H	-.579610	-3.763941	3.353548
H	.038204	-2.272671	5.206451
H	.169020	.154489	4.836465
H	-.302640	1.084929	2.622711
C	-2.941634	.256968	.083942
C	-3.723268	-.052038	1.185198
C	-5.085934	.203412	1.160554
C	-5.669308	.758513	.037759
C	-4.890138	1.065874	-1.067162
C	-3.531026	.821635	-1.042758
H	-3.281173	-.489443	2.056109
H	-5.684744	-.036410	2.015924
H	-6.722916	.951698	.019913
H	-5.339581	1.494882	-1.940064
H	-2.932488	1.063589	-1.899815
C	3.303508	-1.325092	1.514649
C	3.694533	.025410	.889383
H	2.245186	-1.520107	1.411515
H	3.856306	-2.145885	1.073152
H	3.529782	-1.308992	2.574181
C	5.190238	.323023	1.122447
H	3.112372	.799668	1.375932
H	5.472939	1.287128	.712195
H	5.404679	.335763	2.184007
H	5.818016	-.437119	.670101
H	-.163572	3.794239	.784820
C	-1.884609	3.939559	-.572372
H	-2.101799	3.743144	-1.614780
H	-2.536400	3.326055	.032667
H	-2.122034	4.979731	-.367796
H	2.534143	3.348444	-1.807405
C	2.609375	3.740639	.352831
H	1.959742	3.718854	1.216233
H	3.421696	3.047379	.520239
H	3.040264	4.736099	.287743

66 exoanan

Pd	.721057	1.407611	.021994
N	1.927726	-.213818	-.716336
P	-1.137928	-.175479	.073648
C	1.617194	-1.246733	-1.392412
H	3.167182	3.013969	.403150
H	-.769840	3.148388	1.641753
C	1.201890	3.378287	.969304
C	-.194729	3.265892	.738701
C	2.183426	3.192187	.004605

H	1.521227	3.242847	1.988629
C	3.412635	-.208111	-.452005
C	-1.062354	-1.248369	1.600945
C	-.937295	-1.377903	-1.359189
C	-2.913230	.387525	-.052145
O	2.668054	-2.020977	-1.766901
C	.313322	-1.748594	-1.872488
C	-.995653	3.955978	-.357939
C	2.207148	3.648969	-1.445588
C	3.915361	-1.357239	-1.365476
C	-2.077106	-1.939308	-1.910582
C	-1.998302	-2.848387	-2.954083
C	.379690	-2.672807	-2.909611
C	-.767999	-3.214878	-3.454310
H	-3.037640	-1.663732	-1.529784
H	-2.897099	-3.263804	-3.362942
H	1.337478	-2.963320	-3.280168
H	-.694104	-3.918641	-4.257691
H	4.526066	-2.085854	-.867772
H	4.396873	-.999278	-2.260260
H	3.802448	.741256	-.782141
C	-1.310248	-2.612632	1.558532
C	-1.260992	-3.361133	2.722458
C	-.970650	-2.751561	3.930045
C	-.723711	-1.389879	3.976627
C	-.764277	-.640461	2.815104
H	-1.538059	-3.092921	.629325
H	-1.451085	-4.414751	2.683756
H	-.935746	-3.333127	4.829114
H	-.498864	-.914861	4.910307
H	-.565115	.412879	2.854668
C	-3.845567	.073901	.922613
C	-5.147489	.538448	.809668
C	-5.520130	1.307012	-.276064
C	-4.589916	1.617508	-1.256509
C	-3.290267	1.163703	-1.143828
H	-3.567718	-.527140	1.763473
H	-5.863918	.293808	1.567704
H	-6.527129	1.662223	-.362360
H	-4.876812	2.209165	-2.102495
H	-2.575940	1.405292	-1.907329
C	3.175616	-1.719678	1.609425
C	3.711908	-.392197	1.047574
H	2.101899	-1.791370	1.499217
H	3.634490	-2.573588	1.124423
H	3.402610	-1.783360	2.667113
C	5.228240	-.257861	1.296855
H	3.211720	.419978	1.563940
H	5.609973	.685757	.920561
H	5.434085	-.301541	2.359303
H	5.779035	-1.063115	.822980
H	2.937199	3.070069	-1.997415
H	1.261527	3.564903	-1.952649
H	2.518433	4.689282	-1.485368
H	-1.984210	3.522245	-.408521
H	-1.109197	5.006798	-.105544
H	-.547088	3.898104	-1.335216

