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Supporting Information

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Rhodium Catalyzed Conversion of Carbenes into Ketenes and Ketene Imines using PNN Pincer Complexes

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Content

Table S1. Energies (and imaginary frequencies) of the calculated species (with disp3)

		SCF au	G Au	ZPE au	SCF+ZPE au	Imaginary Frequency (cm^{-1})
MDA		-376.83	-376.78	0.07401	-376.75	--
N_2		-109.58	-109.59	0.00543	-109.58	--
CO		-113.37	-113.38	0.00484	-113.36	--
Imine		-173.34	-173.28	0.09310	-173.25	--
ketene		-380.68	-380.64	0.07394	-380.61	--
β-lactam		-554.07	-553.93	0.17379	-553.90	--
TS-uncatalized [2+2] ketene imine cyclization	**$TS_{uncatal.}$**	-553.98	-553.85	0.16885	-553.81	-449.77
Rh(CO)PNN	**^{NH}INT0**	-1066.49	-1066.27	0.26208	-1066.23	--
	^{N}INT0	-1066.05	-1065.86	0.24586	-1065.81	--
Rh(CO)PNN–MDA	**^{NH}INT1**	-1443.34	-1443.05	0.34469	-1443.34	--
	^{N}INT1	-1442.88	-1442.62	0.32088	-1442.56	--
TS-N_2 loss	**^{NH}TS1-2**	-1443.30	-1443.01	0.33724	-1442.96	-242.29
	^{N}TS1-2	-1442.87	-1442.6	0.31883	-1442.55	-357.47
Rh(CO)PNN-carbene	**^{NH}INT2^{b}**	-1333.76	-1333.48	0.32787	-1333.43	--
	^{N}INT2^{b}	-1333.32	-1333.06	0.31164	-1333.01	--
Reaction with coordinated CO						
TS-ketene formation	**^{NH}TS2-3**	-1333.74	-1333.46	0.32699	-1333.41	-360.11
	^{N}TS2-3	-1333.30	-1333.04	0.31109	-1332.99	-300.89
Rh(PNN)-ketene	**^{NH}INT3**	-1333.79	-1333.5	0.33592	-1333.45	--
	^{N}INT3	-1333.35	-1333.09	0.31353	-1333.04	--

Rh(PNN)-ketene-imine, $\mathbf{P_{II}}$	^{NH}**INT4**	-1507.14	-1506.77	0.4269	-1506.72	--
	^{N}**INT4**	-1506.72	-1506.37	0.41275	-1506.31	--
TS-cycloaddition, $\mathbf{P_{II}}$	^{NH}**TS4-5**	-1507.13	-1506.76	0.37097	-1506.76	-263.11
	^{N}**TS4-5**	-1506.7	-1506.34	0.41122	-1506.29	-285.91
Rh(PNN)-metallocycle, $\mathbf{P_{II}}$	^{NH}**INT5**	-1507.15	-1506.78	0.37052	-1506.78	--
	^{N}**INT5**	-1506.72	-1506.36	0.41478	-1506.31	--
TS-cycloaddition lactam, $\mathbf{P_{II}}$	^{NH}**TS5-0**	-1507.13	-1506.76	0.4282	-1506.7	-168.17
	^{N}**TS5-0**	-1506.69	-1506.34	0.41173	-1506.28	-214.18
TS-imine coupling, $\mathbf{P_{IO}}$	^{NH}**TS3-7**	-1507.14	-1506.77	0.42475	-1506.71	-167.56
	^{N}**TS3-7**	-1506.69	-1506.34	0.40914	-1506.28	-193.23
Rh(PNN)-zwitterion, $\mathbf{P_{IO}}$	^{NH}**INT7**	-1507.14	-1506.77	0.42549	-1506.72	--
	^{N}**INT7**	-1506.69	-1506.34	0.41006	-1506.28	--
Rh(PNN)-zwitterion rotamer, $\mathbf{P_{IO}}$	^{NH}**INT8**	-1507.14	-1506.77	0.42599	-1506.71	--
	^{N}**INT8**	-1506.69	-1506.34	0.41059	-1506.28	--
TS-cycloaddition, $\mathbf{P_{IO}}$	^{NH}**TS8-0**	-1507.09	-1506.72	0.42351	-1506.66	-454.20
	^{N}**TS8-0**	-1506.65	-1506.3	0.40774	-1506.24	-522.51
Reaction with external CO						
TS-ketene formation ext. CO	^{NH}**TS2-6**	-1447.13	-1446.84	0.33579	-1446.79	-205.94
	^{N}**TS2-6**	-1446.69	-1446.43	0.31984	-1446.37	-406.83
Rh(CO)PNN-ketene	^{NH}**INT6**	-1447.19	-1446.9	0.33863	-1446.85	--
	^{N}**INT6**	-1446.75	-1446.48	0.32189	-1446.43	--
Rh(CO)PNN-ketene-imine, $\mathbf{P_{OI}}$	^{NH}**INT9**	-1620.54	-1620.17	0.4349	-1620.11	--
	^{N}**INT9**	-1620.10	-1619.74	0.41942	-1619.68	--
TS-cycloaddition, $\mathbf{P_{OI}}$	^{NH}**TS9-10**	-1620.52	-1620.14	0.43487	-1620.09	-236.87

	^{N}TS9-10	-1620.08	-1619.72	0.41938	-1619.66	-282.90
Rh(CO)PNN-metallocycle, **P_{OI}**	**^{NH}INT10**	-1620.55	-1620.17	0.43663	-1620.12	--
	^{N}INT10	-1620.11	-1619.74	0.421	-1619.69	--
TS-cycloaddition lactam, **P_{OI}**	**^{NH}TS10-0**	-1620.53	-1620.15	0.43736	-1620.09	-169.22
	^{N}TS10-0	-1620.09	-1619.73	0.41925	-1619.67	-174.98
TS-cycloaddition, **P_{OO}**	**^{NH}TS6-0**	-1620.54	-1620.17	0.43391	-1620.11	-349.64
	^{N}TS6-0	-1620.09	-1619.73	0.41772	-1619.67	-313.08

Cartesian coordinates of the calculated species (with disp3):

N_2

2

Energy = -109.5804240180

N 1.9083652 4.4465698 -8.8585874

N 1.6456348 5.4754302 -9.1554126

CO

2

Energy = -113.3653361964

O 0.0000000 0.0000000 0.9548681

C 0.0000000 0.0000000 -0.1815681

MDA

11

Energy = -376.8251413399

C	-0.1511229	-0.1010885	0.9789029
C	-0.2158662	0.2769121	-0.4280202
O	-1.2100147	-0.3889450	-1.0878096
C	-1.3258493	-0.0589901	-2.4899431
H	0.5839844	0.3351276	1.6472479
H	-1.5487494	1.0087720	-2.6184335
H	-0.3939871	-0.2956646	-3.0209196
H	-2.1507178	-0.6736814	-2.8639747
N	-0.9789069	-0.9816072	1.4832299
N	-1.7097885	-1.7496179	1.8985323
O	0.5322330	1.0898372	-0.9426851

Imine

11

Energy = -173.3412481737

C	0.5059105	-0.0123277	2.4466947
N	0.2659279	-1.2345958	2.1875659
C	-1.1137844	-1.6850523	2.2237268
C	1.8922032	0.5525358	2.4360341
H	-0.3136136	0.6979294	2.6952781
H	-1.2058664	-2.5043293	2.9532944
H	2.1411726	0.9804719	3.4205402
H	1.9663323	1.3767533	1.7083193
H	2.6238100	-0.2237687	2.1814550
H	-1.8427277	-0.8904966	2.4833696
H	-1.3809705	-2.1050333	1.2417206

ketene

11

Energy = -380.6787201969

C	0.8843631	0.2254153	-0.3117727
C	-0.1712893	-0.5752201	-0.2186994
C	1.0766819	1.1146985	-1.4641849
O	0.0527721	0.9855191	-2.3621673
C	0.1609860	1.8280598	-3.5313063
H	-0.7235036	1.5997021	-4.1343350
H	0.1707739	2.8879487	-3.2436787
H	1.0794968	1.5995643	-4.0882405
O	2.0197275	1.8685145	-1.6065711
H	1.6249023	0.2230861	0.4840271
O	-1.0968722	-1.2763929	-0.1383684

β-lactam

22

Energy = -554.0688457988

C	0.6713349	0.4368642	1.2142301
C	1.4014908	-0.0527953	-0.0781432
N	-0.1273032	-0.8048461	1.1567653
C	0.4376586	-1.2922654	0.0088758
C	-1.2132868	-1.2890165	1.9721327
C	1.5249000	0.6002623	2.4607378
C	1.2791920	0.7574770	-1.3410732

O	0.0197674	1.2562825	-1.4838267
C	-0.2068604	1.9933244	-2.7071271
H	-1.2527853	2.3130097	-2.6652873
H	0.4639223	2.8610448	-2.7641549
H	-0.0315132	1.3488847	-3.5785301
O	2.1687568	0.9249234	-2.1504856
H	2.4545681	-0.3182820	0.0692175
H	0.0496373	1.3278994	1.0323756
H	-0.8978894	-1.4198634	3.0185882
H	0.8963532	0.7485555	3.3509344
H	2.1799793	1.4772063	2.3623333
H	2.1512881	-0.2885463	2.6242704
H	-2.0703700	-0.5971645	1.9428918
H	-1.5262610	-2.2610619	1.5706965
O	0.2438529	-2.2889105	-0.6527195

TS-uncatalyzed ketene-imine cyclization

22

Energy = -553.9787602427

C	0.4584907	0.1602427	2.1391731
C	1.0608206	0.1872741	-0.2845388
N	0.1374725	-1.0636890	1.6449651
C	0.0214678	-0.7034481	0.0630078
C	-1.1345759	-1.6161801	2.1281250
C	1.8187539	0.5583768	2.5794459

C	1.1362146	0.9984614	-1.4897764
O	0.0221294	0.9366622	-2.2777813
C	0.0597826	1.7970772	-3.4326694
H	-0.8836534	1.6175208	-3.9588800
H	0.1419419	2.8515763	-3.1332283
H	0.9154618	1.5491397	-4.0763846
O	2.0958869	1.7221055	-1.7440675
H	2.0136091	0.0719074	0.2170983
H	-0.3703391	0.7913128	2.5089758
H	-0.9679418	-2.0564223	3.1196857
H	1.8203868	0.4891536	3.6866416
H	2.0481105	1.6025652	2.3282998
H	2.5972168	-0.1126933	2.2013844
H	-1.9357943	-0.8582105	2.1964958
H	-1.4601915	-2.3938567	1.4281965
O	-0.9788133	-1.0958907	-0.4814644

Rh(CO)PNN

^{N}INT0			**^{NH}INT0**		
32			33		
Energy = -1066.0548199190			Energy = -1066.4907301270		
Rh	0.0759014	-0.4457169	0.8231977	Rh	0.2331660	-0.3689912	0.7380732
C	-1.2483658	3.9761441	2.2471365	C	-1.1036447	4.0123611	2.2578403
C	-0.3353587	1.7886881	2.6659719	C	-0.2713661	1.7968746	2.6550155
C	-0.8373321	2.4270475	0.4450471	C	-0.7653778	2.4639788	0.4421696

C	-1.2799447	3.6709859	0.8793113	C	-1.1728885	3.7188322	0.8954642
C	-0.7604798	3.0288640	3.1441742	C	-0.6376276	3.0448879	3.1501193
C	0.2338614	0.6984157	3.5186379	C	0.1443213	0.6423217	3.5294078
C	-0.7453133	2.0331245	-1.0040729	N	0.9893248	-0.3340263	2.7799505
P	-0.6509618	0.1735789	-1.1775854	C	-0.7306709	2.0756993	-1.0104969
C	0.6723820	-2.0778881	0.2483048	P	-0.6908066	0.2177165	-1.1929030
O	1.0494341	-3.0932212	-0.1861465	C	0.6953483	-2.0572155	0.1624270
H	1.2388240	1.0608716	3.8539449	O	0.9721536	-3.1119637	-0.2245189
H	-0.3615941	0.6211579	4.4562330	H	1.9212630	0.0804040	2.6599549
H	-0.7106727	3.2361600	4.2131719	H	0.6504257	0.9967898	4.4423224
H	-1.5967112	4.9463495	2.6019225	H	-0.7613860	0.1027291	3.8498170
H	-1.6347887	4.4000846	0.1512303	H	-0.5701843	3.2504821	4.2179173
H	-1.5546260	2.4753198	-1.6035896	H	-1.4070161	4.9936685	2.6226970
H	0.2071015	2.4171532	-1.4072785	H	-1.5259311	4.4619179	0.1815745
C	-2.3600272	-0.2940707	-1.6892704	H	-1.5590432	2.5284822	-1.5740827
C	0.2715178	-0.0548191	-2.7489297	H	0.2055570	2.4492815	-1.4575173
C	0.9562035	-1.5827993	3.6158764	C	-2.4312579	-0.2664525	-1.4704515
H	-0.2007823	0.4807955	-3.5854840	C	0.1262539	-0.0825368	-2.7936269
H	1.3025943	0.2940338	-2.6128881	C	1.1483890	-1.6105612	3.5255042
H	0.3013275	-1.1283080	-2.9794067	H	-0.3877406	0.4524674	-3.6043407
H	0.4580778	-1.7118530	4.6002512	H	1.1734008	0.2392992	-2.7389338
H	0.9143967	-2.5454775	3.0927846	H	0.1035809	-1.1600788	-3.0037521
H	-2.6699172	0.2181074	-2.6129267	H	0.1795067	-2.1203824	3.5695920
H	-2.3958879	-1.3804184	-1.8447780	H	1.8574337	-2.2484234	2.9875494
H	-3.0517857	-0.0438352	-0.8747333	H	-2.8328187	0.2150833	-2.3731865

H 2.0252324 -1.3574527 3.8254834	H -2.4846686 -1.3568326 -1.5845841
N -0.3952941 1.4961669 1.3404685	H -3.0330034 0.0196596 -0.5984136
N 0.3013813 -0.5610449 2.8284151	H 1.5166028 -1.4347782 4.5487334
	N -0.3352955 1.5243060 1.3276783

Rh(CO)PNN–MDA

^{N}INT1	**^{NH}INT1**
43	44
Energy = -1442.8812101390	Energy = -1443.3405250070
C -1.3850724 4.7063400 1.3990754	C -2.0741988 3.8951313 1.9147372
C -0.9121650 2.6243719 2.5081888	C -1.1445688 1.8003554 2.6221873
C -1.4657866 2.6131625 0.2136191	C -1.4457094 2.2032249 0.3149579
C -1.6165374 3.9978892 0.2173744	C -1.9784784 3.4631192 0.5933371
C -1.0530940 4.0114941 2.5604003	C -1.6637179 3.0488920 2.9470469
C -0.6781376 1.7361783 3.6944170	C -0.7873256 0.7548244 3.6436456
C -1.7764107 1.7369155 -0.9704248	C -1.3762362 1.6459167 -1.0786486
P -0.8597862 0.1246825 -0.8299619	P -0.4276988 0.0395208 -1.1449649
H -0.0535974 2.2571894 4.4511573	H -0.5279098 1.2079481 4.6139496
H -1.6843230 1.6319551 4.1855301	H -1.6800089 0.1252025 3.7965164
H -0.9063517 4.5312936 3.5067869	H -1.7469223 3.3511061 3.9903483
H -1.4884220 5.7915433 1.4164739	H -2.4790500 4.8818021 2.1401464
H -1.9281965 4.5091681 -0.6928078	H -2.3240853 4.0929686 -0.2250444
H -2.8433013 1.4563412 -0.9254718	H -2.4047063 1.4378242 -1.4129799
H -1.5998779 2.2490248 -1.9275676	H -0.9403697 2.3749462 -1.7768139

