Supporting Information

Energy decomposition.

We employed the scheme developed by Ziegler and Rauk in C_s symmetry which allows to separate the orbital interaction contributions to the bond energy within the irreducible representations A′ and A″, corresponding to σ and π interactions. We first reoptimized all complexes in C_s symmetry and the results of the bond analysis are presented in Table S1 together with the analogous bonding contributions for the parent diphenyl complex. Table S1 shows small steric energies indicating that the bonding dissociation energy is mainly due to the orbital interaction. It is worth noting that the small decrease of the bonding energy upon the insertion of one or two *p*-nitro groups on the phenyls comes from the compensation of two opposite effects: an increase of the attractive orbital interaction and a slightly larger increase of the steric repulsion between the metal fragment and the allenylidene unit.

Stereoisomers and Rotamers for the α-phosphonioallenyl adducts.

In the α-phosphonioallenyl species, rotation is in principle possible around Re–C_α and C_α–P bonds: the rotation around Re–C_α leads to three possible relative orientations of the phosphonioallenyl ligand with (i) the phosphonio unit pointing toward the triphos phenyl groups (and the allenyl unit toward the carbonyl ligands), (ii) the phosphonio unit pointing toward the carbonyl ligands (and the allenyl unit toward the triphos phenyl groups), or (iii) the phosphonio and allenyl moieties lying both in between one CO and one triphos phenyl group, respectively, **A**, **B** and **C** in Chart S1.

No clear possibility can be envisaged for the rotation around the C_α–P bond, but one of the substituents has likely to be almost eclipsed with either the C_α=C_β or the C_α–Re bond, in order to keep the other two substituents staggered, respectively **D** and **E** in Chart S2.

These forecasts were checked against a detailed analysis of all the minima obtained from geometry optimizations of the most plausible orientations of the rotatable bonds of the phosphine addition (as discussed in the manuscript). Moreover, in order to determine the existence of different rotamers and estimate the energy barriers involved in their interconversion, we performed an energy scan around each of the corresponding rotatable bonds and the results are reported in Figures S2 and S3 and discussed in the following. Indeed, for atropoisomerism to be observed, the involved rotamers have to be separated by sufficiently high barriers both for the clockwise and anticlockwise rotation of the corresponding dihedral angle. All the scans were performed using the experimental {C=C=C(Ph)(*p*-$C_6H_4NO_2$)} species with the bulkier $PMePh_2$ phosphine, the only one experimentally showing the presence of different rotamers at low temperature. The scans were carried out at the PBE/BS1 level of theory and, whenever necessary, the energies corresponding to minima and transition states were also re-evaluated at the MP2/BS2 level of theory.

The results of the optimizations of the different conformers arising from the rotation around the Re–C_α bond in the α-phosphonio allenyl species indicate that the most stable conformations show orientation **C**, see Chart S1, with the phosphonio and allenyl moieties lying both in between one CO and one triphos phenyl group, while the lowest conformations showing orientation **A** are significantly higher in energy and orientation **B** was only found (high in energy) for the bulkier $PMePh_2$ phosphine complex. These results suggest that the stability of the various possible conformations depends on a subtle balance between steric repulsion and π-stacking among phenyl rings. Indeed, the most stable conformations with orientation **C** show one or more tight π-stacking between the protruding phenyl rings on the triphos ligand and those on the allenyl and/or on the phosphonium units. Finally, when the rotation around the C_α-P bond is considered, all the optimized conformers only show orientation **D**, see Chart S2.

This analysis is confirmed by the energy scans: the scan performed by rotating around the Re-C_α bond (Fig S2) shows two minima within 2 kcal mol^{-1} corresponding to orientation **C**, distorted to allow the allenylidene terminal *p*-nitrophenyl to interact with one of the triphos phenyl groups, and

a further minimum higher in energy (*ca*. 7 kcal mol^{-1}) corresponding approximately to conformation **B**. These three minima are separated by two low barriers, less than 10 kcal mol^{-1}, too small to account for any possible atropoisomerism.

The energy scan for the rotation around the C_α-P bond for the experimental phenyl *p*-nitrophenyl phosphonio species (see Fig. S3) shows the presence of three minima very close in energy and separated by energy barriers of, at most, 11 and 8 kcal mol^{-1}, values indicating that no atropoisomerism can be observed for these rotamers in agreement with the experiment.