66 endoanan

Pd	.643428	1.379780	-.606737
N	1.862986	-.390092	-.772805

P	-1.147161	-.135911	.066422
C	1.531452	-1.541163	-1.203941
C	.731271	3.462105	-1.418061
C	2.054373	3.146104	-1.136648
C	-.350116	3.321594	-.509368
H	.463589	3.457958	-2.460768
H	-1.315574	3.337275	-.983660
H	2.672656	3.005892	-2.006579
C	3.346293	-.360792	-.507133
C	-1.018761	-1.616094	-1.088153
C	-.940856	-.855813	1.776183
C	-2.932536	.392337	-.044366
O	2.567594	-2.394210	-1.409878
C	.211876	-2.108497	-1.546029
C	-.416891	3.809219	.932878
C	2.855200	3.461134	.116981
C	3.825435	-1.661935	-1.200809
C	-2.181781	-2.251072	-1.487072
C	-2.144487	-3.353488	-2.328156
C	.237232	-3.224279	-2.373777
C	-.934326	-3.840409	-2.771049
H	-3.127026	-1.884187	-1.146808
H	-3.060353	-3.823132	-2.625149
H	1.180621	-3.604211	-2.698513
H	-.893929	-4.693577	-3.416519
H	4.465522	-2.278642	-.599968
H	4.262244	-1.481434	-2.169304
H	3.754324	.509516	-.995044
C	-1.140657	-2.203649	2.037104
C	-.990417	-2.688799	3.325703
C	-.646382	-1.831906	4.355748
C	-.448188	-.485480	4.099326
C	-.590824	.001151	2.812974
H	-1.409505	-2.873926	1.246658
H	-1.144292	-3.730833	3.521266
H	-.533198	-2.209626	5.351882
H	-.183497	.180920	4.895461
H	-.431738	1.044099	2.619853
C	-3.829981	.158049	.984506
C	-5.142451	.590204	.868704
C	-5.559771	1.248364	-.272326
C	-4.664376	1.480269	-1.305374
C	-3.354274	1.058751	-1.190430
H	-3.515310	-.353908	1.870301
H	-5.831934	.408929	1.668390
H	-6.574708	1.579976	-.359735
H	-4.986195	1.987542	-2.192570
H	-2.664705	1.240550	-1.992505
C	3.110383	-1.516649	1.775742
C	3.633962	-.292271	1.005196
H	2.040674	-1.628723	1.665103
H	3.593891	-2.430412	1.450509
H	3.318817	-1.393920	2.832011
C	5.146773	-.102393	1.239583
H	3.119392	.585908	1.379070
H	5.522015	.775028	.722903
H	5.345452	.022137	2.296979
H	5.709303	-.965215	.899511
H	-1.298954	3.396742	1.406518
H	.442090	3.548076	1.528601
H	-.514344	4.891169	.945330
H	2.311489	3.329990	1.036578
H	3.740802	2.840807	.154501

H	3.187380	4.494822	.070319
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Calculated geometries of the isomers of complex 7