C	-1.6778783	-0.9472482	-2.0691828	C	-1.4977935	-1.1185750	-2.0566266
C	0.7557944	0.4712895	-1.6347992	C	0.9728057	0.3534923	-2.2747292
C	-0.1324580	-0.4622732	4.4221187	C	0.4104562	-1.3723971	3.9780589
H	0.6303222	0.7932170	-2.6797462	H	0.6134819	0.6784113	-3.2612539
H	1.2739639	1.2504925	-1.0618751	H	1.6298939	1.1205807	-1.8465346
H	1.3680467	-0.4393853	-1.6026555	H	1.5490547	-0.5740672	-2.3890308
H	0.3455994	-0.0233775	5.3215110	H	0.5210551	-1.1303780	5.0469644
H	-1.1641801	-0.7628270	4.7389243	H	-0.4902903	-1.9798240	3.8357551
H	-1.6635755	-0.4830284	-3.0659350	H	-1.7429713	-0.7230636	-3.0524522
H	-1.1338812	-1.9006629	-2.1109678	H	-0.9709429	-2.0754012	-2.1675862
H	-2.7113505	-1.1365806	-1.7548281	H	-2.4160453	-1.2677861	-1.4760310
H	0.4119561	-1.3809441	4.1645582	H	1.2799745	-1.9473481	3.6423282
N	-1.0582789	1.9630781	1.3346867	N	-1.0124488	1.4081127	1.3295474
Rh	-0.7320752	-0.0961401	1.4168937	Rh	0.0354474	-0.3382293	0.9951051
N	-0.0992389	0.4644099	3.3153935	C	-4.5735755	1.1502272	2.0405869
C	-2.8081626	-0.3931917	2.0814432	H	-4.8372542	1.1736746	3.0937335
H	-2.6524844	-0.8342103	3.0747775	N	-4.9739790	2.1544820	1.2996149
N	-3.6081909	0.7204312	2.1993447	N	-5.2939449	3.0193842	0.6373853
N	-3.9266996	1.8235948	2.0905126	C	-3.8986118	0.0447782	1.3818631
C	-3.3977655	-1.3233419	1.0760086	O	-3.5582283	-0.8955565	2.3053893
O	-3.0959288	-2.6095082	1.3955239	C	-2.9456389	-2.0917787	1.7615802
C	-3.4218482	-3.5850174	0.3849427	H	-2.8559042	-2.7802703	2.6072086
H	-3.1692581	-4.5544185	0.8253537	H	-1.9502081	-1.8425586	1.3454233
H	-2.8203210	-3.4122216	-0.5184940	H	-3.5774317	-2.5251074	0.9759613
H	-4.4873356	-3.5380858	0.1238254	O	-3.6590459	-0.0402257	0.1834809

O -4.0314589 -0.9944853 0.0816568	C 1.0111515 -1.8516439 0.6181502
C -0.0410442 -1.8029630 1.3793964	O 1.6200551 -2.7986105 0.3462821
O 0.3570416 -2.8954604 1.2937010	N 0.2955961 -0.1438874 3.1510191
	H 1.1849539 0.3654210 3.2098531

TS-N_2 loss

^{N}**TS1-2**	^{NH}**TS1-2**
43	44
Energy = -1442.8666244600	Energy = -1443.2955226940
C -1.5094856 4.6529379 1.4047456	C -1.4438949 4.6700964 1.4252056
C -0.9149205 2.6069291 2.5177205	C -0.8755637 2.6183187 2.5337600
C -1.4855588 2.5531057 0.2305407	C -1.4551554 2.5692483 0.2486394
C -1.7118253 3.9279161 0.2281906	C -1.6702377 3.9472368 0.2532973
C -1.1379735 3.9829922 2.5693590	C -1.0661832 3.9960562 2.5881922
C -0.6343301 1.7292801 3.7023439	C -0.6489068 1.7617135 3.7542192
C -1.7926575 1.6418889 -0.9270693	C -1.7696833 1.6697391 -0.9156060
P -0.8058110 0.0762609 -0.7948511	P -0.7758846 0.1099057 -0.8205203
H -0.0042001 2.2607450 4.4444432	H -0.1181701 2.3149116 4.5454572
H -1.6248066 1.5849132 4.2040341	H -1.6422479 1.4964107 4.1528952
H -1.0238370 4.5139797 3.5140473	H -0.9334656 4.5294810 3.5288609
H -1.6752313 5.7303890 1.4190141	H -1.5915483 5.7496100 1.4404179
H -2.0648759 4.4160985 -0.6794754	H -2.0207394 4.4428627 -0.6510069
H -2.8409956 1.3060009 -0.8252867	H -2.8189353 1.3349786 -0.8173124
H -1.6796117 2.1409276 -1.9001269	H -1.6583047 2.1737490 -1.8854792

C	-1.5700924	-1.0374373	-2.0263967	C	-1.5551734	-1.0605721	-1.9696855
C	0.8032590	0.4944831	-1.5765483	C	0.8329422	0.5008918	-1.5916500
C	0.1136343	-0.4125515	4.4580465	C	-0.0675075	-0.4935284	4.5547869
H	0.6727838	0.8269766	-2.6172065	H	0.6940018	0.8157224	-2.6361943
H	1.2859336	1.2869276	-0.9903874	H	1.3251590	1.3013945	-1.0257076
H	1.4507624	-0.3918160	-1.5535199	H	1.4709044	-0.3916551	-1.5611288
H	0.6866242	0.0858817	5.2654095	H	0.2895895	-0.0584827	5.5011059
H	-0.8575745	-0.7244527	4.9013647	H	-1.1152732	-0.7930480	4.6720121
H	-1.5277171	-0.5958274	-3.0322994	H	-1.4895034	-0.6749801	-2.9965028
H	-1.0205016	-1.9880612	-2.0257415	H	-1.0239976	-2.0194207	-1.9105188
H	-2.6136829	-1.2192951	-1.7413657	H	-2.6067563	-1.1994812	-1.6930310
H	0.6583301	-1.3198765	4.1674432	H	0.5281577	-1.3797630	4.3117666
N	-1.0252399	1.9400033	1.3482962	N	-1.0033686	1.9442517	1.3663922
Rh	-0.6462551	-0.1356833	1.4693413	Rh	-0.6025905	-0.1293031	1.4084972
N	-0.0297704	0.4688584	3.3168561	C	-2.5710476	-0.5924270	1.9863253
C	-2.7049327	-0.3928613	1.9791082	H	-2.6770202	-1.1165273	2.9528260
H	-2.7713772	-0.8404505	2.9846235	N	-3.8445127	0.8510908	2.4088587
N	-3.9772748	0.9425698	2.2162724	N	-3.8540635	1.9651616	2.2963115
N	-3.9530971	2.0598894	2.0196221	C	-3.3907834	-1.3094440	0.9542972
C	-3.3972918	-1.2630934	0.9877944	O	-3.2478475	-2.6485511	1.0898857
O	-3.1748757	-2.5900799	1.2476982	C	-3.8624040	-3.4674390	0.0583516
C	-3.6284084	-3.5102478	0.2333641	H	-3.7123622	-4.5004659	0.3836643
H	-3.4137137	-4.5092190	0.6265944	H	-3.3735443	-3.2970416	-0.9099740
H	-3.0837110	-3.3513711	-0.7082481	H	-4.9298461	-3.2298855	-0.0259236
H	-4.7037108	-3.3857522	0.0472102	O	-4.0244449	-0.7731425	0.0557449

O -4.0236117 -0.8865053 0.0025664	C 0.2908383 -1.7253402 1.2608652
C 0.0230729 -1.8407178 1.4740734	O 0.8160533 -2.7573467 1.1626234
O 0.3928097 -2.9459640 1.4472777	N 0.0342424 0.4774988 3.4383131
	H 1.0277048 0.6721532 3.2761358

Rh(CO)PNN-carbene (carbene in basal positions)

^{N}**INT2^{b}**	^{NH}**INT2^{b}**
41	42
Energy = -1333.3207324330	Energy = -1333.7563991670
C -0.7853348 4.2001641 1.7296293	C -0.4778997 4.1750193 1.6795646
C -0.6233554 1.9928267 2.6664364	C -0.4592434 1.9780793 2.6455575
C -0.9582770 2.2386641 0.3429424	C -0.9217723 2.2197166 0.3452197
C -0.9545396 3.6285064 0.4655064	C -0.7955023 3.6068270 0.4448583
C -0.6287028 3.3756504 2.8454292	C -0.3165945 3.3540301 2.7997678
C -0.4822611 0.9634263 3.7509437	C -0.4280843 0.9869438 3.7825289
C -1.2222165 1.4960280 -0.9352733	C -1.3284580 1.4822110 -0.8984113
P -0.4410955 -0.2189500 -0.9527414	P -0.5648669 -0.2270979 -0.9826786
C -2.1765937 -1.2653553 1.3324185	C -2.2753898 -1.1615446 1.4375056
O -3.1823815 -1.8511206 1.2693121	O -3.2734217 -1.7448217 1.4589312
H 0.0792566 1.3872562 4.6073149	H 0.0927650 1.3984143 4.6611895
H -1.5135397 0.7574879 4.1427575	H -1.4713159 0.7898429 4.0817561
H -0.4988673 3.7948626 3.8430406	H -0.0866289 3.7760810 3.7776290
H -0.7754303 5.2848005 1.8424059	H -0.3637535 5.2550111 1.7718987
H -1.0915060 4.2508474 -0.4183590	H -0.9493992 4.2302600 -0.4349593
H -2.3088715 1.3108271 -1.0000089	H -2.4196801 1.3216826 -0.8614890

H	-0.9413576	2.0835666	-1.8211870	H	-1.1144221	2.0546044	-1.8110666
C	-1.4953684	-1.0220982	-2.2122202	C	-1.6775070	-1.1110066	-2.1149186
C	1.1629673	0.0958266	-1.7770568	C	0.9910303	0.0808875	-1.8812530
C	0.3468975	-1.2064451	4.2934813	C	-0.1439300	-1.3851271	4.3724196
H	1.0115815	0.5011975	-2.7884174	H	0.7675217	0.5082151	-2.8693941
H	1.7298253	0.8156209	-1.1727309	H	1.5995169	0.7888016	-1.3045476
H	1.7091766	-0.8516412	-1.8314895	H	1.5333638	-0.8612936	-2.0028866
H	0.8435010	-0.7486215	5.1714376	H	0.2199869	-1.1105983	5.3748354
H	-0.6109488	-1.6441653	4.6522608	H	-1.2287487	-1.5425161	4.4090400
H	-1.5913907	-0.3790764	-3.0990042	H	-1.8040570	-0.5343356	-3.0419516
H	-1.0457076	-1.9825579	-2.4792088	H	-1.2413608	-2.0902366	-2.3350636
H	-2.4884551	-1.1983314	-1.7781187	H	-2.6532680	-1.2463290	-1.6310337
H	0.9855971	-2.0292048	3.9483790	H	0.3339129	-2.3193425	4.0589670
N	-0.7723642	1.4616360	1.4351606	N	-0.7248986	1.4422085	1.4346969
Rh	-0.4470306	-0.6482147	1.3254536	Rh	-0.4514863	-0.6716548	1.2524115
C	0.8887150	-3.0665523	0.0778761	C	1.1205645	-2.9662793	-0.0308438
O	0.5938147	-2.8263036	-1.1071814	O	0.6603597	-2.8816834	-1.1679887
O	1.6731637	-4.1661587	0.3865777	O	2.0388219	-3.8992948	0.3230576
C	2.1473174	-4.9086895	-0.7467254	C	2.4577875	-4.7968830	-0.7366085
H	2.7654762	-5.7145876	-0.3344820	H	3.1856666	-5.4705104	-0.2757812
H	2.7463925	-4.2723724	-1.4155900	H	2.9146638	-4.2285790	-1.5578065
H	1.3095270	-5.3259932	-1.3245683	H	1.5949626	-5.3551907	-1.1227828
C	0.5647576	-2.3001116	1.2472593	C	0.7747588	-2.0991413	1.1086900
H	0.7838654	-2.8265814	2.1828905	H	1.2379434	-2.4567032	2.0429258
N	0.1754912	-0.2281156	3.2439639	N	0.1502627	-0.3262908	3.3761484

	H 1.1685178 -0.2230147 3.3065003

TS-ketene formation

^{N}**TS2-3**	^{NH}**TS2-3**
41	42
Energy = -1333.3009709070	Energy = -1333.7352855540
C -1.2479777 4.0330847 2.0377146	C -2.3174366 3.4013924 1.5047662
C -0.1104207 2.0239344 2.7187677	C -0.8264748 1.6597348 2.2200003
C -1.0347437 2.1528431 0.5422265	C -1.7854976 1.5414504 0.0669083
C -1.4777942 3.4520932 0.7873731	C -2.4446312 2.7513071 0.2752171
C -0.5668980 3.3046871 3.0167752	C -1.4929689 2.8495905 2.4889487
C 0.7044594 1.1116012 3.6150505	C 0.2522355 1.0919211 3.1095132
C -1.3253694 1.4077726 -0.7378051	C -1.8756632 0.7326600 -1.1923160
P -0.3817322 -0.2149730 -0.8755979	P -0.3776757 -0.3664180 -1.4372782
H 1.7707043 1.3181358 3.3985182	C -0.6201566 -2.4075736 0.6751948
H 0.5359116 1.3767932 4.6771515	O -1.2316094 -3.3638096 0.4563368
H -0.3759630 3.7280295 4.0031988	H 1.2036455 1.5753391 2.8306227
H -1.6023495 5.0431352 2.2462706	H 0.0605629 1.3258568 4.1688069
H -2.0147854 3.9938727 0.0087613	H -1.3477237 3.3510400 3.4455719
H -2.3977953 1.1518589 -0.7569315	H -2.8427562 4.3380484 1.6886709
H -1.1416983 2.0421815 -1.6178055	H -3.0627855 3.1714139 -0.5172811