Table S1. Bond dissociation energy decomposition (kcal mol^{-1}) calculated at the PBE/BS4//PBE/BS3 level in C_s symmetry, for the $[(triphos)(CO)_2Re(C{=}C{=}CRR')]^+$ allenylidenes with R = R' = Ph; R = Ph, R' = *p*-$C_6H_4NO_2$; R = R' = *p*-$C_6H_4NO_2$, and R = H, R' = *p*-$C_6H_4NO_2$.

R, R'	E^*	E_{Pauli}	E_{elect}	E_{Ster}	E_{orb}	$E_{A'}$	$E_{A''}$
Ph, Ph	-87	220	-198	22	-109	-80	-29
Ph, *p*-$C_6H_4NO_2$	-86	220	-193	27	-113	-80	-33
p-$C_6H_4NO_2$, *p*-$C_6H_4NO_2$	-85	213	-184	29	-114	-79	-35
H, *p*-$C_6H_4NO_2$,	-92	206	-183	23	-115	-78	-37

Table S2. Breakdown of the contributions from rhenium and allenylidene carbon atoms (at the PBE/BS4//PBE/BS3 level) to the LUMO of the $[(triphos)(CO)_2Re(C{=}C{=}CRR')]^+$ allenylidenes with R = R' = Ph; R = Ph, R' = *p*-$C_6H_4NO_2$; R = R'=*p*-$C_6H_4NO_2$, and R=H, R'=*p*-$C_6H_4NO_2$.

R, R'	MO	ε	M	C_α	C_β	C_γ

Ph, Ph	HOMO	-7.49	33.3	8.0	21.7	-
	LUMO	-6.11	8.4	21.3	-	26.8
	Mulliken Charge		0.35	-0.39	0.08	-0.17
Ph, *p*-$C_6H_4NO_2$	HOMO	-7.72	31.2	9.3	22.9	-
	LUMO	-6.46	6.7	18.6	2.4	21.7
	Mulliken Charge		0.37	-0.36	0.09	-0.17
p-$C_6H_4NO_2$, *p*-$C_6H_4NO_2$	HOMO	-7.98	37.6	9.4	24.4	-
	LUMO	-6.79	7.6	20.8	3.4	18.5
	Mulliken Charge		0.39	-0.35	0.09	-0.17
H, *p*-$C_6H_4NO_2$,	HOMO	-7.96	38.8	9.4	25.0	-
	LUMO	-6.73	9.32	20.6	3.8	23.6

Table S3. Energies, enthalpies and free energies for the formation of the adducts of the addition of PMe_3 to the C_γ atom of the considered $[(triphos)(CO)_2Re(=C=C=CRR')]^+$ allenylidenes (R=R'=Ph, R=Ph, R'=*p*-$C_6H_4NO_2$, R=R'=*p*-$C_6H_4NO_2$, and R=H, R'=*p*-$C_6H_4NO_2$), calculated at the LMP2/BS2//PBE/BS1 level of theory (kcal mol^{-1}).

R, R'	**ΔE_{gas}**	**ΔE_{sol}**	**ΔH_{sol}**	**ΔG_{sol}**
R=R'=Ph	-5.6	-3.4	-3.6	11.5
R=Ph, R'=*p*-$C_6H_4NO_2$	-7.2	-5.0	-2.7	10.9
R=R'= *p*-$C_6H_4NO_2$	-9.8	-6.2	-4.9	8.2