69 tbuexosynsyn

Pd	.525226	1.622609	-.451931
N	1.825073	-.092817	-.763117
P	-1.212736	-.034134	.019420
C	1.544795	-1.171590	-1.379640
O	2.618400	-1.926445	-1.728806
C	3.835072	-1.159040	-1.430467
C	3.309837	-.054890	-.476347
C	.250904	-1.744395	-1.801905
C	-1.000897	-1.370786	-1.291093
C	-2.132174	-2.010979	-1.766934
C	-2.044635	-2.999921	-2.735313
C	.326478	-2.746106	-2.762658
C	-.814320	-3.366748	-3.234393
H	-3.093256	-1.735714	-1.387731
H	-2.937707	-3.475263	-3.087525
H	1.285806	-3.035580	-3.130414
H	-.734494	-4.130581	-3.980294
H	4.543287	-1.834381	-.993443
H	4.206288	-.760160	-2.361105
H	3.680713	.913880	-.764577
C	.861205	3.866163	-.254481
C	-.514160	3.498613	-.270566
C	1.675338	3.500551	-1.299812
H	1.303669	4.204493	.666340
C	-1.391361	3.794540	.931584
H	-1.016463	3.553234	-1.224647
C	3.171393	3.703006	-1.295072
H	1.223795	3.345538	-2.267555
C	-1.027765	-.927648	1.647758
C	-1.060445	-2.310677	1.741607
C	-.933508	-2.923228	2.978102
C	-.781602	-2.159032	4.120613
C	-.752977	-.776953	4.030631
C	-.871446	-.162347	2.798196
H	-1.184477	-2.910330	.863441
H	-.957765	-3.992231	3.044897
H	-.686955	-2.635384	5.075538
H	-.638262	-.182083	4.914301
H	-.846721	.908347	2.733952
C	-3.021080	.414642	-.089116
C	-3.942496	-.021713	.849563
C	-5.274899	.342918	.732417
C	-5.688729	1.136867	-.320432
C	-4.769644	1.573230	-1.262051
C	-3.440050	1.217666	-1.144764
H	-3.630365	-.638287	1.666945
H	-5.982537	.004309	1.462040
H	-6.719135	1.416373	-.409072
H	-5.087765	2.187913	-2.079947

H	-2.732552	1.558624	-1.875956
H	-2.276902	3.174253	.923064
H	-.857749	3.625435	1.859862
H	-1.715256	4.831529	.915000
H	3.668983	2.940882	-1.880998
H	3.412015	4.661534	-1.745783
H	3.573165	3.692633	-.289960
C	3.134992	-1.666671	1.502826
C	3.640391	-.295897	1.017957
H	2.054579	-1.717279	1.467169
H	3.540703	-2.482007	.915730
H	3.438468	-1.817456	2.532317
C	5.174686	-.209595	1.182911
H	5.549049	.750238	.840856
H	5.432105	-.314228	2.229997
H	5.691370	-.993268	.641574
C	3.006097	.809130	1.883316
H	1.926793	.753220	1.857631
H	3.321380	.688641	2.913425
H	3.319103	1.793485	1.550218

69 tbuendosynsyn

Pd	.499835	1.719311	-.010319
N	1.857189	.165399	-.685455
P	-1.185853	-.086996	.067769
C	1.623730	-.754607	-1.535403
O	2.730225	-1.355610	-2.044723
C	3.909464	-.618072	-1.572840
C	3.339976	.188236	-.378635
C	.357889	-1.289734	-2.073754
C	-.904823	-1.112714	-1.489793
C	-2.000664	-1.717985	-2.081839
C	-1.869121	-2.475193	-3.235954
C	.478185	-2.058761	-3.225882
C	-.628760	-2.641957	-3.811256
H	-2.969923	-1.593882	-1.648352
H	-2.736269	-2.928076	-3.672485
H	1.446716	-2.200514	-3.651297
H	-.514777	-3.224237	-4.702391
H	4.659286	-1.339379	-1.316046
H	4.243166	.016210	-2.378785
H	3.674032	1.210560	-.407500
C	.419492	3.981511	-.061834
C	1.756985	3.595689	-.012447
C	-.476501	3.499552	.901024
H	.030387	4.421269	-.963443
C	2.715273	3.938220	-1.133145
H	2.198303	3.437179	.958671
C	-1.956884	3.798562	.833669
H	-.085556	3.321628	1.892345
C	-.976072	-1.290681	1.479960
C	-.977161	-2.664347	1.290199
C	-.833702	-3.513087	2.375863
C	-.697588	-2.995059	3.650997
C	-.700484	-1.623625	3.845003
C	-.834220	-.773510	2.762971
H	-1.089304	-3.074879	.307907
H	-.833121	-4.573502	2.223097
H	-.590461	-3.654071	4.488835
H	-.597574	-1.218997	4.831724
H	-.832248	.288260	2.919280