C	-1.6006448	-1.3083263	-1.6902163	H	-2.7241688	0.0312763	-1.1084186
C	0.8635147	0.0994270	-2.1756247	H	-2.0635289	1.3593782	-2.0755348
C	-0.8522860	-0.7072230	3.8780796	C	-1.0485995	-1.6319303	-2.5569676
H	0.3905246	0.4088168	-3.1184291	C	0.8393814	0.5829785	-2.3995419
H	1.5545337	0.8802312	-1.8333658	C	-0.5053752	-1.1751955	3.7462747
H	1.4189759	-0.8357298	-2.3172890	H	0.4251502	0.8477249	-3.3826865
H	-0.9820536	-1.7897355	3.7455064	H	1.1157912	1.4947961	-1.8554455
H	-0.9262247	-0.4859588	4.9629151	H	1.7218024	-0.0557727	-2.5271578
H	-1.9606904	-0.8641911	-2.6297468	H	-0.3079791	-2.2410080	3.5870694
H	-1.1006421	-2.2634357	-1.8888717	H	-0.3826917	-0.9340783	4.8137784
H	-2.4459838	-1.4758460	-1.0112113	H	-1.5587887	-1.1292333	-3.3910634
H	-1.7266478	-0.2012475	3.3984667	H	-0.2294590	-2.2551826	-2.9258515
N	0.4622700	-0.3120710	3.3793084	H	-1.7685683	-2.2602403	-2.0183484
N	-0.3555778	1.4716984	1.4993820	H	-1.5353730	-0.9562961	3.4405488
Rh	0.3502441	-0.4819889	1.2856559	N	-1.0070447	1.0026041	1.0446010
C	1.0462280	-3.2415278	0.1551946	Rh	0.1377631	-0.7187935	0.7501876
O	0.9642275	-2.9290100	-1.0439603	C	2.0738533	-2.7087836	-0.5755852
O	1.3027707	-4.5511373	0.5243870	O	1.6803290	-2.4794486	-1.7248794
C	1.3854517	-5.4800153	-0.5674883	O	3.0915152	-3.5713596	-0.3064907
H	1.5688700	-6.4584289	-0.1089138	C	3.7401532	-4.1487252	-1.4649292
H	2.2068968	-5.2152326	-1.2490177	H	4.5564037	-4.7584294	-1.0666145
H	0.4488381	-5.4985045	-1.1447558	H	4.1277415	-3.3589222	-2.1226611
O	3.2177259	-0.4634252	0.4697795	H	3.0303970	-4.7683110	-2.0288371
C	0.8528800	-2.4054463	1.3111645	N	0.4273152	-0.3766998	2.9079737
H	1.2616916	-2.7851843	2.2532993	H	1.3893026	-0.6216006	3.1595841

C 2.1335596 -0.5375579 0.8780841	C 1.6063613 -2.0561268 0.6356770 H 1.9562521 -2.5085744 1.5726363

Rh(PNN)-ketene

^{N}**INT3**	^{NH}**INT3**
41	42
Energy = -1333.3487473640	Energy = -1333.7877724410
C -1.3649771 3.9835657 2.0273013	C -2.0071271 3.5214702 1.4960208
C -0.2038888 1.9871628 2.7061436	C -0.6477837 1.6673913 2.1847673
C -1.1475139 2.1037680 0.5336377	C -1.6713878 1.6194584 0.0546092
C -1.6016948 3.3994515 0.7807794	C -2.2308192 2.8781395 0.2791559
C -0.6656707 3.2684248 3.0010944	C -1.2092927 2.9080997 2.4651583
C 0.6598766 1.1058184 3.5887634	C 0.3359638 0.9742025 3.0977811
C -1.4065980 1.3637864 -0.7544700	C -1.8978141 0.8091075 -1.1867174
P -0.3134842 -0.1591677 -0.9145756	P -0.5424296 -0.4601605 -1.4240509
H 1.7059574 1.4110913 3.3918006	C -0.2941025 -2.7103760 0.5476619
H 0.4623097 1.3317799 4.6555953	O -1.2791006 -3.3682719 0.4477323
H -0.4635242 3.7001839 3.9815142	H 1.3445493 1.3529783 2.8682133
H -1.7253948 4.9918792 2.2357707	H 0.1266706 1.2141218 4.1529931
H -2.1453281 3.9370857 0.0042019	H -1.0141149 3.3928389 3.4214061
H -2.4481466 1.0005802 -0.7508454	H -2.4522457 4.4972800 1.6903779
H -1.3093652 2.0301542 -1.6246548	H -2.8488326 3.3379718 -0.4908341

C	-1.3823193	-1.3089662	-1.8593226	H	-2.8256271	0.2248557	-1.0639285
C	0.9634832	0.3161412	-2.1330267	H	-2.0321516	1.4443384	-2.0737074
C	-0.6800677	-0.8713251	3.8999954	C	-1.3476518	-1.7350616	-2.4390477
H	0.5202574	0.6911773	-3.0662644	C	0.6883448	0.3320542	-2.5112421
H	1.6194596	1.0757888	-1.6894693	C	-0.7202674	-1.1948635	3.6451385
H	1.5627954	-0.5823805	-2.3303579	H	0.2303829	0.6168614	-3.4689898
H	-0.7536223	-1.9431418	3.6647146	H	1.1025259	1.2215923	-2.0203159
H	-0.6330738	-0.7796067	5.0045376	H	1.4902863	-0.3954385	-2.6872078
H	-1.7297214	-0.8576713	-2.8002110	H	-0.6658644	-2.2723947	3.4541290
H	-0.7874657	-2.2065987	-2.0714068	H	-0.6097216	-1.0073619	4.7250789
H	-2.2468153	-1.5916557	-1.2444045	H	-1.8088619	-1.2734732	-3.3232118
H	-1.6404775	-0.3924692	3.5890843	H	-0.5845715	-2.4592827	-2.7443733
N	0.5327621	-0.3186272	3.2978236	H	-2.1121307	-2.2482293	-1.8430216
N	-0.4571955	1.4309230	1.4905066	H	-1.6999420	-0.8337072	3.3117084
Rh	0.3167591	-0.4570078	1.2443440	N	-0.8942685	1.0384499	1.0080399
C	1.3012247	-3.1690061	0.1092249	Rh	0.0624556	-0.7671321	0.7189705
O	1.2346091	-2.9660668	-1.1017775	C	1.9532748	-2.8430517	-0.5863068
O	1.1393904	-4.4172281	0.6484178	O	1.5961542	-2.6957729	-1.7474627
C	0.8824843	-5.4612322	-0.3109869	O	3.1841053	-3.2629371	-0.2229227
H	0.8014076	-6.3830454	0.2751650	C	4.0888766	-3.5573380	-1.3210989
H	1.7034178	-5.5365413	-1.0376234	H	5.0252053	-3.8639501	-0.8463497
H	-0.0531621	-5.2694466	-0.8558503	H	4.2384375	-2.6638402	-1.9410375
O	3.1026295	-0.3304349	0.3600032	H	3.6820282	-4.3660249	-1.9411941
C	1.5489449	-2.1778986	1.1558714	N	0.3437248	-0.5012239	2.8680754
H	1.7747024	-2.5426871	2.1614581	H	1.2542602	-0.8620716	3.1676346

C 2.1390357 -0.9125576 0.7634983	C 1.1305904 -2.5862852 0.6216513 H 1.5971966 -2.8683223 1.5707823

Rh(PNN)-ketene-imne, P_{II}

^{N}**INT4**	^{NH}**INT4**
52 Energy = -1506.7226717150 C -0.9837886 4.3716831 1.1233486 C -0.6480630 2.4210836 2.4892062 C -0.6752860 2.1915682 0.1449519 C -0.8901236 3.5599329 -0.0088909 C -0.8504789 3.7962063 2.3853986 C -0.4470038 1.6831269 3.7726714 C -0.4771351 1.2422180 -0.9950586 P -0.8997897 -0.4903362 -0.4610017 H 0.6280884 1.8269628 4.0452988 H -1.0367330 2.1579626 4.5838023 H -0.9033448 4.3998155 3.2908656 H -1.1527010 5.4439556 1.0194530 H -0.9658918 3.9808350 -1.0111579 H -1.0105593 1.5600520 -1.9023771 H 0.6004004 1.1998030 -1.2304819	53 Energy = -1507.1424033380 C -0.5659753 3.3479354 1.0044649 C -0.2294400 1.1644872 1.9415215 C -1.2883778 1.3672524 -0.1519292 C -1.1560687 2.7557261 -0.1165874 C -0.1014222 2.5478376 2.0534909 C 0.3588846 0.1677865 2.9140101 C -1.9731529 0.5771343 -1.2368449 P -1.2078158 -1.1269488 -1.3717084 C -0.1224426 -3.3673812 0.9042414 O -0.3900335 -4.5167779 1.1211857 H 1.3742430 -0.0713458 2.5600083 H 0.4469194 0.6006375 3.9230720 H 0.3674063 2.9918046 2.9316491 H -0.4669099 4.4319400 1.0601251 H -1.5229451 3.3650903 -0.9420916

C	-2.7238152	-0.5666272	-0.7232483	H	-3.0301834	0.4246939	-0.9635549
C	-0.2791982	-1.4349006	-1.9021183	H	-1.9564396	1.0951075	-2.2054120
C	-0.6679935	-0.4143405	4.8848253	C	-2.3738827	-2.0749986	-2.4001892
H	-0.7185625	-1.0311593	-2.8263397	C	0.2078024	-0.7933712	-2.4705021
H	0.8135393	-1.3491007	-1.9321141	C	-1.5273713	-1.0876682	3.9184299
H	-0.5286304	-2.4946004	-1.7879365	H	-0.1474548	-0.2360597	-3.3482468
H	-0.9537693	-1.4675877	4.7720054	H	0.9515469	-0.1957009	-1.9275263
H	0.3520681	-0.3844231	5.3271160	H	0.6712518	-1.7349779	-2.7824283
H	-2.9961461	-0.3216175	-1.7605963	H	-2.0615791	-2.0432184	3.8843187
H	-3.0766906	-1.5796136	-0.4892559	H	-1.1665757	-0.9051204	4.9426279
H	-3.2133364	0.1358110	-0.0361500	H	-2.5383112	-1.5801361	-3.3674779
H	-1.3524395	0.0357099	5.6318796	H	-1.9434266	-3.0703684	-2.5734378
N	-0.7726624	0.2799242	3.6200206	H	-3.3322497	-2.1843819	-1.8775557
N	-0.5863895	1.6420714	1.3833059	H	-2.2167753	-0.2851262	3.6395409
Rh	-0.3716671	-0.3632442	1.7502402	N	-0.8231736	0.6126238	0.8671300
C	2.0297208	-2.5881082	0.0805329	Rh	-0.8999455	-1.5716064	0.8333966
O	0.9459381	-3.1888002	0.0629473	C	1.8146971	-2.7134475	-0.5164075
O	3.1704096	-3.2283409	-0.4254427	O	1.4151543	-3.3266597	-1.4991974
C	2.9377103	-4.5454197	-0.9331059	O	3.0591521	-2.1671915	-0.4312391
H	3.9147696	-4.9060743	-1.2770050	C	3.9125758	-2.4105337	-1.5774254
H	2.2227414	-4.5356277	-1.7704564	H	4.8724749	-1.9485120	-1.3280574
H	2.5405277	-5.2147305	-0.1542703	H	3.4853834	-1.9527920	-2.4799276
O	2.1108847	0.7633864	1.6541659	H	4.0307726	-3.4884557	-1.7468496
C	2.3848091	-1.2873967	0.5377083	N	-0.4042787	-1.1214322	2.9518226
H	3.4434939	-1.0388533	0.4390033	H	0.2497384	-1.8473112	3.2604953

C 1.6519562 -0.2936359 1.2120705	C 1.0420424 -2.4797953 0.7119857
C 0.5182284 -2.9199733 3.0784377	H 1.6682874 -2.2633041 1.5851770
N -0.3439373 -2.3252834 2.3327411	N -2.8997571 -1.8948957 1.1131590
C -1.4685370 -3.1234010 1.8377284	C -3.9164242 -1.1575952 1.4186705
H -2.4069306 -2.5898015 2.0371867	C -3.2261775 -3.3324451 0.9418978
H -1.5001806 -4.1158653 2.3152370	H -2.8444906 -3.6855595 -0.0216675
H -1.3349927 -3.2544013 0.7570836	H -4.3097040 -3.5103592 1.0059155
C 1.7457703 -2.3135613 3.6519263	H -2.7068281 -3.9153748 1.7114306
H 0.3475305 -3.9854611 3.2911784	C -3.9363849 0.3032187 1.6956451
H 1.8634894 -2.6284314 4.6997469	H -2.9458922 0.7596409 1.7180318
H 1.7430730 -1.2207470 3.5827711	H -4.5530884 0.8178171 0.9406760
H 2.6195754 -2.6811001 3.0901871	H -4.4439034 0.4807139 2.6568686
	H -4.8952959 -1.6555939 1.4958603

TS-cycloaddition, P_{II}

^{N}TS4-5	**^{NH}TS4-5**
52	53
Energy = -1506.6983532640	Energy = -1507.1260154570
C -0.9258539 4.4408789 1.1902721	C -0.2730678 4.2228453 0.7947976
C -0.6815926 2.4523506 2.5213583	C -0.5597311 2.4021329 2.3333862
C -0.6399983 2.2769837 0.1712339	C -0.3971416 1.9437796 0.0222710
C -0.8265071 3.6516412 0.0422554	C -0.2756276 3.3062086 -0.2551082
C -0.8503124 3.8340601 2.4426791	C -0.4170865 3.7662400 2.1070121
C -0.6101156 1.6800863 3.8037882	C -0.8441890 1.8105700 3.6883203

C	-0.4835985	1.3343430	-0.9798903	C	-0.3821399	0.8726805	-1.0344207
P	-1.0090281	-0.3780080	-0.4638927	P	-1.1979712	-0.6240526	-0.3181254
H	0.3676833	1.9142908	4.2901404	H	-0.4665835	2.4620245	4.4916873
H	-1.3816840	2.0638242	4.5053831	H	-1.9390847	1.7562325	3.8098256
H	-0.9310131	4.4176179	3.3595128	H	-0.4245825	4.4608789	2.9461582
H	-1.0664634	5.5188901	1.1063153	H	-0.1581865	5.2878673	0.5936129
H	-0.8814076	4.0952420	-0.9516090	H	-0.1653700	3.6353683	-1.2874709
H	-0.9948091	1.6898667	-1.8854750	H	-0.8462118	1.2174826	-1.9691266
H	0.5925718	1.2348042	-1.2031704	H	0.6505069	0.5548840	-1.2542958
C	-2.8453442	-0.3248732	-0.5915568	C	-2.9649774	-0.1148120	-0.1614869
C	-0.5530290	-1.3264267	-1.9596697	C	-1.3413540	-1.8829562	-1.6304684
C	-0.8315715	-0.4989345	4.7906737	C	-0.9957006	-0.3057220	4.9274347
H	-1.0066183	-0.8531083	-2.8437309	H	-1.7967061	-1.4122353	-2.5137145
H	0.5376067	-1.3514478	-2.0554880	H	-0.3618479	-2.2968652	-1.8808917
H	-0.8933987	-2.3619544	-1.8613306	H	-2.0094976	-2.6777105	-1.2744445
H	-0.9100184	-1.5669852	4.5570357	H	-0.5660458	-1.3076819	5.0122299
H	0.0612664	-0.3511645	5.4342220	H	-0.8972150	0.2245723	5.8879394
H	-3.1723769	-0.0579683	-1.6072754	H	-3.3816287	0.1036698	-1.1552196
H	-3.2453301	-1.3130749	-0.3287471	H	-3.5424086	-0.9350158	0.2853348
H	-3.2336827	0.4065932	0.1287362	H	-3.0672527	0.7743614	0.4721659
H	-1.7156646	-0.2055548	5.3914539	H	-2.0610744	-0.4085964	4.6836736
N	-0.7722948	0.2632026	3.5626502	N	-0.5362084	1.5184695	1.3062546
N	-0.5732817	1.7012772	1.3999390	Rh	-0.4431262	-0.4717167	1.8120702
Rh	-0.3589049	-0.3221539	1.7112030	C	2.1541255	-2.1992897	0.0152611
C	1.9426972	-2.9034346	0.0967713	O	1.4410526	-1.8278184	-0.9184780