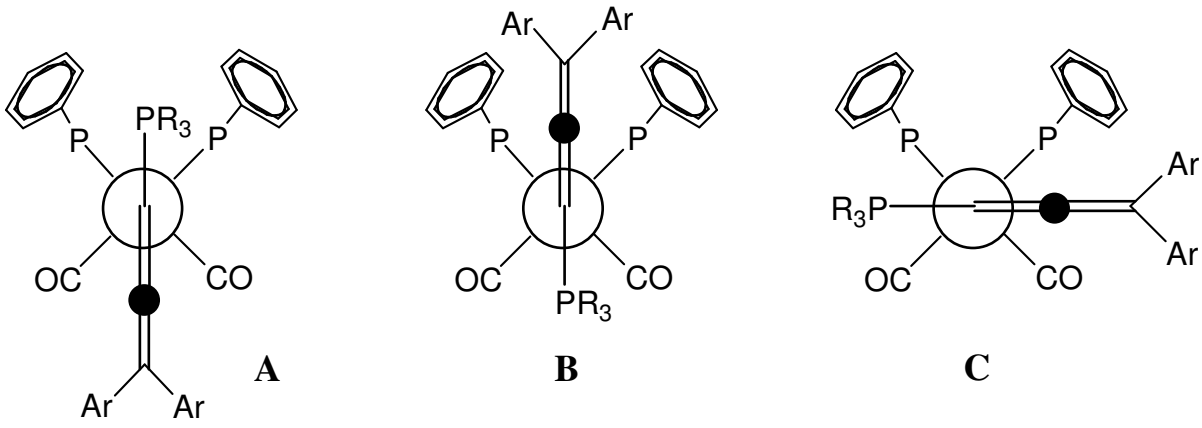

Chart S1. Possible orientations of the phosphonioallenyl ligand with respect to the $[(triphos)(CO)_2Re]^+$ metal fragment through rotation around the Re–C_α bond in the α-phosphonio allenyl product.

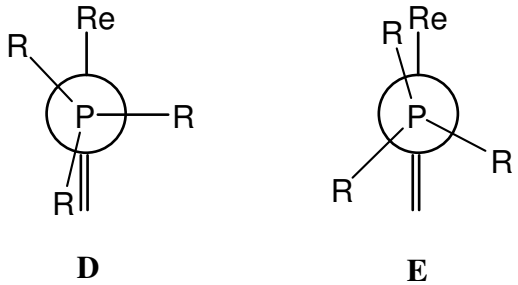

Chart S2. Possible orientations of the PR_3 group with respect to the allenyl unit through rotation around the C_α–P bond in the α-phosphonio allenyl product.

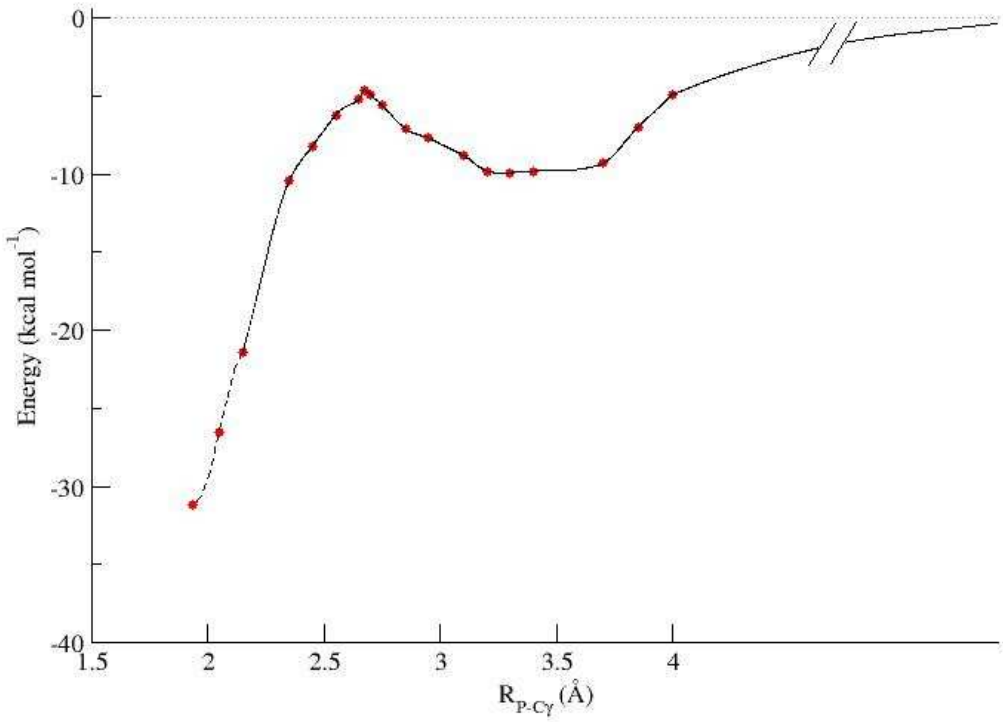

Figure S1. Energy scan for the attack of PMe_3 to the C_γ atom of the bis-*p*-nitro-phenyl allenylidene, using as reaction coordinate the P-C_γ distance.