C	-3.017131	.279542	.011247
C	-3.902843	-.268493	.924191
C	-5.252056	.045757	.854232
C	-5.717673	.897503	-.128675
C	-4.833651	1.444019	-1.046830
C	-3.488537	1.141141	-.974216
H	-3.552498	-.935980	1.683861
H	-5.931915	-.380331	1.564191
H	-6.760765	1.135738	-.182926
H	-5.192036	2.102604	-1.812298
H	-2.808830	1.567689	-1.686879
H	3.523351	3.221867	-1.191733
H	2.211043	3.960921	-2.091251
H	3.160617	4.913463	-.959146
H	-2.536239	3.021992	1.312574
H	-2.164199	4.733051	1.347641
H	-2.297386	3.891848	-.189013
C	3.217339	-1.878861	1.125637
C	3.675973	-.413758	1.009420
H	2.138569	-1.953269	1.080397
H	3.641538	-2.501752	.347288
H	3.535282	-2.279363	2.081180
C	5.206187	-.322777	1.208005
H	5.550017	.702874	1.116996
H	5.462689	-.673441	2.200397
H	5.750774	-.932998	.497461
C	3.004325	.413211	2.121258
H	1.926889	.349993	2.057733
H	3.303517	.029073	3.089647
H	3.305341	1.454589	2.068134

69 tbuexosyan

Pd	.467008	1.691933	-.183171
N	1.871750	.130161	-.707244
P	-1.171545	-.114124	.045011
C	1.665099	-.881871	-1.453347
O	2.788495	-1.500010	-1.900411
C	3.948050	-.685077	-1.515727
C	3.355109	.254055	-.432593
C	.414453	-1.498405	-1.942067
C	-.861627	-1.277094	-1.402799
C	-1.943202	-1.940415	-1.956123
C	-1.784242	-2.806450	-3.027460
C	.561791	-2.378436	-3.008447
C	-.530521	-3.024626	-3.554510
H	-2.921712	-1.778965	-1.556439
H	-2.640278	-3.303203	-3.437352
H	1.538977	-2.553705	-3.400155
H	-.395022	-3.692646	-4.380081
H	4.709603	-1.353209	-1.166232
H	4.277287	-.150292	-2.392300
H	3.642773	1.277403	-.610331
C	.686906	3.860790	.363974
C	-.674676	3.542671	.191490
C	1.620765	3.593042	-.632362
H	1.047109	4.011210	1.366653
C	-.921949	-1.167603	1.565731
C	-.849433	-2.550949	1.506091
C	-.675509	-3.285149	2.668451
C	-.580957	-2.642719	3.889382
C	-.657124	-1.260929	3.952649

C	-.822900	-.524539	2.794721
H	-.928043	-3.057396	.566137
H	-.618618	-4.353757	2.616757
H	-.449636	-3.213230	4.786612
H	-.586969	-.760522	4.897421
H	-.879462	.545611	2.849072
C	-3.006501	.216140	-.026916
C	-3.898258	-.406868	.831858
C	-5.252903	-.125689	.745436
C	-5.718292	.771419	-.197504
C	-4.828992	1.395189	-1.058618
C	-3.477525	1.122395	-.970976
H	-3.545714	-1.103407	1.564245
H	-5.937604	-.608668	1.413016
H	-6.765824	.986247	-.262612
H	-5.187071	2.090427	-1.791010
H	-2.792854	1.608705	-1.639069
C	3.332133	-1.584305	1.344201
C	3.733081	-.133986	1.019048
H	2.256724	-1.704091	1.320419
H	3.776183	-2.294358	.656591
H	3.670468	-1.835032	2.342829
C	5.261039	.040360	1.174208
H	5.562323	1.056648	.940052
H	5.545228	-.163717	2.199462
H	5.819668	-.638844	.541301
H	-1.113541	3.681768	-.781527
H	2.653394	3.627398	-.335138
C	1.389587	3.776483	-2.124274
H	.348243	3.709687	-2.403763
H	1.749534	4.758924	-2.417369
H	1.945422	3.042165	-2.694316
C	-1.644341	3.651815	1.351649
H	-2.489368	2.992466	1.209084
H	-1.165246	3.404185	2.291542
H	-2.026329	4.666096	1.425899
C	3.044070	.814031	2.018441
H	1.970300	.690062	1.997786
H	3.386047	.590951	3.022567
H	3.286597	1.850177	1.804634