O	0.8668562	-3.2431408	-0.3949600	O	2.9389413	-3.3065998	-0.0647481
O	3.0803020	-3.6850873	-0.0773599	C	2.9194334	-3.9938943	-1.3374690
C	2.8634099	-4.8853031	-0.8338649	H	3.6436553	-4.8079167	-1.2377393
H	3.8353277	-5.3909608	-0.8681140	H	3.2084772	-3.3139132	-2.1496199
H	2.5173944	-4.6566533	-1.8529541	H	1.9172053	-4.3948329	-1.5432125
H	2.1136235	-5.5312399	-0.3526561	O	2.0673064	0.5985905	2.2951604
O	2.1464097	0.5710886	0.7971859	C	2.3184311	-1.5463768	1.3030531
C	2.2400116	-1.7857440	0.9564321	H	3.3456183	-1.5649655	1.6793488
H	3.3118021	-1.6510560	1.1293584	C	1.6130570	-0.3557612	1.6899051
C	1.5429281	-0.4819916	0.9663688	C	1.0968731	-2.7693422	2.6880758
C	1.1456650	-2.6082976	2.6051747	N	-0.1546798	-2.4530010	2.3216097
N	-0.1071233	-2.2716687	2.2842130	C	-0.8007518	-3.4597690	1.4671676
C	-1.0520397	-3.2777676	1.8270922	H	-1.8688508	-3.2276363	1.3687624
H	-1.9907138	-3.1790104	2.3985636	H	-0.7236577	-4.4601723	1.9204827
H	-0.6557967	-4.2949845	1.9851450	H	-0.3512892	-3.4963108	0.4604630
H	-1.2805152	-3.1711881	0.7567005	C	1.7552915	-2.3050594	3.9579521
C	1.9273900	-1.9053293	3.6893191	H	1.4434504	-3.7671268	2.3778034
H	1.3727772	-3.6855572	2.5407131	H	1.2766632	-2.8191699	4.8076599
H	1.5582669	-2.2417936	4.6729311	H	1.6998998	-1.2257299	4.1328172
H	1.8119662	-0.8156396	3.6396072	H	2.8150550	-2.5854006	3.9556324
H	2.9921322	-2.1585392	3.6173176	N	-0.3212101	0.4204516	3.8281736
				H	0.6858035	0.4879543	4.0123220

Rh(PNN)-metallocycle, P_{II}

^{N}**INT5**			^{NH}**INT5**		
52			53		
Energy = -1506.7240660400			Energy = -1507.1514571640		
C	-0.6305690	4.4217809	0.9316802	C	-0.3686232	4.3926833	0.8467641
C	-0.4875347	2.5353961	2.4158867	C	-0.4604615	2.5395397	2.3727539
C	-0.5111285	2.1698114	0.0863451	C	-0.5015833	2.1225640	0.0576003
C	-0.6137327	3.5388313	-0.1523044	C	-0.4491579	3.4896386	-0.2131181
C	-0.5652849	3.9156995	2.2292582	C	-0.3644843	3.9122968	2.1568181
C	-0.4675257	1.8529971	3.7544627	C	-0.6103368	1.9487235	3.7535345
C	-0.4308575	1.1257181	-0.9893576	C	-0.4762327	1.0699816	-1.0147033
P	-0.9967428	-0.5273242	-0.3350576	P	-1.0579479	-0.5637715	-0.3503813
H	0.5254756	2.0441617	4.2272046	H	-0.0887160	2.5666815	4.5012103
H	-1.2043098	2.3478682	4.4225053	H	-1.6810081	1.9834994	4.0143940
H	-0.5898236	4.5770582	3.0954422	H	-0.3008401	4.5940430	3.0047434
H	-0.7035299	5.4966153	0.7622293	H	-0.3033407	5.4633477	0.6530982
H	-0.6691442	3.9069270	-1.1765676	H	-0.4461127	3.8365113	-1.2457300
H	-0.9486432	1.4288709	-1.9102597	H	-1.0232731	1.3785132	-1.9166208
H	0.6348884	0.9624452	-1.2257234	H	0.5763013	0.9032944	-1.3018870
C	-2.8104330	-0.5623861	-0.6171757	C	-2.8806459	-0.5538727	-0.4985479
C	-0.3560485	-1.6593430	-1.6230765	C	-0.4992023	-1.7487785	-1.6109353
C	-0.8638635	-0.2336796	4.8969818	C	-0.8712482	-0.2005640	4.9367138
H	-0.7676199	-1.4069342	-2.6108518	H	-0.9859509	-1.5322889	-2.5720983
H	0.7376688	-1.5657531	-1.6480939	H	0.5879773	-1.6583199	-1.7263183

H	-0.6079094	-2.6943729	-1.3615287	H	-0.7314959	-2.7720740	-1.2933872
H	-0.9979550	-1.3069304	4.7059917	H	-0.6346141	-1.2660171	4.8430335
H	0.0298757	-0.0977806	5.5411491	H	-0.5744994	0.1882741	5.9223923
H	-3.0614442	-0.4113305	-1.6772211	H	-3.1814036	-0.3914178	-1.5431181
H	-3.1908503	-1.5373481	-0.2852586	H	-3.2706330	-1.5208520	-0.1555979
H	-3.2813187	0.2194767	-0.0075938	H	-3.3029078	0.2419432	0.1285350
H	-1.7363038	0.1515802	5.4615829	H	-1.9562085	-0.0860389	4.8159915
N	-0.7432775	0.4388449	3.6225258	N	-0.5162738	1.6697789	1.3376995
N	-0.4469853	1.6966181	1.3569446	Rh	-0.4396851	-0.3955505	1.7866375
Rh	-0.3851236	-0.3396274	1.8269895	C	1.8739762	-3.0042309	0.2640189
C	1.8566193	-3.1361392	0.3152632	O	1.0976254	-3.9055151	0.0177507
O	1.0564747	-4.0202898	0.0661652	O	2.8725058	-2.6122016	-0.5523536
O	2.8998975	-2.8317695	-0.5064976	C	3.0352239	-3.4012850	-1.7625315
C	2.9928817	-3.6437614	-1.6968643	H	3.8599090	-2.9299143	-2.3039124
H	3.8731965	-3.2743225	-2.2327290	H	2.1141919	-3.3891632	-2.3595829
H	2.0903115	-3.5360641	-2.3145739	H	3.2787779	-4.4392582	-1.5032469
H	3.1125873	-4.7038255	-1.4342282	O	2.1186886	0.1021355	0.7174252
O	2.1409077	-0.0602742	0.4973953	C	1.8706558	-2.1721422	1.5524706
C	1.8496434	-2.2428485	1.5408484	H	2.9249291	-2.0743595	1.8583509
H	2.9058239	-2.1149446	1.8303267	C	1.4124635	-0.7290131	1.2298055
C	1.3952836	-0.7908837	1.1243334	C	0.9812126	-2.7944011	2.6474167
C	0.9905292	-2.7515967	2.6602680	N	-0.3872425	-2.2478319	2.5863113
N	-0.3870911	-2.2374333	2.5920311	C	-1.3732542	-3.1922227	2.0753922
C	-1.3434463	-3.1394491	1.9753854	H	-2.3742073	-2.7348063	2.1098926
H	-2.3571745	-2.7243007	2.0953297	H	-1.4134214	-4.0871636	2.7217227

H -1.3323975 -4.1214127 2.4862134	H -1.1728097 -3.5470334 1.0445366
H -1.1797027 -3.3512078 0.8949446	C 1.6221860 -2.5613488 4.0226555
C 1.6268070 -2.3624129 4.0069742	H 0.9435714 -3.8804115 2.4670619
H 0.9532910 -3.8543349 2.6054398	H 0.9847679 -2.9741485 4.8145600
H 1.0106036 -2.7336863 4.8348978	H 1.7707088 -1.4881284 4.2235917
H 1.6912998 -1.2673439 4.0953409	H 2.6074683 -3.0455928 4.0888785
H 2.6417051 -2.7785893 4.1066280	N -0.1942886 0.5217542 3.8321343
	H 0.8173595 0.4843271 3.9879595

TS-cycloaddition lactam, P_{II}

^{N}TS5-0	**^{NH}TS5-0**
52	53
Energy = -1506.6934026660	Energy = -1507.1331030420
C 0.1217824 4.1856016 0.4559346	C -0.3487250 4.0956178 0.0842788
C 0.1839879 2.3233976 1.9813557	C -0.4922369 2.5440306 1.9150605
C -0.6595881 2.0004481 -0.2046050	C -0.2951328 1.7140760 -0.2824505
C -0.4293174 3.3386043 -0.5101582	C -0.2772860 3.0118683 -0.7905875
C 0.4412986 3.6652829 1.7095816	C -0.4545114 3.8562690 1.4551686
C 0.5091783 1.6347813 3.2708912	C -0.6881660 2.1889504 3.3644715
C -1.1767222 0.9901982 -1.1840655	C -0.2090984 0.4866994 -1.1414967
P -2.0518511 -0.3552122 -0.2464692	P -1.0372659 -0.9050342 -0.2339727
H 1.6201027 1.4951430 3.2915235	H -0.2901555 2.9851864 4.0167318
H 0.2893895 2.3115039 4.1240548	H -1.7693603 2.1158157 3.5716756
H 0.8846638 4.2909148 2.4842290	H -0.5151241 4.6796588 2.1662327

H	0.3047406	5.2359479	0.2285003	H	-0.3222388	5.1159289	-0.2974891
H	-0.6685514	3.7057328	-1.5078603	H	-0.1970115	3.1651244	-1.8661205
H	-1.7780901	1.4508764	-1.9809811	H	-0.6205497	0.6575666	-2.1464695
H	-0.3217837	0.4671986	-1.6483653	H	0.8448166	0.1837069	-1.2456015
C	-3.7235257	0.3614022	0.0451176	C	-2.8280763	-0.5248912	-0.4060968
C	-2.3798515	-1.6060124	-1.5444822	C	-0.8558999	-2.3553278	-1.3279816
C	0.0760061	-0.2787112	4.6319923	C	-0.3372054	0.4605891	5.0659631
H	-2.8480937	-1.1453168	-2.4265765	H	-1.2602061	-2.1061420	-2.3196630
H	-1.4232660	-2.0721889	-1.8070861	H	0.1866231	-2.6747964	-1.4241614
H	-3.0523556	-2.3739483	-1.1407911	H	-1.4366437	-3.1906650	-0.9145911
H	-0.5393443	-1.1817314	4.7164738	H	0.2127149	-0.4666217	5.2595740
H	1.1449116	-0.5711344	4.7520537	H	-0.0020702	1.2290381	5.7816599
H	-4.2254036	0.6176245	-0.8998421	H	-3.1136124	-0.4913264	-1.4671612
H	-4.3368689	-0.3645469	0.5951167	H	-3.4162444	-1.3010521	0.0993933
H	-3.6215040	1.2625425	0.6638676	H	-3.0528347	0.4430049	0.0595841
H	-0.1661403	0.3806798	5.4906523	H	-1.4109758	0.2893209	5.2138130
N	-0.2059516	0.3850184	3.3831133	N	-0.3992256	1.4911380	1.0603417
N	-0.3773762	1.5145063	1.0427199	Rh	-0.4292431	-0.4117028	1.8456327
Rh	-0.7377062	-0.3906322	1.5953420	C	2.1942611	-2.4887216	0.1841931
C	2.8740600	-2.6573495	1.0923036	O	2.1588116	-3.4419939	-0.5685279
O	3.1337233	-3.8235266	0.8650354	O	2.6543476	-1.2626194	-0.1585095
O	3.6968823	-1.6241205	0.7560506	C	3.2367492	-1.1792912	-1.4887949
C	4.8901795	-2.0117140	0.0412737	H	3.5662301	-0.1416168	-1.5948376
H	5.4247518	-1.0786162	-0.1651103	H	2.4931883	-1.4391633	-2.2542324
H	4.6263872	-2.5232741	-0.8942328	H	4.0867676	-1.8673507	-1.5730201

H	5.5070107	-2.6849909	0.6524165	O	2.1495359	-0.6119862	3.0734200
O	0.5593646	-2.0193586	-0.5093341	C	1.7564089	-2.5640411	1.6269179
C	1.6175627	-2.1337431	1.7263723	H	2.6043849	-3.0268896	2.1613285
H	1.8465242	-1.3076768	2.4104456	C	1.4171013	-1.2875457	2.3861652
C	0.5046012	-1.7188136	0.6803062	C	0.4494481	-3.3115777	1.9519488
C	0.6565988	-3.1690582	2.3110158	N	-0.1641134	-2.2222203	2.7656453
N	-0.6111674	-2.5024053	1.8965423	C	-1.0651865	-2.6074745	3.8459018
C	-1.6262781	-3.4122272	1.3992088	H	-1.5510147	-1.7214763	4.2656727
H	-1.6607898	-4.3262146	2.0158104	H	-0.5445012	-3.1365463	4.6598413
H	-1.4090398	-3.7162168	0.3538611	H	-1.8642339	-3.2656761	3.4618420
H	-2.6219106	-2.9507787	1.4361022	C	0.6931777	-4.6157846	2.7030672
C	0.7992118	-3.5925360	3.7650491	H	-0.1455830	-3.5279714	1.0497321
H	0.7730686	-4.0675012	1.6765089	H	-0.2463214	-5.1092273	2.9838105
H	-0.0609021	-4.2074698	4.0689110	H	1.2886060	-4.4512058	3.6128565
H	0.8680953	-2.7352853	4.4414144	H	1.2487506	-5.3000744	2.0477051
H	1.7072960	-4.2020939	3.8828131	N	-0.0825814	0.8762265	3.6721643
				H	0.9391017	0.9280101	3.5597563

TS-imine coupling, P_{IO}

^{N}**TS3-7**			^{NH}**TS3-7**		
52			53		
Energy = -1506.6929711300			Energy = -1507.1369406160		
C	-1.6882057	3.8582725	1.1270523	C	-0.6262844	4.1347333	0.7456665
C	-0.9215262	1.7996408	2.1081510	C	-0.5036528	2.0496577	1.9320128