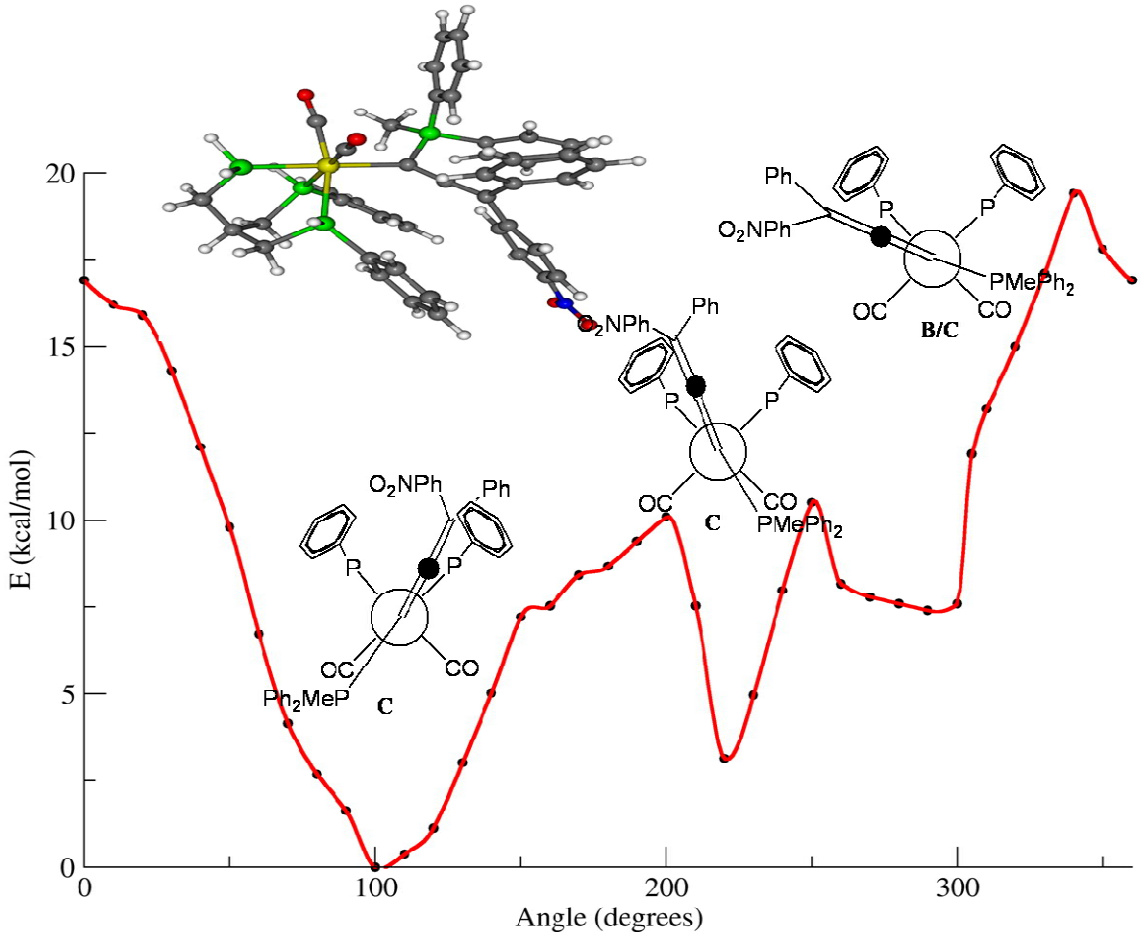

Figura S2. Energy scan for the rotation around Re–C_α bond in the α-phosphonio allenyl product of the addition of $PMePh_2$ to the asymmetric {C=C=C(Ph)(*p*-$C_6H_4NO_2$)} allenylidene. Angle in degrees, energies in kcal mol^{-1}.