69 tbuendoansy

Pd	.520192	1.643229	-.279918
N	1.815227	-.040056	-.728397
P	-1.232823	-.025445	.034305
C	1.524004	-1.045856	-1.453901
O	2.589645	-1.775681	-1.873355
C	3.814954	-1.060911	-1.492085
C	3.299001	-.048490	-.436107
C	.225547	-1.554379	-1.942528
C	-1.027027	-1.219145	-1.406996
C	-2.161743	-1.790193	-1.956324
C	-2.077407	-2.674238	-3.021680
C	.297280	-2.451894	-3.001547
C	-.846842	-3.004218	-3.545118
H	-3.122824	-1.541743	-1.558527
H	-2.972875	-3.097796	-3.429496
H	1.256179	-2.715068	-3.389544
H	-.769207	-3.687433	-4.365712
H	4.509159	-1.787522	-1.119608
H	4.199667	-.577223	-2.375694

H	3.682573	.939144	-.629931
C	.496415	3.857348	-.743088
C	1.826805	3.591737	-.504119
C	-.507828	3.473836	.190775
H	-.193612	4.084374	-1.750283
C	2.887149	3.771784	-1.566961
H	2.180794	3.552903	.510883
C	-1.071390	-1.090954	1.558744
C	-1.151077	-2.474451	1.504059
C	-1.041445	-3.220514	2.666420
C	-.859645	-2.589524	3.883572
C	-.783387	-1.207741	3.942372
C	-.884800	-.460456	2.783819
H	-1.297738	-2.971695	.567433
H	-1.102120	-4.289048	2.617924
H	-.778364	-3.168926	4.781027
H	-.644834	-.715554	4.883909
H	-.821166	.608937	2.835921
C	-3.030618	.470319	-.033037
C	-3.959365	-.015436	.872795
C	-5.281282	.396017	.795640
C	-5.677013	1.284462	-.185881
C	-4.750409	1.768526	-1.096642
C	-3.431232	1.367251	-1.017963
H	-3.661713	-.706144	1.634381
H	-5.994837	.019366	1.500434
H	-6.699204	1.599853	-.243852
H	-5.055158	2.454851	-1.860927
H	-2.717611	1.744023	-1.725477
H	3.674885	3.037455	-1.460407
H	2.470046	3.684807	-2.562311
H	3.345080	4.752052	-1.473226
C	3.085774	-1.836669	1.379525
C	3.621475	-.436885	1.028493
H	2.004517	-1.859779	1.341857
H	3.472751	-2.599266	.714084
H	3.386871	-2.094091	2.388339
C	5.156568	-.398914	1.203688
H	5.553093	.579332	.950217
H	5.407267	-.602636	2.237736
H	5.658466	-1.142033	.595554
H	-1.520582	3.543089	-.162125
C	-.367936	3.698002	1.692404
H	-1.076435	3.080433	2.229194
H	.624652	3.484951	2.065831
H	-.595040	4.734530	1.925646
C	3.008292	.594498	1.993864
H	1.928000	.576820	1.948717
H	3.302618	.360205	3.010392
H	3.359461	1.596296	1.767104

69 tbuexoansy

Pd	.512446	1.638794	-.218665
N	1.786853	-.028271	-.795447
P	-1.231319	-.039823	.087304
C	1.482931	-1.031330	-1.519799
O	2.545087	-1.709327	-2.028902
C	3.762846	-.948123	-1.721688
C	3.286148	-.008048	-.587019
C	.177115	-1.603265	-1.906845
C	-1.050120	-1.303526	-1.297383