C	-1.0457479	1.9777749	-0.2455615	C	-1.0539384	2.0309786	-0.3599095
C	-1.5129431	3.2863298	-0.1367984	C	-0.9657676	3.4228799	-0.4041410
C	-1.3793782	3.1056848	2.2611158	C	-0.4022090	3.4363326	1.9342155
C	-0.5867515	0.8722214	3.2434147	C	-0.3734492	1.2157294	3.1766562
C	-0.7748050	1.2954024	-1.5586577	C	-1.4888829	1.1933940	-1.5240054
P	-0.5872986	-0.5669079	-1.3385250	P	-0.9107106	-0.5700730	-1.3155116
C	-1.6255236	-2.4634488	1.0332654	C	-1.7235107	-2.7054150	1.0136034
O	-2.5785776	-2.7252808	0.3153000	O	-2.6292587	-2.9763393	0.2744725
H	-0.0939395	1.4478577	4.0569858	H	0.2122591	1.7441545	3.9480346
H	-1.5717727	0.5414149	3.6952657	H	-1.3817752	1.0465140	3.5917318
H	-1.4930069	3.5211761	3.2628190	H	-0.1518389	3.9610140	2.8558451
H	-2.0512123	4.8819258	1.2229413	H	-0.5448737	5.2210210	0.7193610
H	-1.7312837	3.8530236	-1.0419825	H	-1.1708628	3.9406145	-1.3406177
H	-1.5471241	1.5390695	-2.3028953	H	-2.5915447	1.1547287	-1.5339200
H	0.1808836	1.6719460	-1.9600663	H	-1.1752021	1.6260517	-2.4845292
N	-0.7789256	1.2475533	0.8745036	N	-0.7931514	1.3546319	0.7977452
Rh	-0.2956503	-0.7359010	0.8625154	Rh	-0.5816646	-0.6772343	0.8714031
C	0.3542153	-3.6331622	0.0071552	C	0.4613386	-3.4525937	0.0316145
O	-0.0419531	-3.7361901	-1.1476486	O	0.1166621	-3.6031533	-1.1300354
O	1.4868719	-4.2875779	0.4444752	O	1.6561873	-3.8865512	0.5205800
C	2.1739882	-5.0375137	-0.5731158	C	2.5125622	-4.5416760	-0.4482730
H	2.5064143	-4.3779865	-1.3880219	H	2.7662078	-3.8518427	-1.2641707
H	1.5233840	-5.8153420	-0.9974434	H	2.0135967	-5.4246736	-0.8673438
H	3.0376409	-5.4895034	-0.0728433	H	3.4104313	-4.8296011	0.1067794
C	-0.2191797	-2.8427860	1.0994601	C	-0.2976674	-2.7792443	1.1126621

H	0.2155007	-3.0605020	2.0742343	H	0.1146134	-2.9529955	2.1057945
N	0.1981798	-0.2408384	2.7983350	N	-2.3985054	-2.7146188	2.7496114
N	-2.2209041	-2.2583815	2.7078712	C	-3.3691918	-1.9441522	3.0724645
C	-3.1625490	-1.4140344	2.9485103	C	-2.0553910	-3.8955907	3.5269463
C	-1.8641742	-3.2843787	3.6709078	H	-1.0070366	-3.8362261	3.8476931
H	-0.8019510	-3.2081345	3.9288321	H	-2.1602821	-4.7809549	2.8849362
H	-2.0364445	-4.2676843	3.2113427	H	-2.7016563	-4.0017576	4.4102660
H	-2.4640114	-3.1938519	4.5894458	H	-3.9274486	-2.1741760	3.9941799
H	-3.6399193	-1.4480017	3.9385010	C	-3.8031757	-0.7851908	2.2549965
C	-3.6705945	-0.4568361	1.9342120	H	-2.9735617	-0.4257285	1.6187584
H	-2.8394466	-0.1076494	1.3004229	H	-4.6206197	-1.1076093	1.5883970
H	-4.3598425	-0.9868834	1.2562225	H	-4.1951005	0.0162991	2.8945069
H	-4.1926410	0.3824489	2.4068491	C	0.6273181	-0.6419483	-2.3065446
C	0.7647108	-0.9539119	-2.5225318	C	-2.1079131	-1.5288485	-2.2954185
C	-2.0482175	-1.2422265	-2.2139135	C	0.1995748	-0.9894863	4.0733132
C	0.6991417	-1.0102921	3.9067706	H	1.3785917	0.0314075	-1.8752785
H	1.7004133	-0.5065255	-2.1633999	H	0.4267729	-0.3539376	-3.3481600
H	0.5370194	-0.5823304	-3.5328367	H	1.0018562	-1.6723817	-2.2796332
H	0.8747017	-2.0455199	-2.5481409	H	-2.1652299	-1.1291929	-3.3179181
H	-2.0989647	-0.8741977	-3.2491324	H	-3.0925217	-1.4914045	-1.8155296
H	-2.9561355	-0.9689913	-1.6627537	H	-1.7680547	-2.5707203	-2.3101704
H	-1.9593665	-2.3350976	-2.1918958	H	-0.8345372	-1.2198849	4.3548839
H	-0.0926430	-1.3625278	4.6131826	H	0.7021503	-0.5044910	4.9258497
H	1.4038256	-0.4140900	4.5235912	H	0.7249342	-1.9232250	3.8434008
H	1.2527187	-1.8882561	3.5455137	N	0.1928748	-0.1251875	2.8743720

	H 1.1685391 0.0029633 2.5773572

Rh(PNN)-zwitterion, P_{IO}

^{N}**INT7**	^{NH}**INT7**
52	53
Energy = -1506.6941270790	Energy = -1507.1406715500
C -1.6858107 3.8201667 1.1456797	C -0.1478626 4.0930722 0.5801342
C -0.9197434 1.7631918 2.1302727	C -0.1898417 2.0668289 1.8704184
C -0.9610838 1.9683243 -0.2253097	C -0.9630563 2.0226800 -0.3561787
C -1.4587072 3.2658030 -0.1178538	C -0.6999906 3.3859978 -0.4879444
C -1.4077463 3.0577217 2.2822130	C 0.0959732 3.4248105 1.7819747
C -0.6419814 0.8089943 3.2618251	C -0.1028486 1.2936528 3.1583723
C -0.6499344 1.2873441 -1.5291044	C -1.6165220 1.1906266 -1.4194832
P -0.5854730 -0.5819196 -1.3011383	P -1.1089095 -0.5923245 -1.2089070
C -1.6897340 -2.5976697 1.1767163	C -1.8745842 -3.1186242 1.1648930
O -2.6046151 -2.8513908 0.3925940	O -2.6458868 -3.4231351 0.2812998
H -0.2438864 1.3634476 4.1377487	H 0.6353535 1.7393567 3.8454654
H -1.6582788 0.4248533 3.6105569	H -1.0853720 1.3611356 3.6545465
H -1.5735818 3.4562111 3.2835511	H 0.4986184 3.9521853 2.6464617
H -2.0709766 4.8357595 1.2404061	H 0.0765143 5.1549815 0.4830917
H -1.6611411 3.8376831 -1.0234842	H -0.9341219 3.8863832 -1.4270107
H -1.3492490 1.5900672 -2.3221114	H -2.7092366 1.2228552 -1.2703111
H 0.3585785 1.5929597 -1.8551246	H -1.4143431 1.5731321 -2.4295718
N -0.7100690 1.2333432 0.8961784	N -0.6659048 1.3672367 0.8052322
Rh -0.2588354 -0.7446489 0.8847449	Rh -0.6776418 -0.6567997 0.9604723
C 0.3061244 -3.6328007 0.0270881	C 0.4153627 -3.3034146 0.1300201

O	-0.1507803	-3.7962626	-1.0967539	O	0.0941796	-3.6083756	-1.0065304
O	1.5186464	-4.1770145	0.4020014	O	1.7031218	-3.3631666	0.5856678
C	2.2076439	-4.8788021	-0.6473897	C	2.6743982	-3.8134741	-0.3897584
H	2.4247987	-4.2071108	-1.4907762	H	2.7322471	-3.1071966	-1.2291931
H	1.6081837	-5.7218942	-1.0193317	H	2.4038955	-4.8048124	-0.7749601
H	3.1399780	-5.2388057	-0.1982458	H	3.6281166	-3.8519823	0.1455361
C	-0.2553762	-2.8616039	1.1409326	C	-0.4676960	-2.8063294	1.2138588
H	0.2465257	-3.0541548	2.0897666	H	-0.0156107	-2.9303856	2.2010396
N	0.1987616	-0.2658718	2.8407449	N	-2.5104025	-3.0528894	2.5944576
N	-2.1980089	-2.2494347	2.6360659	C	-3.3754040	-2.1223029	2.8883159
C	-3.1452463	-1.3685117	2.8260757	C	-2.2203896	-4.1833440	3.4737400
C	-1.8448412	-3.1964177	3.6891265	H	-1.1360299	-4.2727072	3.6159078
H	-0.7673297	-3.1768155	3.8763596	H	-2.5864480	-5.1062333	3.0031700
H	-2.1289172	-4.2066995	3.3634702	H	-2.7115527	-4.0453669	4.4446171
H	-2.3724989	-2.9431425	4.6178087	H	-3.8247932	-2.1693675	3.8862782
H	-3.5900342	-1.3313340	3.8239067	C	-3.6722252	-1.0268339	1.9757960
C	-3.6421403	-0.4969687	1.7445711	H	-2.6538106	-0.5836691	1.6290053
H	-2.7747629	-0.1408201	1.1514143	H	-4.0930296	-1.3959937	1.0302516
H	-4.2390724	-1.0919094	1.0337650	H	-4.3211449	-0.2686812	2.4223395
H	-4.2308616	0.3371618	2.1405639	C	0.3634311	-0.7219924	-2.2909217
C	0.6780895	-1.0682356	-2.5443361	C	-2.3774753	-1.5547468	-2.0874167
C	-2.1289033	-1.1734068	-2.0921924	C	-0.1338243	-0.9378236	4.1558520
C	0.7277678	-1.0134856	3.9508045	H	1.1592530	-0.0706717	-1.9077881
H	1.6598364	-0.6913777	-2.2298894	H	0.1069655	-0.4248253	-3.3176287
H	0.4321434	-0.6797606	-3.5439234	H	0.7076592	-1.7629553	-2.2875266
H	0.7063861	-2.1650022	-2.5730372	H	-2.4819761	-1.2036832	-3.1238056
H	-2.1991243	-0.8491789	-3.1408401	H	-3.3390813	-1.4768226	-1.5655710

H -2.9909884 -0.8048808 -1.5218803	H -2.0611282 -2.6050285 -2.0674626
H -2.1236564 -2.2681422 -2.0185646	H -1.2167529 -0.9250703 4.3356884
H -0.0469228 -1.3802469 4.6677894	H 0.3804642 -0.5308685 5.0415724
H 1.4232132 -0.3951197 4.5550633	H 0.1872200 -1.9744801 4.0097809
H 1.3001243 -1.8797536 3.5902278	N 0.1572912 -0.1551807 2.9353846
	H 1.1519324 -0.2732131 2.7078974

Rh(PNN)-zwitterion rotamer, P_{IO}

^{N}INT8	**^{NH}INT8**
52	53
Energy = -1506.6940675670	Energy = -1507.1361995650
C -0.9637486 3.9908394 1.0960888	C -0.4030705 4.0743284 0.7148438
C -0.5704392 1.8495353 2.1214656	C -0.3100440 2.0076083 1.9372354
C -1.1484500 1.9395281 -0.1672208	C -1.0845136 1.9860832 -0.2884967
C -1.2238146 3.3294634 -0.1077853	C -0.9090090 3.3668244 -0.3754791
C -0.6421968 3.2366020 2.2247761	C -0.1109656 3.3829514 1.8924662
C -0.2744453 0.9285878 3.2695748	C -0.1459966 1.2009293 3.1958152
C -1.4908699 1.1442396 -1.3959659	C -1.6770025 1.1529229 -1.3845933
P -0.8880959 -0.6288434 -1.2437136	P -1.0854578 -0.6085886 -1.2169646
C -1.7137621 -2.8685812 1.1216779	C -1.7705171 -3.0182041 1.0920966
O -2.5497868 -3.2435611 0.3022566	O -2.5803779 -3.3642584 0.2618465
H 0.4223429 1.4218512 3.9792425	H 0.5632270 1.6834481 3.8896107
H -1.2362333 0.8222831 3.8418079	H -1.1225959 1.1652831 3.7074302
H -0.4392007 3.7146073 3.1834214	H 0.2646267 3.9051522 2.7721058

H	-1.0143932	5.0785604	1.1512519	H	-0.2483294	5.1510896	0.6525100
H	-1.4947308	3.8869781	-1.0044445	H	-1.1743734	3.8801472	-1.2991198
H	-2.5896075	1.0849050	-1.4784732	H	-2.7720800	1.1233518	-1.2532709
H	-1.1317380	1.6376157	-2.3116550	H	-1.4793450	1.5748382	-2.3801010
N	-0.8016836	1.2160294	0.9392439	N	-0.7516934	1.3109515	0.8534906
Rh	-0.4725517	-0.7827257	0.9255212	Rh	-0.6299498	-0.7125998	0.9388320
C	0.4530628	-3.5611004	0.0129517	C	0.4974532	-3.3681827	0.0634725
O	0.1007110	-3.7157256	-1.1482956	O	0.1574748	-3.6173121	-1.0818568
O	1.6855312	-3.9966247	0.4578389	O	1.7750007	-3.5383709	0.5187762
C	2.5253595	-4.5616915	-0.5646873	C	2.7188391	-4.0028873	-0.4768002
H	2.7322470	-3.8229438	-1.3524423	H	2.8095157	-3.2703411	-1.2901393
H	2.0507099	-5.4395880	-1.0251694	H	2.3971014	-4.9643231	-0.8970625
H	3.4539041	-4.8479043	-0.0581402	H	3.6709927	-4.1087909	0.0517997
C	-0.2573905	-2.8996427	1.1154165	C	-0.3463572	-2.8318039	1.1560019
H	0.2476506	-3.0320537	2.0697869	H	0.0978526	-2.9671259	2.1441558
N	0.2235128	-0.3490550	2.8156924	N	-2.4537785	-2.8380925	2.5593825
N	-2.3069158	-2.3708456	2.4532285	C	0.3930485	-0.6539438	-2.2993205
C	0.5430271	-0.6952119	-2.3998404	C	-2.3110017	-1.5910863	-2.1371528
C	-2.1571201	-1.5577760	-2.1817588	C	0.1236840	-1.0469104	4.1220460
C	0.4570166	-1.2459198	3.8991048	H	1.1614435	0.0210585	-1.9021272
H	1.3439850	-0.0451639	-2.0252451	H	0.1278757	-0.3508996	-3.3222277
H	0.2583363	-0.3901465	-3.4178988	H	0.7792576	-1.6803050	-2.3125803
H	0.9000724	-1.7334367	-2.4158258	H	-2.4331840	-1.1932679	-3.1547917
H	-2.2892299	-1.1465825	-3.1938156	H	-3.2714564	-1.5846766	-1.6089126
H	-3.1049431	-1.5344308	-1.6299640	H	-1.9444167	-2.6241218	-2.1720330