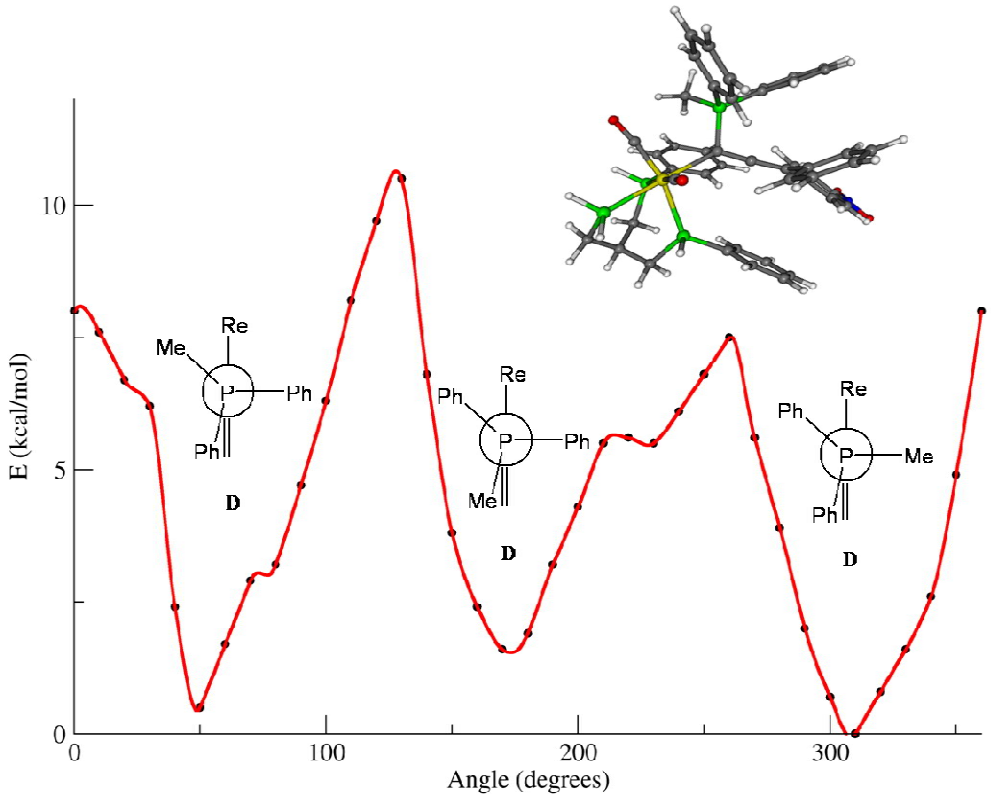

Figura S3. Energy scan for the rotation around RC_{α}–P bond in the α-phosphonio allenyl product of the addition of $PMePh_2$ to the asymmetric {C=C=C(Ph)(*p*-$C_6H_4NO_2$)} allenylidene. Angle in degrees, energies in kcal mol^{-1}.

Cartesian coordinates

We report below the cartesian coordinated for all considered nitrosubstituted allenylidenes and their adducts with PMe_3 and $PMePh_2$.

The cartesian coordinates for the unsubstituted $[(triphos)(CO)_2Re(=C=C=CPh_2)]^+$ allenylidene complex and all its adducts with PMe_3 and $PMePh_2$ can be found in ref. Coletti, C.; Gonsalvi, L.; Guerriero, A.; Marvelli, L.; Peruzzini, M.; Reginato, G.; Re, N. *Organometallics,* **2010***, 29,* 5982 – 5993.

$[(triphos)(CO)_2Re\{C=C=C(C_6H_5)(p\text{-}C_6H_4NO_2)\}]^*$ (3)

C	1.4774410428	-0.6250351061	1.2419324974
C	1.3751381326	-1.9788906452	1.6063101991
C	0.5120166438	-2.3632211970	2.6432647459
C	-0.2600628532	-1.4050616434	3.3043085127
C	-0.1701000359	-0.0352508346	2.9440264973
C	0.7227996949	0.3394131501	1.9083827311
C	-0.9440894000	0.9929398127	3.6556358141
C	-0.4737204279	2.2792811540	3.7398463752
C	-0.0287700338	3.4648233012	3.8383359263
Re	0.7298975025	5.2894168147	4.0753444366
P	-1.4832181066	6.3498322698	4.1082275018
C	-3.0686870360	5.4354697471	4.0846218508
C	-4.0853761780	5.7558609214	5.0070996646
C	-5.3031436821	5.0628966775	4.9788630190
C	-5.5143610211	4.0517525810	4.0309956504
C	-4.5034826219	3.7262642797	3.1144006433
C	-3.2799440481	4.4074318871	3.1433410788
C	2.5305850126	4.5514340529	4.0195836647
O	3.6166738677	4.1219969659	3.9704125804
C	0.6005123355	5.1286067808	6.0152929734
O	0.5174552694	5.0732424016	7.1789055980
P	0.9635205154	5.8026525597	1.6761004678
C	0.4306422079	4.6623889956	0.3390798065
C	-0.9252521714	4.5394539478	-0.0238764464
C	-1.3092177258	3.6313458066	-1.0196200761
C	-0.3472713820	2.8326272695	-1.6563008811