C	-2.186950	-1.966166	-1.729496				
C	-2.131602	-2.899189	-2.753520	Pd	.429828	1.760126	-.332508
C	.219639	-2.544832	-2.929412	N	1.815183	.153055	-.779529
C	-.927309	-3.184325	-3.357989	P	-1.176153	-.088864	.105452
H	-3.129285	-1.749348	-1.273161	C	1.581244	-.827833	-1.560060
H	-3.028608	-3.393435	-3.067653	O	2.686983	-1.394272	-2.109185
H	1.160458	-2.775651	-3.376968	C	3.843499	-.553712	-1.767201
H	-.871597	-3.901341	-4.151053	C	3.310749	.252077	-.558755
H	4.520513	-1.651579	-1.439422	C	.317125	-1.470526	-1.967056
H	4.047010	-.410856	-2.612759	C	-.919766	-1.288403	-1.329899
H	3.634680	.998186	-.742956	C	-2.010114	-2.013414	-1.779973
C	.884171	3.792477	.423599	C	-1.900744	-2.892375	-2.847164
C	-.501146	3.450130	.282233	C	.414704	-2.357890	-3.032987
C	1.745064	3.677358	-.635275	C	-.688383	-3.060052	-3.478563
H	1.293599	3.895457	1.413308	H	-2.959236	-1.888404	-1.304492
C	-1.007740	-1.014732	1.664398	H	-2.763709	-3.436825	-3.173519
C	-1.099750	-2.397895	1.697979	H	1.363978	-2.497966	-3.500250
C	-.943596	-3.072515	2.897837	H	-.592180	-3.733948	-4.304851
C	-.704577	-2.370237	4.065202	H	4.665151	-1.206919	-1.551423
C	-.615627	-.988406	4.036022	H	4.058107	.070906	-2.620169
C	-.760961	-.312197	2.838767	H	3.596131	1.288260	-.621977
H	-1.291449	-2.949881	.801075	C	.249620	3.919449	-.922308
H	-1.013233	-4.141404	2.917756	C	1.608712	3.594860	-.766206
H	-.588122	-2.894765	4.992047	C	-.653359	3.707418	.116702
H	-.431824	-.441224	4.938648	H	-.138821	4.048922	-1.917089
H	-.684539	.757952	2.819937	C	-.824826	-1.092859	1.640311
C	-3.043758	.412672	.042778	C	-.757738	-2.477739	1.620593
C	-3.874153	.183594	1.126931	C	-.515719	-3.175857	2.792690
C	-5.205008	.570854	1.074153	C	-.349598	-2.496257	3.985763
C	-5.708771	1.177352	-.059890	C	-.420676	-1.113244	4.010204
C	-4.881671	1.400319	-1.150376	C	-.652444	-.412895	2.840796
C	-3.554061	1.023299	-1.099088	H	-.894214	-3.013083	.703611
H	-3.496292	-.294083	2.006836	H	-.463041	-4.245717	2.771118
H	-5.841483	.391363	1.917034	H	-.166745	-3.039066	4.891121
H	-6.737759	1.472765	-.099353	H	-.294604	-.583623	4.932982
H	-5.270330	1.863878	-2.034778	H	-.702349	.658924	2.865632
H	-2.922370	1.191931	-1.949855	C	-3.028964	.163817	.119301
C	3.221521	-1.909669	1.125298	C	-3.821038	-.289685	1.161270
C	3.695233	-.473651	.833917	C	-5.189641	-.066105	1.139488
H	2.140517	-1.963370	1.152290	C	-5.768811	.600552	.077151
H	3.586558	-2.617664	.391127	C	-4.979323	1.051392	-.969816
H	3.590611	-2.218263	2.096430	C	-3.615106	.838884	-.946678
C	5.235632	-.395407	.933465	H	-3.383223	-.815148	1.984173
H	5.588204	.609241	.721787	H	-5.795988	-.418650	1.949335
H	5.545960	-.652739	1.938986	H	-6.826754	.768536	.060682
H	5.727802	-1.082937	.255954	H	-5.425378	1.565794	-1.797186
H	1.354022	3.721318	-1.636760	H	-3.009722	1.189305	-1.760282
C	3.237767	3.867268	-.510312	C	3.384310	-1.813966	.955227
H	3.584847	3.668951	.495255	C	3.744542	-.322501	.815440
H	3.773144	3.227371	-1.200036	H	2.310993	-1.954117	.968450
H	3.495076	4.892454	-.760711	H	3.804621	-2.415373	.158826
H	-1.057793	3.417635	1.203004	H	3.774628	-2.186778	1.894958
C	-1.328542	3.940749	-.901775	C	5.273380	-.137841	.946027
H	-.818085	3.835373	-1.849942	H	5.549756	.906629	.840403
H	-2.261374	3.399104	-.951503	H	5.594434	-.469751	1.926026
H	-1.563371	4.992819	-.766132	H	5.822441	-.715019	.211425
C	3.101210	.472899	1.893470	C	3.067790	.457715	1.956892
H	2.021968	.416281	1.905788	H	1.993385	.350489	1.917169
H	3.461065	.187852	2.875529	H	3.406730	.068214	2.910113
H	3.401753	1.499187	1.711950	H	3.323187	1.509710	1.917897
				H	-.300142	3.785731	1.130809
				H	2.186662	3.561015	-1.673294
				C	-2.139993	3.910139	-.062328