H -1.8249207 -2.6019780 -2.2248129	H -0.9339023 -1.1371787 4.4002465
H -0.4858917 -1.7322435 4.2952342	H 0.6778853 -0.6195097 4.9736954
H 0.9212011 -0.7432072 4.7697268	H 0.5222182 -2.0458483 3.9120627
H 1.1210025 -2.0686234 3.5939865	N 0.2349986 -0.2082798 2.9100799
C -2.0419573 -3.1050156 3.5132181	H 1.2157829 -0.2194182 2.6038366
C -3.3324990 -1.3350159 2.4463136	C -2.3442172 -3.8577464 3.3401579
C -1.3083240 -4.4010789 3.5400920	C -1.5315326 -5.0742176 3.1042792
H -3.4757778 -1.0279212 1.4053302	C -3.3847750 -1.7349970 2.7424268
H -2.9904267 -0.4694471 3.0319146	H -2.8309719 -0.7961685 2.5870150
H -4.2720321 -1.7246411 2.8647260	H -4.1492135 -1.8126865 1.9573537
H -2.5083632 -2.7687771 4.4450263	H -3.8533675 -1.7798053 3.7333206
H -1.7634589 -5.0448871 4.3067435	H -2.9244437 -3.8211969 4.2731773
H -0.2479074 -4.2758290 3.8113641	H -2.1201599 -5.9501678 3.4140566
H -1.3396130 -4.9097769 2.5687995	H -0.6433863 -5.0548643 3.7579903
	H -1.2047449 -5.1933549 2.0674625

TS-cycloaddition, P_{IO}

^{N}TS8-0	**^{NH}TS8-0**
52	53
Energy = -1506.6473979770	Energy = -1507.0859224060
C -0.0221905 4.1453045 0.7522499	C -0.9675505 4.3127118 0.5435845
C 0.1163456 2.0291473 1.8944078	C -0.7701427 2.3038158 1.8453454
C -0.7922573 2.1103896 -0.2943931	C -0.4066019 2.2013366 -0.4822545
C -0.5759972 3.4873888 -0.3480244	C -0.6713553 3.5653398 -0.5960552

C	0.3184803	3.4052784	1.8883846	C	-1.0074089	3.6719201	1.7831636
C	0.5124207	1.0550983	2.9874436	C	-0.8984079	1.5032968	3.1115962
C	-1.4416541	1.3175477	-1.3956476	C	-0.0291934	1.3272374	-1.6375181
P	-1.0293912	-0.5024576	-1.2047230	P	-0.4156471	-0.4495162	-1.2304680
C	-2.2595124	-2.9993455	1.3563969	C	-2.1836385	-2.5153570	1.5367329
O	-3.2060702	-2.9378631	0.5838386	O	-3.1520016	-2.0765275	0.9421186
H	1.5568912	0.7537219	2.7857277	H	-0.6735272	2.1222656	3.9968062
H	0.5093771	1.5634283	3.9722691	H	-1.9383209	1.1510565	3.2074162
H	0.7534049	3.8863837	2.7647583	H	-1.2368126	4.2229787	2.6946562
H	0.1390076	5.2234294	0.7243571	H	-1.1647042	5.3816283	0.4675231
H	-0.8570814	4.0375860	-1.2460317	H	-0.6303931	4.0361046	-1.5777594
H	-2.5371284	1.3816179	-1.2837876	H	-0.5083949	1.6504833	-2.5725582
H	-1.1921131	1.7166110	-2.3900597	H	1.0617938	1.3810666	-1.7914617
N	-0.4376458	1.4016536	0.8145884	N	-0.4648006	1.5817708	0.7325207
Rh	-0.6352886	-0.5917885	0.9935216	Rh	-0.2513515	-0.4192295	0.9836690
C	0.0280985	-3.3878657	0.1599797	C	-0.2694018	-3.3695728	0.0488509
O	-0.3454764	-3.8402690	-0.9136663	O	-0.9572391	-3.7608923	-0.8799569
O	1.3199176	-3.4952320	0.6043941	O	1.0315516	-3.7237237	0.2337774
C	2.2238031	-4.1292311	-0.3219658	C	1.5518331	-4.6856138	-0.7189135
H	2.3150828	-3.5335659	-1.2412690	H	1.6121994	-4.2419953	-1.7207805
H	1.8727000	-5.1357647	-0.5875431	H	0.9077114	-5.5732233	-0.7595548
H	3.1868678	-4.1784785	0.1968052	H	2.5507139	-4.9421341	-0.3544386
C	-0.8081515	-2.6729891	1.1323754	C	-0.7287700	-2.4684754	1.1286100
H	-0.2655065	-2.2542002	2.0513210	H	-0.0095658	-2.3961053	2.0085831
N	-0.3321229	-0.1403389	2.9773089	N	-2.1820119	-3.1454196	2.7747787

N	-2.2873240	-3.3915383	2.6849182	C	0.6983445	-1.3650545	-2.3556427
C	0.3561715	-0.7597159	-2.3874676	C	-2.0787077	-0.7530825	-1.9128782
C	-2.4102490	-1.3595634	-2.0369431	C	-0.2388348	-0.5867977	4.2226670
C	-1.5943937	0.1175430	3.6635558	H	1.7282904	-1.3211985	-1.9817652
H	1.2301476	-0.1859853	-2.0538426	H	0.6498192	-0.9261020	-3.3623732
H	0.0816387	-0.4625064	-3.4105672	H	0.3674471	-2.4083959	-2.4123925
H	0.6049820	-1.8295746	-2.3752598	H	-2.0981323	-0.5803504	-2.9984080
H	-2.5483421	-1.0037243	-3.0687202	H	-2.8008589	-0.1000063	-1.4080926
H	-3.3244118	-1.2238860	-1.4476441	H	-2.3479047	-1.7929282	-1.6872314
H	-2.1745845	-2.4320382	-2.0286429	H	-1.2477877	-1.0128973	4.1746963
H	-2.1755120	0.9764653	3.2604940	H	-0.1197275	-0.0413195	5.1729914
H	-1.4162000	0.3267264	4.7398063	H	0.4966909	-1.3995085	4.1897502
H	-2.2407482	-0.7686188	3.5964385	N	-0.0352561	0.2917846	3.0521648
C	-0.9584762	-3.5828290	3.1311150	H	0.9447871	0.5989492	3.0496503
C	-3.4733115	-3.4538334	3.5138352	C	-0.9466873	-3.7733592	2.9943658
C	-0.2991483	-4.9178377	2.9940741	C	-0.6584081	-5.1337309	2.4631242
H	-4.3258999	-3.1627491	2.8860693	C	-3.2948096	-3.1512930	3.7117353
H	-3.3912883	-2.7599832	4.3667844	H	-4.0808045	-2.5154490	3.2849213
H	-3.6427914	-4.4704163	3.8993094	H	-3.6909146	-4.1662259	3.8532740
H	-0.6560594	-2.9593342	3.9845123	H	-2.9823140	-2.7523817	4.6899983
H	-0.5494710	-5.5661116	3.8552161	H	-0.4438104	-3.5076882	3.9361056
H	0.7940422	-4.8108094	2.9662588	H	-0.9969286	-5.8807110	3.2070107
H	-0.6264266	-5.4312472	2.0793530	H	0.4200233	-5.2888080	2.3227530
				H	-1.1900296	-5.3332366	1.5236109

TS-ketene formation ext. CO

^{N}**TS2-6**			^{NH}**TS2-6**		
43			44		
Energy = -1446.6940351610			Energy = -1447.1252132980		
C	-0.9535924	4.0831493 1.7684342	C	-0.8298181	4.0002298 1.4953648
C	-0.1162301	2.0031332 2.6401941	C	-0.0687751	2.0244532 2.6181446
C	-1.1015619	2.0479636 0.4864189	C	-0.9911794	1.8335758 0.4462467
C	-1.3214415	3.4219444 0.5935249	C	-1.1840687	3.2186130 0.3949990
C	-0.3482535	3.3676904 2.8040930	C	-0.2781315	3.3997873 2.6319200
C	0.6487053	1.0830019 3.5723558	C	0.6382861	1.2511042 3.7063606
C	-1.5148388	1.2074421 -0.6883656	C	-1.4134664	0.8547106 -0.5956789
P	-0.4858376	-0.3668798 -0.8586573	P	-0.2754065	-0.7272605 -0.8060626
C	-1.5239875	-1.8204171 1.5555607	C	-1.6419933	-1.7131649 1.6478772
O	-2.4151916	-2.5628345 1.5647910	O	-2.5885835	-2.3621881 1.7172227
H	1.7125418	1.1639078 3.2706605	H	1.7184671	1.2547533 3.4877686
H	0.5854365	1.4543022 4.6126935	H	0.4975338	1.7318161 4.6878543
H	-0.0398413	3.8611274 3.7257457	H	0.0002809	3.9913254 3.5034607
H	-1.1356452	5.1535665 1.8719437	H	-0.9908842	5.0781132 1.4732208
H	-1.7907287	3.9599509 -0.2296531	H	-1.6303033	3.6697071 -0.4902923
H	-2.5431997	0.8472176 -0.5092373	H	-2.3899596	0.4419814 -0.2858308

H	-1.5367492	1.7887639	-1.6217645	H	-1.5664095	1.3389545	-1.5716591
C	-1.6310878	-1.3772403	-1.8573470	C	-1.5144137	-1.6335837	-1.8106271
C	0.8699332	0.1246516	-1.9737344	C	0.9901105	0.0993681	-1.8318537
C	-0.9842011	-0.5336982	4.2488535	C	-1.0627320	-0.3555957	4.5066711
H	0.4756932	0.4633557	-2.9421219	H	0.5174787	0.4165917	-2.7719060
H	1.4404902	0.9365615	-1.5041513	H	1.3424548	0.9960401	-1.3052994
H	1.5156515	-0.7504898	-2.1077209	H	1.8287596	-0.5680180	-2.0445105
H	-1.2471448	-1.6000949	4.2274051	H	-1.3288508	-1.4180685	4.5204804
H	-0.8166675	-0.2543899	5.3074664	H	-0.9487232	0.0060532	5.5403403
H	-2.0151922	-0.7866716	-2.7020494	H	-2.2791383	-0.9616912	-2.2178734
H	-1.0883256	-2.2606370	-2.2066968	H	-0.9900360	-2.1546814	-2.6176807
H	-2.4694685	-1.6989547	-1.2258410	H	-1.9956750	-2.3914017	-1.1792279
H	-1.8691939	0.0428971	3.8963462	H	-1.8678559	0.2059416	4.0173790
N	0.2495933	-0.3220299	3.4944980	N	-0.4228246	1.2881159	1.5457192
N	-0.5142897	1.3782017	1.5059800	Rh	0.0239886	-0.7635583	1.5375142
Rh	-0.0088517	-0.6507442	1.4042338	C	0.8265932	-3.1780826	0.1215526
C	0.8905307	-3.2575804	0.1493986	O	0.7631018	-2.3892662	-0.9357696
O	0.7607126	-2.7776053	-1.0100908	O	1.2404808	-4.4478278	-0.0885102
O	1.3609998	-4.5559427	0.3016967	C	1.4986722	-4.8491790	-1.4520849
C	1.6647029	-5.2361140	-0.9217079	H	1.7995660	-5.8992658	-1.3845627
H	2.0306950	-6.2259376	-0.6229618	H	2.3070007	-4.2507787	-1.8933914

H 2.4377728 -4.7046232 -1.4969625	H 0.5940771 -4.7541591 -2.0684561
H 0.7716293 -5.3404733 -1.5568029	O 3.0713357 -0.7962712 1.1212259
O 3.0423008 -0.7964310 0.9596978	C 0.5331915 -2.7751698 1.3973069
C 0.6276679 -2.6291947 1.3734932	H 0.6105054 -3.4380344 2.2551783
H 0.8658141 -3.0869559 2.3299195	C 1.9380776 -0.7166035 1.2805272
C 1.9053576 -0.7058296 1.1564842	N 0.1921546 -0.1747042 3.7325728
	H 0.9287183 -0.7351271 4.1689108

Rh(CO)PNN-ketene

^{N}INT6	**^{NH}INT6**
43	44
Energy = -1446.7491984670	Energy = -1447.1852719360
C -0.9571748 4.0267901 1.8526447	C -0.9657562 4.0508094 1.8124271
C -0.1102722 1.9058701 2.6148440	C -0.1160372 1.9490459 2.6003832
C -1.2056990 2.0396426 0.5171761	C -1.1934467 2.0434851 0.5023114
C -1.3965103 3.4119114 0.6765607	C -1.3948876 3.4166392 0.6453202
C -0.3111710 3.2691780 2.8314171	C -0.3199850 3.3102300 2.8057194
C 0.6903255 0.9443562 3.4703274	C 0.6989089 1.0643767 3.5088240
C -1.6553506 1.2416226 -0.6766746	C -1.6382712 1.2284357 -0.6778621
P -0.5560084 -0.2592819 -0.8980425	P -0.5311737 -0.2594089 -0.8946077
C -1.8349467 -1.7730681 1.4503019	C -1.8977319 -1.7106654 1.4501469

O	-2.6025528	-2.6309205	1.3167348	O	-2.6869901	-2.5414449	1.3335553
H	1.7279922	1.0024321	3.0892342	H	1.7362980	1.0686586	3.1369278
H	0.7154998	1.2948577	4.5198359	H	0.7041516	1.4480408	4.5412584
H	0.0565782	3.7292787	3.7484376	H	0.0373023	3.7854375	3.7187145
H	-1.1101586	5.0970463	1.9976327	H	-1.1276140	5.1203810	1.9452084
H	-1.8899488	3.9860066	-0.1071577	H	-1.8908524	3.9770956	-0.1460942
H	-2.6605762	0.8314144	-0.4750653	H	-2.6461037	0.8240167	-0.4789655
H	-1.7231038	1.8582449	-1.5845111	H	-1.6996293	1.8256443	-1.5982488
C	-1.5039615	-1.3261387	-2.0336953	C	-1.4735055	-1.3731820	-1.9724094
C	0.8450571	0.3437253	-1.8969706	C	0.8893125	0.3293816	-1.8598378
C	-0.9537656	-0.6312692	4.2121912	C	-0.9618072	-0.5714355	4.3408759
H	0.4996782	0.8120562	-2.8290965	H	0.5453986	0.7782032	-2.8016927
H	1.4256742	1.0595554	-1.3012850	H	1.4498669	1.0667937	-1.2717971
H	1.4838322	-0.5213410	-2.1148647	H	1.5366404	-0.5316060	-2.0641365
H	-1.2618921	-1.6851503	4.1783630	H	-1.2520043	-1.6262423	4.2934101
H	-0.7181281	-0.3860281	5.2671188	H	-0.7356618	-0.2969290	5.3830122
H	-1.7493575	-0.8053141	-2.9703936	H	-1.7127396	-0.8667795	-2.9181966
H	-0.8778638	-2.2024557	-2.2455310	H	-0.8529563	-2.2548490	-2.1723450
H	-2.4254158	-1.6576730	-1.5380159	H	-2.4003176	-1.6804382	-1.4722851
H	-1.8340662	-0.0127782	3.9230908	H	-1.7947344	0.0410263	3.9768056
N	0.2381753	-0.4470494	3.3872401	N	-0.5695049	1.3431573	1.4797674