C	1.0035385309	2.9509669591	-1.2982601199
C	1.3946482159	3.8614119502	-0.3055228679
P	1.5675661821	7.5781129471	4.2662208699
C	0.5452914479	8.8826644648	3.3776926272
C	-0.3959154012	8.3435912274	2.2684984701
C	0.3142957431	7.5004711131	1.1789538240
C	-1.6931213956	7.6840802381	2.8067358115
C	-2.2441405241	0.6564095143	4.2799007658
C	-2.6715810226	1.3362445231	5.4459858270
C	-3.9118123854	1.0607740534	6.0195597623
C	-4.7391595134	0.1116167463	5.4076096336
C	-4.3585414778	-0.5738661601	4.2502995938
C	-3.1073182646	-0.3037072858	3.6931930210
N	-6.0761116720	-0.1599725863	5.9925323840
O	-6.7670086865	-1.0296018538	5.4437020214
O	-6.4055078336	0.5104229969	6.9814393875
H	2.3352477360	5.9264043384	1.3119231425
H	2.8765334694	7.8577107779	3.7708024395
H	1.7267085143	8.1691177833	5.5525711648
H	-1.6888247534	7.1158885950	5.2934217283
H	-2.2444534643	7.2182308597	1.9708599022
H	-2.3631155164	8.4536815505	3.2261921314
H	1.2405909755	9.6264520714	2.9550876125
H	-0.0512391029	9.4091495698	4.1420477382
H	-0.3830500137	7.3345577320	0.3401839500
H	1.1651996429	8.0673813644	0.7638241610
H	-0.7410760542	9.2481046018	1.7322655427
H	-2.0066724032	2.0753470048	5.9005979877
H	-2.8064078548	-0.8137934333	2.7748383553
H	-5.0466796593	-1.2970806624	3.8071125828
H	-4.2571125442	1.5634051737	6.9253464050
H	-1.6908371868	5.1552282721	0.4611150507
H	2.4537742117	3.9512971844	-0.0408660317
H	1.7615571856	2.3424775051	-1.8008977213
H	-2.3633819370	3.5506326327	-1.3009809406
H	-0.6491716040	2.1265399546	-2.4350200807
H	-3.9276952960	6.5432552757	5.7520077580
H	-2.4827152537	4.1234070230	2.4504679310
H	-4.6617513405	2.9262262349	2.3848243502
H	-6.0861136859	5.3130875314	5.7007139931
H	-6.4656438561	3.5115921049	4.0125084913
H	1.9725254917	-2.7331023882	1.0851430092
H	0.7907713242	1.3945225420	1.6257405745
H	-0.9048866196	-1.7071858424	4.1340082835
H	0.4469617836	-3.4132454032	2.9425943833
H	2.1485498604	-0.3263653241	0.4311358142

α-phosphonioallenyl complex [(triphos) $(CO)_2Re\{C(PMe_3)=C=CPh(p\text{-}C_6H_4NO_2)\}]^+$ (7)