H	-2.438748	3.770616	-1.093054
H	-2.707091	3.225757	.552171
H	-2.406171	4.921161	.233080
C	2.416512	3.961265	.471486
H	1.860996	3.858966	1.392696
H	3.306846	3.353430	.542953
H	2.736106	4.996379	.387942

H	-5.602925	.808834	-.942397
H	-5.628253	-.627063	-1.948750
H	-5.831335	-.780990	-.221111
H	-2.734975	3.533523	-.557561
H	1.158933	3.139399	-1.874784
C	-1.657937	4.114323	1.243226
H	-2.427083	3.633954	1.835321
H	-.710391	3.948555	1.725787
H	-1.858046	5.182336	1.254047
C	1.525751	4.022854	.070749
H	2.472390	3.502981	.105228
H	1.723736	5.048052	-.230052
H	1.112117	4.044637	1.064961
C	-3.130888	.356567	-2.067032
H	-2.055659	.245844	-2.064183
H	-3.507013	-.065749	-2.991810
H	-3.380181	1.412670	-2.056225

69 tbuexoanan

Pd	-.471728	1.658272	-.156804
N	-1.837283	.205069	.689183
P	1.196954	-.121363	-.094244
C	-1.599851	-.669847	1.584895
O	-2.705043	-1.185231	2.183872
C	-3.873981	-.424564	1.725645
C	-3.332385	.286278	.459505
C	-.334376	-1.232561	2.100527
C	.920565	-1.104263	1.487054
C	2.012339	-1.728697	2.066551
C	1.885953	-2.460784	3.237089
C	-.448172	-1.974697	3.271425
C	.654503	-2.579824	3.842379
H	2.974817	-1.638944	1.609503
H	2.749345	-2.930542	3.663058
H	-1.409159	-2.077988	3.723522
H	.543725	-3.141300	4.747165
H	-4.664989	-1.125387	1.548054
H	-4.140902	.268721	2.507457
H	-3.614860	1.326010	.448224
C	-.756399	3.632300	-1.178024
C	.624889	3.364530	-.966840
C	-1.727033	3.611296	-.189323
H	-1.114059	3.488511	-2.183172
C	.936243	-1.350233	-1.476197
C	.934253	-2.719573	-1.258060
C	.750605	-3.588967	-2.320970
C	.577218	-3.095840	-3.601484
C	.582424	-1.728712	-3.823577
C	.755968	-.857607	-2.764036
H	1.074375	-3.111077	-.271634
H	.747723	-4.646026	-2.146586
H	.439010	-3.770949	-4.421768
H	.450109	-1.343446	-4.814540
H	.753650	.200869	-2.940288
C	3.030912	.231094	-.087092
C	3.876086	-.294903	-1.049742
C	5.227488	.016694	-1.029431
C	5.736030	.843950	-.047071
C	4.893254	1.366182	.922470
C	3.545596	1.064836	.901046
H	3.493066	-.943074	-1.810291
H	5.875653	-.392354	-1.777969
H	6.780697	1.080815	-.031915
H	5.285154	2.003265	1.689698
H	2.900070	1.468529	1.657049
C	-3.372318	-1.862770	-.926763
C	-3.769430	-.376016	-.872256
H	-2.295643	-1.975814	-.939294
H	-3.770897	-2.423033	-.089477
H	-3.760958	-2.304582	-1.836841
C	-5.303906	-.233532	-.992996