N -0.5856639 1.3253049 1.4859470	Rh -0.1639563 -0.7150358 1.3078521
Rh -0.1646731 -0.7194292 1.3238167	C 1.2680598 -3.1835156 -0.0300213
C 1.2959691 -3.1633714 0.0769972	O 1.1851708 -2.8189274 -1.1986224
O 1.1868417 -2.8654434 -1.1121490	O 1.3801099 -4.4734725 0.3486595
O 1.4062699 -4.4606538 0.4934411	C 1.4141474 -5.4417315 -0.7340431
C 1.3771831 -5.4422471 -0.5621515	H 1.5149488 -6.4145221 -0.2449244
H 1.4825942 -6.4109389 -0.0621990	H 2.2687441 -5.2445139 -1.3931687
H 2.2029084 -5.2801926 -1.2686004	H 0.4853005 -5.3925885 -1.3167127
H 0.4265664 -5.3945431 -1.1116737	O 2.7985944 -0.3033793 0.8162973
O 2.7693549 -0.2257048 0.7270688	C 1.2696269 -2.2898490 1.1464749
C 1.3340414 -2.2434926 1.2122569	H 1.4461380 -2.7938645 2.1016784
H 1.5138153 -2.6742824 2.1991879	C 1.8008881 -0.9397431 0.9976611
C 1.7946107 -0.8734668 1.0022333	N 0.2172269 -0.3513137 3.4618764
	H 0.9804386 -0.9478671 3.7953453

Rh(CO)PNN-ketene-imine, P_{OI}

^{N}INT9	**^{NH}INT9**
54	55
Energy = -1620.0973832360	Energy = -1620.5422037200
C -0.4998207 4.3947117 1.1120037	C -0.4831750 4.3067091 0.9441093
C -0.5805836 2.4299880 2.4931812	C -0.6103464 2.4081321 2.4094013

C	-0.5475724	2.1881734	0.1484955	C	-0.4865787	2.0565417	0.0841186
C	-0.5170903	3.5730770	-0.0152903	C	-0.4473464	3.4332762	-0.1402766
C	-0.5130559	3.8180801	2.3801840	C	-0.5488843	3.7872733	2.2366499
C	-0.6805219	1.6739398	3.7756049	C	-0.7370352	1.7568407	3.7552714
C	-0.4153966	1.2211425	-0.9874251	C	-0.3252074	1.0428414	-1.0038248
P	-1.0189471	-0.4698438	-0.5070592	P	-0.9950073	-0.5971855	-0.4722309
H	-0.2752091	2.2711130	4.6152232	H	-0.3242769	2.4081997	4.5422320
H	-1.7850702	1.5823988	3.9754377	H	-1.8077114	1.6123968	3.9816830
H	-0.4707270	4.4288518	3.2808100	H	-0.5503188	4.4416080	3.1072098
H	-0.4550581	5.4785382	0.9994459	H	-0.4391649	5.3839746	0.7848980
H	-0.4722079	3.9932062	-1.0196444	H	-0.3597989	3.8063139	-1.1597700
H	-0.8928100	1.5906070	-1.9062143	H	-0.7624596	1.3761118	-1.9550554
H	0.6612657	1.0894581	-1.1896875	H	0.7537874	0.8726571	-1.1618549
C	-2.8126978	-0.3580741	-0.9070983	C	-2.7832945	-0.4812144	-0.8547830
C	-0.4064786	-1.4603978	-1.9193283	C	-0.3895580	-1.7087310	-1.7819708
C	-0.5310387	-0.3908251	4.8525582	C	-0.3794261	-0.2799712	5.0479005
H	-0.8080037	-1.0409741	-2.8535537	H	-0.8625053	-1.3985986	-2.7249702
H	0.6882102	-1.4270162	-1.9275834	H	0.6983483	-1.6255543	-1.8660660
H	-0.7132698	-2.5047182	-1.8038155	H	-0.6379195	-2.7505081	-1.5576815
H	-0.0803777	-1.3872740	4.9006161	H	0.1387378	-1.2411460	5.0664043
H	-0.2685605	0.1334492	5.7924193	H	-0.0541564	0.3186818	5.9134588

H	-2.9572405	-0.1442347	-1.9754384	H	-2.9299843	-0.3464063	-1.9348469
H	-3.3099689	-1.3032405	-0.6549993	H	-3.2925155	-1.4004431	-0.5376735
H	-3.2748548	0.4362357	-0.3085324	H	-3.2300794	0.3653093	-0.3203684
H	-1.6417094	-0.5215811	4.8538851	H	-1.4591190	-0.4612044	5.1255679
N	-0.0489795	0.3634079	3.7094128	N	-0.6035035	1.5719612	1.3442420
N	-0.6189629	1.6523757	1.3881699	Rh	-0.5870512	-0.4548707	1.7988442
Rh	-0.5263440	-0.3761285	1.7994197	C	2.0496051	-2.4472877	0.0241645
C	1.9223244	-2.5857167	-0.0087668	O	1.0660141	-3.1824363	0.1835249
O	0.8500120	-3.2062977	0.0151982	O	3.1223184	-2.8708885	-0.7306867
O	3.0637775	-3.2186794	-0.5203018	C	3.0142557	-4.2065595	-1.2586127
C	2.8431448	-4.5497929	-0.9971320	H	3.9404050	-4.3741160	-1.8172746
H	3.8172273	-4.8985182	-1.3604572	H	2.1442838	-4.3003837	-1.9237980
H	2.1058107	-4.5689510	-1.8146331	H	2.9164238	-4.9437816	-0.4494416
H	2.4796051	-5.2115129	-0.1958882	O	1.9645177	0.6939150	1.9755658
O	1.9887158	0.8716698	1.3109542	C	2.3104294	-1.1316482	0.5359635
C	2.2545169	-1.2581216	0.3820999	H	3.3364678	-0.7796379	0.4040019
H	3.2916812	-0.9739867	0.1900621	C	1.5468465	-0.3042332	1.3531995
C	1.5370691	-0.2440460	1.0477737	C	0.5184343	-3.0673651	2.9844968
C	0.8520108	-2.8121308	3.0087593	N	-0.4229798	-2.4718801	2.3422284
N	-0.1759169	-2.3561804	2.3857404	C	-1.4806683	-3.3393186	1.8030662
C	-1.2031776	-3.3291773	2.0026291	H	-2.4696400	-2.9478802	2.0668006

H -2.1174701 -3.1333466 2.5783796	H -1.3861521 -4.3657648 2.1832093
H -0.8640941 -4.3582144 2.1889908	H -1.3689258 -3.3645363 0.7123154
H -1.4128185 -3.2187135 0.9346979	C 1.7806588 -2.5106303 3.5234077
C 2.0153971 -2.0472647 3.5232868	H 0.4008014 -4.1517744 3.1175657
H 0.8808129 -3.9008844 3.1672080	H 1.9381776 -2.8691916 4.5520485
H 2.2353949 -2.3773313 4.5513909	H 1.8626840 -1.4231929 3.4776614
H 1.8558012 -0.9626969 3.5007856	H 2.6051278 -2.9216338 2.9176006
H 2.8945110 -2.2930890 2.9066325	C -2.5640224 -0.4424527 2.2912727
C -2.5032860 -0.5309777 2.2675956	O -3.7118070 -0.4953413 2.2411548
O -3.5663952 -0.9496151 2.0636353	N -0.0952814 0.4165546 3.7782924
	H 0.9180832 0.5564158 3.6154610

TS-cycloaddition, P_{OI}

***N*TS9-10**	***NH*TS9-10**
54	55
Energy = -1620.0787750100	Energy = -1620.5208065820
C -0.4120881 4.4091384 1.0651795	C -0.0604997 4.1854643 0.7272944
C -0.5915677 2.4543302 2.4510244	C -0.5593328 2.4166093 2.2707057
C -0.5302246 2.2022193 0.1099391	C -0.2849482 1.9054003 -0.0191863
C -0.4444664 3.5845406 -0.0592427	C -0.0459819 3.2495197 -0.3061331
C -0.4694691 3.8380453 2.3355642	C -0.3121323 3.7650537 2.0337741

C	-0.7398280	1.6990724	3.7295238	C	-0.8900276	1.8472207	3.6207647
C	-0.4432460	1.2254704	-1.0220094	C	-0.2245271	0.8117060	-1.0512972
P	-1.1250085	-0.4339599	-0.5331104	P	-1.2395602	-0.5894266	-0.4154889
H	-0.3562659	2.2891578	4.5842196	H	-0.5579965	2.5224594	4.4251979
H	-1.8502555	1.6122875	3.8963424	H	-1.9866035	1.7502590	3.7038391
H	-0.4213806	4.4506340	3.2347483	H	-0.3112528	4.4713611	2.8628311
H	-0.3246225	5.4900892	0.9498667	H	0.1390034	5.2362778	0.5176430
H	-0.3741897	3.9991887	-1.0644737	H	0.1718534	3.5481251	-1.3305761
H	-0.9119380	1.6102463	-1.9392152	H	-0.5558316	1.1625198	-2.0385517
H	0.6255380	1.0519657	-1.2332740	H	0.8026322	0.4223168	-1.1410303
C	-2.9294005	-0.1923504	-0.8089095	C	-2.9394984	0.1102832	-0.5173562
C	-0.6725218	-1.4115906	-2.0143501	C	-1.3900366	-1.9107798	-1.6622925
C	-0.6129062	-0.3848469	4.7939094	C	-0.7778567	-0.1476280	5.0431503
H	-1.0956737	-0.9278686	-2.9078563	H	-1.7296787	-1.4514285	-2.6019468
H	0.4166804	-1.4784439	-2.0939811	H	-0.4422191	-2.4302723	-1.8128463
H	-1.0548739	-2.4326719	-1.9151396	H	-2.1638911	-2.6086784	-1.3167557
H	-0.2661684	-1.4205880	4.7440179	H	-0.3982866	-1.1710574	5.0949729
H	-0.2650657	0.0539698	5.7494453	H	-0.4392135	0.4162425	5.9260889
H	-3.1327199	0.0821844	-1.8535229	H	-3.1658513	0.3785943	-1.5587699
H	-3.4656076	-1.1183250	-0.5651278	H	-3.6681076	-0.6400135	-0.1845622
H	-3.2955634	0.5995112	-0.1432264	H	-3.0368866	1.0001079	0.1152602

H	-1.7293799	-0.4113067	4.8320329	H	-1.8740697	-0.1836942	5.0451179
N	-0.1066989	0.3900199	3.6729459	N	-0.5611945	1.5234970	1.2545770
N	-0.6356011	1.6721345	1.3488370	Rh	-0.6302525	-0.4801317	1.8156341
Rh	-0.5684652	-0.3739569	1.7715498	C	2.1615916	-2.1577220	-0.0032163
C	1.8920834	-2.7362308	0.0743607	O	1.3187341	-1.9343594	-0.8800934
O	0.8032714	-3.1197975	-0.3504727	O	3.0921691	-3.1409744	-0.1374994
O	3.0541389	-3.4402463	-0.2178950	C	3.0462251	-3.8799159	-1.3787525
C	2.8489054	-4.6214788	-1.0076485	H	3.9096122	-4.5513565	-1.3482336
H	3.8413508	-5.0705314	-1.1283348	H	3.1134499	-3.2013676	-2.2392918
H	2.4218039	-4.3730578	-1.9907886	H	2.1141193	-4.4582222	-1.4490843
H	2.1691212	-5.3252433	-0.5045169	O	1.9790296	0.5998152	2.3264505
O	2.0239584	0.7083769	1.0694255	C	2.3201816	-1.4468741	1.2422912
C	2.1940547	-1.6357728	0.9583983	H	3.3390602	-1.4374937	1.6377981
H	3.2693612	-1.4699691	1.0754269	C	1.5163439	-0.3361828	1.6632291
C	1.4533242	-0.3736504	1.1174018	C	1.0860258	-2.7508100	2.6347823
C	1.2318516	-2.5522086	2.6122180	N	-0.1660455	-2.4789083	2.2625377
N	-0.0637779	-2.3042676	2.3631825	C	-0.7872956	-3.4962652	1.4001860
C	-0.9317137	-3.3989318	1.9487913	H	-1.8699541	-3.3283294	1.3498460
H	-1.7843506	-3.4786223	2.6435382	H	-0.6311219	-4.4996056	1.8233098
H	-0.3868459	-4.3561359	1.9572392	H	-0.3760817	-3.4752826	0.3804411
H	-1.3237232	-3.2459679	0.9333571	C	1.7467590	-2.2731463	3.8947642

C 2.0491243 -1.8604239 3.6761379	H 1.4662738 -3.7302757 2.3065722
H 1.5121694 -3.6117885 2.4874119	H 1.2802303 -2.7915094 4.7492222
H 1.7786302 -2.2785963 4.6615545	H 1.6862767 -1.1943842 4.0653485
H 1.8701434 -0.7781942 3.7021738	H 2.8083460 -2.5454904 3.8810856
H 3.1157260 -2.0580721 3.5112158	C -2.5151159 -0.8368801 2.3795051
C -2.4826585 -0.6891205 2.2573685	O -3.4838766 -1.3126812 2.7728107
O -3.5013977 -1.2374947 2.2645850	N -0.3108931 0.4866019 3.7930897
	H 0.7165997 0.5908792 3.7690621

Rh(CO)PNN-metallocycle, P_{OI}

^{N}INT10	**^{NH}INT10**
54	55
Energy = -1620.1071296100	Energy = -1620.5516746390
C 0.0192220 4.3208644 0.8079106	C -0.0537932 4.3520605 0.7868385
C -0.2849859 2.4942883 2.3403947	C -0.3737344 2.5334215 2.3210776
C -0.4726810 2.0985517 0.0244956	C -0.4514528 2.1075704 0.0108706
C -0.2292904 3.4451982 -0.2500367	C -0.2309137 3.4584335 -0.2669183
C 0.0087735 3.8396078 2.1164817	C -0.1085280 3.8818779 2.1001573
C -0.4434139 1.8514081 3.6819654	C -0.5594616 1.9485555 3.6967902
C -0.6098040 1.0595998 -1.0552687	C -0.5112907 1.0612986 -1.0670660
P -1.1977116 -0.5877467 -0.4038159	P -1.1584878 -0.5622797 -0.4396227

H	0.0941280	2.4327424	4.4570870	H	-0.0697208	2.5747520	4.4592287
H	-1.5359708	1.9723312	3.9295592	H	-1.6390202	1.9534173	3.9229180
H	0.2186595	4.4941374	2.9619778	H	0.0446112	4.5529725	2.9449900
H	0.2349136	5.3714926	0.6093470	H	0.1404231	5.4059195	0.5873491
H	-0.2064406	3.7906356	-1.2832748	H	-0.1721954	3.7938589	-1.3016292
H	-1.2374180	1.4113127	-1.8871787	H	-1.0756359	1.4033989	-1.9461028
H	0.3996764	0.8723402	-1.4553342	H	0.5233580	0.8639097	-1.3924172
C	-2.9822761	-0.6276062	-0.8236292	C	-2.9452667	-0.5564751	-0.8152633
C	-0.4725443	-1.7244676	-1.6425015	C	-0.4709153	-1.7636765	-1.6176844
C	-0.6359669	-0.1743751	4.8694037	C	-0.6545534	-0.1574211	4.9719146
H	-0.8594644	-1.4993217	-2.6470981	H	-0.8926881	-1.5800061	-2.6158146
H	0.6167802	-1.5962213	-1.6350463	H	0.6180282	-1.6458528	-1.6568884
H	-0.6952967	-2.7637579	-1.3742021	H	-0.6991078	-2.7863816	-1.2962281
H	-0.5905164	-1.2649588	4.7734449	H	-0.5309205	-1.2369970	4.8321328
H	-0.1002600	0.1281461	5.7906286	H	-0.1619584	0.1776430	5.8965633
H	-3.1439589	-0.5144458	-1.9049547	H	-3.1103054	-0.4651119	-1.8974685
H	-3.4010796	-1.5861805	-0.4900657	H	-3.3906927	-1.4950670	-0.4605012
H	-3.4992107	0.1774686	-0.2866907	H	-3.4306270	0.2809882	-0.2992825
H	-1.7102163	0.1003408	5.0068358	H	-1.7290059	0.0529872	5.0416078
N	-0.0427075	0.4538186	3.6989297	N	-0.5475818	1.6780013	1.2894086
N	-0.5221867	1.6638426	1.3014432	Rh	-0.6781589	-0.4016045	1.7668383