Re	1.75450	-1.06880	2.03060
C	2.07750	-2.92620	1.69480

O	2.38090	-4.04640	1.46640
C	1.77990	-1.29040	3.94860
O	1.80760	-1.39690	5.11780
C	-1.42280	-0.42760	2.43210
C	-2.46610	0.35710	2.74620
P	1.92320	-0.61120	-0.38960
H	2.83130	-1.53940	-0.98210
P	4.12940	-0.79640	1.99540
H	4.94970	-1.95770	1.88690
H	4.74480	-0.24030	3.15800
P	1.81050	1.39940	2.32260
H	2.09150	1.80980	3.65920
C	3.30780	2.18460	1.46410
H	2.98720	3.19540	1.16270
H	4.09800	2.31970	2.22370
C	4.85450	0.29060	0.65480
H	5.09570	-0.34740	-0.21280
H	5.80800	0.70880	1.01790
C	2.80810	0.99050	-0.78540
H	2.04570	1.78500	-0.86360
H	3.25510	0.87930	-1.78760
C	3.88820	1.42930	0.24140
H	4.50900	2.17210	-0.29330
C	-2.70290	0.66110	4.19280
C	-3.12630	1.13830	6.94630
C	-1.62620	0.99200	5.04180
C	-3.99700	0.56320	4.75130
C	-4.20410	0.80250	6.11540
C	-1.83590	1.22790	6.40500
H	-0.62080	1.07450	4.61690
H	-4.84530	0.29440	4.11410
H	-5.21380	0.72460	6.53010
H	-0.98960	1.49190	7.04670
C	-3.37680	0.87280	1.69170
C	-5.03490	1.88670	-0.33520
C	-4.25100	1.95820	1.94160
C	-3.36790	0.31160	0.39010
C	-4.18520	0.81080	-0.62190
C	-5.07930	2.46440	0.93740
H	-4.26320	2.42560	2.92920
H	-2.68700	-0.51660	0.16770
H	-4.18090	0.38980	-1.62970
H	-5.75070	3.30760	1.11520
C	0.59840	-0.73770	-1.67000
C	-1.44380	-1.07950	-3.58490
C	-0.11320	0.37440	-2.15950
C	0.28240	-2.02350	-2.15830
C	-0.73360	-2.19200	-3.10780
C	-1.12800	0.20140	-3.11310
H	0.11940	1.38650	-1.81610
H	0.84570	-2.89660	-1.80980

H	-0.95920	-3.19250	-3.48940
H	-1.66670	1.07470	-3.49370
H	-2.23160	-1.21010	-4.33250
C	0.50000	2.62170	1.91250
C	-1.29780	4.61700	1.08320
C	-0.41340	2.36500	0.87540
C	0.49070	3.87890	2.55190
C	-0.40790	4.86990	2.13790
C	-1.30440	3.36340	0.45660
H	-0.44930	1.37220	0.41600
H	1.18590	4.08760	3.37270
H	-0.41350	5.84140	2.64110
H	-2.01900	3.15080	-0.34440
H	-1.99570	5.39480	0.75900
C	-0.45610	-1.29420	2.18510
P	-1.18740	-2.95240	2.32610
C	-0.99180	-3.95800	0.81020
H	-1.32180	-3.37130	-0.06100
H	-1.61100	-4.86500	0.89810
H	0.05860	-4.25070	0.67650
C	-0.47020	-3.89900	3.71590
H	0.58960	-4.11760	3.52970
H	-1.02260	-4.84510	3.83060
H	-0.56190	-3.30750	4.63960
C	-2.98750	-2.90630	2.65870
H	-3.51400	-2.38810	1.84370
H	-3.18070	-2.36860	3.59890
H	-3.36400	-3.93810	2.74050
N	-5.88130	2.43770	-1.41060
O	-6.62710	3.38510	-1.12120
O	-5.77930	1.92040	-2.53520
H	-3.29160	1.33040	8.01060

γ-phosphonioalkynyl complex [(triphos) $(CO)_2$Re{C≡CCPh(*p*-$C_6H_4NO_2$)(PMe_3)}]$^+$

Re	1.654312	-0.413341	1.023710
C	1.080125	-2.073416	0.218726
O	0.702398	-3.073839	-0.268240
C	2.212467	-1.322716	2.634376
O	2.530528	-1.862695	3.629115
C	-0.243329	-0.194556	1.826889
C	-1.397318	-0.161110	2.296283
P	1.078759	0.815110	-1.021206
H	1.455764	0.092824	-2.195186
P	3.841623	-0.496482	0.026186
H	4.227500	-1.571647	-0.829940
H	4.980116	-0.548275	0.887936
P	2.437488	1.718666	1.947959
H	3.285222	1.607264	3.089680
C	3.624209	2.640603	0.799339
H	3.429731	3.717293	0.938914