69 tbuendoanan

Pd	0.451540	1.590447	-0.674894
N	1.799830	-0.095934	-0.819725
P	-1.206537	-0.057868	0.054268
C	1.530185	-1.204884	-1.386992
O	2.615091	-1.925440	-1.772469
C	3.808304	-1.088611	-1.577194
C	3.293231	-0.008635	-0.594045
C	0.239674	-1.847983	-1.706680
C	-0.999732	-1.487600	-1.155525
C	-2.124856	-2.206417	-1.520015
C	-2.045278	-3.259963	-2.418729
C	0.307172	-2.911578	-2.599008
C	-0.828644	-3.610708	-2.960617
H	-3.076112	-1.941307	-1.109546
H	-2.933756	-3.796006	-2.684912
H	1.257190	-3.187779	-2.999620
H	-0.754933	-4.422296	-3.654921
H	4.585291	-1.718709	-1.192859
H	4.080871	-0.678862	-2.536980
H	3.622008	0.975059	-0.886034
C	0.264297	3.600364	-1.633101
C	1.635168	3.430855	-1.475551
C	-0.694350	3.448047	-0.601014
H	-0.112145	3.480716	-2.634581
C	-0.947016	-0.810239	1.741945
C	-0.944004	-2.181456	1.948017
C	-0.763001	-2.688854	3.224708
C	-0.593055	-1.831526	4.296393
C	-0.599775	-0.461059	4.094632
C	-0.771667	0.048795	2.821296
H	-1.082657	-2.852865	1.125779
H	-0.759942	-3.749177	3.378013
H	-0.456897	-2.226726	5.282805
H	-0.470648	0.205863	4.923145
H	-0.772569	1.111179	2.670895
C	-3.028342	0.344009	-0.029269
C	-3.894934	0.037871	1.006917
C	-5.236249	0.376848	0.910145
C	-5.713183	1.013195	-0.219597
C	-4.848928	1.315548	-1.260986
C	-3.511134	0.986744	-1.164802
H	-3.534869	-0.458266	1.884253

H	-5.901345	0.139727	1.715879
H	-6.750051	1.272612	-0.292382
H	-5.216726	1.804674	-2.140513
H	-2.846987	1.220128	-1.974898
C	3.256429	-1.668700	1.355433
C	3.684200	-0.265970	0.884180
H	2.178044	-1.761643	1.369281
H	3.665474	-2.453946	0.731673
H	3.612421	-1.828560	2.366474
C	5.217681	-0.116325	1.002943
H	5.539897	0.864930	0.668717
H	5.512513	-0.228874	2.039301
H	5.749861	-0.866735	0.430255
H	-1.705262	3.358776	-0.955484
H	2.169456	3.251114	-2.392952
C	-0.621136	3.993829	0.821207
H	-1.484440	3.647064	1.374805
H	0.263593	3.695357	1.362233
H	-0.653882	5.079146	0.804093
C	2.524430	3.980759	-0.373668
H	2.058405	4.016220	0.595058
H	3.432798	3.398114	-0.298798
H	2.815013	4.993464	-0.641139
C	3.027737	0.785793	1.797007
H	1.950217	0.703074	1.772710
H	3.350882	0.628469	2.819748
H	3.315380	1.789503	1.506899