Rh	-0.6759904	-0.3728307	1.8412724	C	1.9191097	-2.8858293	0.2328409
C	1.9294434	-2.9055222	0.2823587	O	1.1987159	-3.8283890	-0.0359532
O	1.2027047	-3.8373156	-0.0162560	O	2.9100466	-2.4363701	-0.5655040
O	2.9623661	-2.4947644	-0.5069369	C	3.1403812	-3.2146150	-1.7705891
C	3.1507851	-3.2662814	-1.7125676	H	3.9545692	-2.7035137	-2.2913581
H	4.0008625	-2.8037800	-2.2241420	H	2.2355588	-3.2462096	-2.3916952
H	2.2527862	-3.2321922	-2.3451712	H	3.4264593	-4.2404684	-1.5066775
H	3.3665071	-4.3156957	-1.4694795	O	1.9772090	0.2247615	0.7047700
O	1.9140498	0.1594652	0.5561924	C	1.8389199	-2.0554222	1.5118871
C	1.8323767	-2.0565544	1.5299226	H	2.8775500	-1.8909192	1.8388447
H	2.8661299	-1.8495284	1.8489003	C	1.2848049	-0.6365056	1.2020719
C	1.2522888	-0.6411843	1.1848277	C	0.9811564	-2.7402444	2.5844269
C	0.9856490	-2.7047868	2.6405246	N	-0.4302244	-2.2842428	2.5444840
N	-0.4335696	-2.3028491	2.5889866	C	-1.3250503	-3.3343114	2.0645103
C	-1.2808356	-3.2989980	1.9493470	H	-2.3721260	-3.0141425	2.1478516
H	-2.3398153	-3.0393278	2.0972581	H	-1.2113006	-4.2347377	2.6925959
H	-1.1228755	-4.2877294	2.4183642	H	-1.1257725	-3.6460206	1.0206279
H	-1.1068641	-3.4420564	0.8606238	C	1.6127924	-2.5302108	3.9673056
C	1.6333835	-2.3830012	3.9962876	H	0.9919341	-3.8203479	2.3731379
H	1.0225413	-3.7975220	2.4932837	H	0.9830752	-2.9706673	4.7505840
H	1.0499710	-2.8288517	4.8121679	H	1.7598870	-1.4639314	4.1981433

H 1.6852957 -1.2962953 4.1519906	H 2.6009317 -3.0105906 4.0139757
H 2.6543722 -2.7945195 4.0383685	C -2.5863197 -0.4140697 2.3377727
C -2.5671374 -0.4014098 2.3924501	O -3.6843109 -0.5620485 2.6369048
O -3.6816052 -0.6246436 2.5904565	N -0.1168159 0.5331330 3.7777279
	H 0.9068101 0.5048864 3.8017344

TS-cycloaddition lactam, P_{OI}

^{N}TS10-0	**^{NH}TS10-0**
54	55
Energy = -1620.0853569450	Energy = -1620.5317500890
C 0.7258569 3.8156726 0.2304233	C -0.2708459 4.0775017 -0.0216528
C 0.2706876 2.1732596 1.9253845	C -0.6095470 2.5707412 1.8176446
C -0.5074925 1.8067059 -0.2764217	C -0.4400239 1.6969129 -0.3648363
C 0.0346650 3.0246945 -0.6890597	C -0.2820594 2.9823327 -0.8843909
C 0.8575652 3.3801358 1.5491897	C -0.4311820 3.8689841 1.3483525
C 0.2329670 1.6094174 3.3088979	C -0.8857732 2.2450903 3.2566194
C -1.1647396 0.8379892 -1.2202176	C -0.4145994 0.4609216 -1.2146858
P -2.1318042 -0.4583365 -0.3032293	P -1.3008819 -0.8973596 -0.3295042
H 1.0545930 2.0221442 3.9263301	H -0.4748412 3.0242392 3.9197735
H -0.7150325 2.0073569 3.7625282	H -1.9794738 2.2306239 3.4090433
H 1.4042486 3.9668409 2.2865597	H -0.4270107 4.7028739 2.0493696

H	1.1704590	4.7600791	-0.0851924	H	-0.1358741	5.0854726	-0.4134897
H	-0.0650370	3.3305804	-1.7301673	H	-0.1553925	3.1140840	-1.9582722
H	-1.7761403	1.3534932	-1.9752652	H	-0.8405333	0.6420784	-2.2121001
H	-0.3721648	0.2731107	-1.7367959	H	0.6223257	0.1108670	-1.3387339
C	-3.8152719	0.2702070	-0.2209602	C	-3.0627291	-0.4998754	-0.6417772
C	-2.3256770	-1.7808570	-1.5562678	C	-1.0859513	-2.4117184	-1.3213711
C	-0.1962075	-0.2928328	4.6276869	C	-0.7047036	0.5486190	5.0080621
H	-2.6628940	-1.3641739	-2.5169722	H	-1.4612578	-2.2210868	-2.3370361
H	-1.3550325	-2.2752443	-1.6760408	H	-0.0309587	-2.6941831	-1.3665693
H	-3.0692170	-2.5073219	-1.2031407	H	-1.6828277	-3.2178408	-0.8738691
H	-0.3731776	-1.3723088	4.6320250	H	-0.1194849	-0.3310477	5.2948243
H	0.5672340	-0.0665817	5.3989736	H	-0.4564007	1.3696404	5.6999768
H	-4.2069546	0.4778884	-1.2267412	H	-3.2674510	-0.4998717	-1.7214543
H	-4.4904950	-0.4222852	0.2980715	H	-3.7015944	-1.2474415	-0.1544752
H	-3.7740067	1.2011689	0.3584239	H	-3.2965519	0.4863758	-0.2229735
H	-1.1440317	0.1989181	4.9494294	H	-1.7765670	0.3272581	5.0931821
N	0.2541793	0.1482668	3.3150808	N	-0.6057643	1.5117449	0.9723521
N	-0.3984346	1.4201007	1.0184485	Rh	-0.7879159	-0.4013997	1.8425646
Rh	-0.9568598	-0.4607480	1.7216941	C	2.4570292	-1.9278431	0.1882552
C	2.9625296	-2.3261983	0.8864767	O	1.8136383	-1.6013700	-0.8011002
O	3.2912601	-3.4680192	0.6217120	O	3.7940338	-2.0631259	0.1927822

O	3.6950472	-1.2348057	0.5240501	C	4.4640028	-1.7846915	-1.0658839
C	4.8666700	-1.5295817	-0.2644187	H	5.5279739	-1.9345532	-0.8641368
H	5.3264823	-0.5595408	-0.4812390	H	4.2673436	-0.7515252	-1.3792593
H	4.5847175	-2.0415444	-1.1945995	H	4.1115932	-2.4751082	-1.8428723
H	5.5615539	-2.1705200	0.2958696	O	1.9166943	-0.2618274	3.0265109
O	0.6432288	-1.5265388	-0.5811483	C	1.8755483	-2.2050454	1.5450242
C	1.7210044	-1.8962548	1.6125058	H	2.6811793	-2.5634063	2.2012372
H	1.9299856	-1.0755587	2.3147352	C	1.2572079	-0.9930716	2.2860449
C	0.5745345	-1.4570661	0.6444336	C	0.6363625	-3.0947385	1.7202281
C	0.8840229	-3.0078700	2.2337714	N	-0.0594952	-2.1633568	2.6744420
N	-0.4520082	-2.5261066	1.8128025	C	-0.7372101	-2.7408260	3.8307413
C	-1.4914415	-3.5217446	1.6790156	H	-1.1613405	-1.9509432	4.4546735
H	-2.0438425	-3.6819722	2.6252819	H	-0.0465104	-3.3289719	4.4528615
H	-1.0689779	-4.4917000	1.3573387	H	-1.5692577	-3.3925325	3.5129632
H	-2.2285840	-3.2070171	0.9269644	C	0.9617407	-4.4770854	2.2733129
C	1.1308249	-3.3547686	3.7000554	H	0.0576228	-3.2142752	0.7959197
H	1.0806286	-3.9170289	1.6327436	H	0.0545701	-5.0574045	2.4871597
H	0.3105100	-3.9677899	4.1021102	H	1.5700917	-4.4234047	3.1865510
H	1.2407095	-2.4597054	4.3208657	H	1.5403665	-5.0288246	1.5195066
H	2.0579551	-3.9412490	3.7822309	C	-2.6742797	-0.5352812	2.4404590
C	-2.6484410	-0.3343252	2.7121488	O	-3.5577992	-0.9110309	3.0818635

O -3.7285820 -0.5595635 3.0734561	N -0.3629305 0.9098180 3.6184662 H 0.6760909 0.8650548 3.5258953

TS-cycloaddition, P_{OO}

^{N}**TS6-0**	^{NH}**TS6-0**
54 Energy = -1620.0882696010 C 0.3554970 3.3597237 2.2317706 C -0.2723472 1.0793964 2.6678502 C -0.2381855 1.8595657 0.4350663 C 0.1650124 3.1217201 0.8674963 C 0.1326548 2.3270629 3.1406816 C -0.5966022 -0.0914013 3.5457555 C -0.4706017 1.5406556 -1.0160735 P -1.0923471 -0.2047675 -1.2549143 C -1.6666521 -2.6857831 0.3028774 O -2.1315407 -3.6860678 -0.0740445 H 0.1309113 -0.1316488 4.3883563 H -1.5748456 0.1542850 4.0345894 H 0.2634530 2.4780631 4.2123540 H 0.6749931 4.3427584 2.5788894	55 Energy = -1620.5401034500 C -0.1565937 3.5959694 -0.6434844 C 0.1265726 2.0896612 1.2078000 C -1.1331917 1.3945795 -0.6688831 C -0.9092870 2.6177146 -1.2966202 C 0.3630320 3.3323929 0.6215783 C 0.7278934 1.6835453 2.5242141 C -1.9814776 0.3116121 -1.2802179 P -1.7718327 -1.3174564 -0.3904205 C -0.9414756 -2.3232258 2.3018291 O -0.9807362 -3.3890869 2.7596960 H 1.7914171 1.4621266 2.3384944 H 0.6790330 2.5164223 3.2428463 H 0.9593256 4.0739854 1.1516542 H 0.0223549 4.5591064 -1.1217612

H	0.3298859	3.9095463	0.1330543	H	-1.3287835	2.8019336	-2.2848340
H	-1.1729909	2.2632947	-1.4603436	H	-3.0432556	0.5928809	-1.1844976
H	0.4851823	1.6195014	-1.5518291	H	-1.7798614	0.2069999	-2.3561333
C	-2.7856007	0.0261535	-1.9347904	C	-3.4448580	-2.0514033	-0.3843855
C	-0.1642592	-0.8124561	-2.7037164	C	-0.8382913	-2.3839356	-1.5427640
C	-1.0739557	-2.4405075	3.6283391	C	-0.7835007	0.7289760	4.2436536
H	-0.3029693	-0.1433879	-3.5656190	H	-1.3615350	-2.4777973	-2.5047080
H	0.8943981	-0.8817124	-2.4257189	H	0.1623127	-1.9588331	-1.6896180
H	-0.5213768	-1.8187846	-2.9574093	H	-0.7373078	-3.3803093	-1.0917771
H	-0.9694931	-3.3768777	3.0654108	H	-1.1403395	-0.2206291	4.6570148
H	-0.4576063	-2.5303010	4.5476193	H	-0.2487647	1.2855134	5.0303880
H	-2.7731209	0.6234866	-2.8583951	H	-3.8503759	-2.1212960	-1.4036600
H	-3.2138267	-0.9623339	-2.1487346	H	-3.3845210	-3.0586466	0.0481367
H	-3.4143345	0.5159454	-1.1806086	H	-4.1107577	-1.4446243	0.2411033
H	-2.1330287	-2.3589607	3.9595402	H	-1.6502009	1.3158270	3.9147993
N	-0.6352081	-1.3288574	2.8128548	N	-0.6095703	1.1488201	0.5639039
N	-0.4415061	0.8596861	1.3371631	Rh	-0.8132177	-0.6706835	1.5089215
Rh	-0.9497064	-1.0770330	0.8040600	C	2.3403743	-0.5989951	0.3123893
C	1.5850812	-2.9144972	-0.2354423	O	2.8609673	0.4033704	0.7913327
O	1.8141460	-2.8980555	-1.4387851	O	1.9534585	-0.6599161	-1.0067436
O	1.1693251	-4.0506219	0.4228052	C	2.2267558	0.5366346	-1.7679025

C	0.9348646	-5.1849049	-0.4313949	H	1.8486825	0.3365488	-2.7757552
H	0.6526744	-6.0034812	0.2390921	H	3.3051231	0.7415322	-1.7956780
H	1.8383420	-5.4423947	-1.0021253	H	1.7156682	1.4022477	-1.3254906
H	0.1175026	-4.9724398	-1.1343119	O	2.1733868	-1.3621343	3.3894141
O	2.1422325	0.2055508	-0.6029807	C	2.1454008	-1.8716582	0.9812751
C	1.7767363	-1.8287735	0.7143666	H	1.6207869	-2.6586899	0.4444888
H	1.4402959	-1.9784727	1.7355936	C	2.3871690	-2.0773916	2.4034062
C	2.3361430	-0.5269258	0.3733004	N	2.9333472	-3.3724656	2.4802053
N	3.1702457	-0.1907203	1.4580675	C	3.6176740	-3.6485501	1.3308048
C	3.6437329	-1.3165463	2.0855279	C	4.8345216	-2.9166675	0.8673147
C	4.5860001	-2.2914325	1.4508638	C	2.6779006	-4.3098851	3.5683014
C	3.3321377	1.1684232	1.9461178	H	4.9031668	-1.9073256	1.2886608
H	4.5591582	-2.2225504	0.3568012	H	5.7256788	-3.4980444	1.1744378
H	5.6220293	-2.0992168	1.7955256	H	3.5192298	-4.6855100	0.9762865
H	3.6542985	-1.2681037	3.1835940	H	4.8647722	-2.8526894	-0.2287036
H	4.3422533	-3.3245447	1.7373211	H	2.6751945	-5.3325653	3.1666338
H	2.7689888	1.8292955	1.2757907	H	3.4615235	-4.2324810	4.3351121
H	2.9217828	1.2575521	2.9651905	H	1.7060352	-4.0801105	4.0196688
H	4.3886977	1.4708125	1.9536247	N	0.1091528	0.4543086	3.0926915
				H	0.8923065	-0.1733025	3.3791032