H	4.649144	2.454775	1.166567
C	4.294958	0.971304	-1.061829
H	4.087927	0.690290	-2.108862
H	5.383455	1.131757	-0.990275
C	2.096395	2.360145	-1.277391
H	1.563419	3.195653	-0.789469
H	2.126355	2.580866	-2.357716
C	3.543084	2.281918	-0.706614
H	4.099392	3.085359	-1.224509
C	-3.714815	-1.175713	2.227240
C	-3.337976	1.216711	2.985236
C	-4.416943	3.798741	2.868633
C	-3.635146	1.925282	4.162529
C	-3.610534	1.829723	1.741375
C	-4.150353	3.113511	1.675574
C	-4.173237	3.219014	4.113428
H	-3.449769	1.491673	5.148543
H	-3.384454	1.289997	0.816809
H	-4.360837	3.598357	0.719430
H	-4.401693	3.784586	5.019477
C	-0.651581	1.247168	-1.482337
C	-3.333584	1.732463	-2.210873
C	-1.054261	2.529792	-1.900875
C	-1.606366	0.209797	-1.425937
C	-2.935447	0.449699	-1.798816
C	-2.391009	2.769430	-2.257887
H	-0.333874	3.350309	-1.964661
H	-1.308060	-0.787354	-1.087345
H	-3.662367	-0.367553	-1.758513
H	-2.690230	3.769641	-2.585664
H	-4.371299	1.919297	-2.503374
C	1.321592	3.044892	2.557282
C	-0.287978	5.205755	3.364245
C	1.752084	3.908283	3.586193
C	0.067697	3.257824	1.952425
C	-0.724916	4.344543	2.348112
C	0.946886	4.980828	3.990369
H	2.720148	3.745129	4.072828
H	-0.300064	2.560959	1.192775
H	-1.691932	4.511694	1.865426
H	1.286846	5.643726	4.791800
H	-0.912348	6.049886	3.673035
C	-2.723232	-0.198634	2.909322
P	-2.328240	-1.000984	4.599457
C	-1.060013	-0.041351	5.495014
H	-0.287719	0.234517	4.760175
H	-0.617132	-0.668061	6.284347
H	-1.483446	0.869094	5.941718
C	-1.609392	-2.636542	4.248814
H	-0.718892	-2.503512	3.617793
H	-2.344300	-3.263240	3.722493

H	-1.328622	-3.112851	5.201348
C	-3.762329	-1.309119	5.700991
H	-3.425137	-1.875246	6.584017
H	-4.506967	-1.905097	5.151258
H	-4.228988	-0.370028	6.030064
N	-4.939228	5.181794	2.807189
O	-5.196265	5.741063	3.883159
O	-5.068345	5.685736	1.681143
C	-5.522357	-2.962962	1.009263
H	-6.224320	-3.653998	0.532947
C	-3.254221	-2.139005	1.312552
H	-2.186885	-2.173611	1.072768
C	-5.091778	-1.112905	2.523790
H	-5.471995	-0.344904	3.205577
C	-5.988887	-2.001972	1.918010
H	-7.056727	-1.935642	2.147932
C	-4.154886	-3.027717	0.707824
H	-3.783976	-3.770578	-0.005223

β-phosphonium cyclopropenyl [(triphos) $(CO)_2Re\{CC(PMe_3)CPh(p\text{-}C_6H_4NO_2)\}]^+$

C	0.874712	0.510483	1.686189
C	0.753003	-0.571997	2.573096
C	0.767378	-1.882729	2.077459
C	0.900730	-2.117608	0.699402
C	0.993899	-1.036931	-0.193707
C	0.989836	0.281735	0.309550
P	1.050722	-1.327112	-2.009796
C	-0.531553	-0.478027	-2.590876
C	-1.714929	-1.411950	-2.965075
C	-1.967551	-2.555171	-1.940083
P	-0.882575	-4.066458	-2.154409
C	-1.356677	-5.185459	-0.761341
C	-1.471238	-4.746448	0.572443
C	-1.803052	-5.655057	1.590259
C	-2.016255	-7.009934	1.292861
C	-1.909818	-7.452725	-0.035014
C	-1.584974	-6.547512	-1.055645
Re	1.342214	-3.545542	-3.049813
C	2.560575	-4.328094	-1.541841
C	3.003294	-5.179115	-0.593325
P	2.913689	-6.773351	0.113037
C	4.610771	-7.412180	0.309991
C	1.374398	-5.281735	-3.890550
O	1.362014	-6.352393	-4.377065
C	2.932514	-2.902196	-3.948262
O	3.851101	-2.445080	-4.515137
P	0.038557	-2.631409	-4.863404
C	-1.636252	-1.905265	-4.432088
C	1.978902	-7.940202	-0.935629
C	2.120191	-6.799536	1.763253

C	4.065803	-4.214593	-1.063441
C	5.164702	-4.745936	-1.953550
C	4.887441	-5.683349	-2.974546
C	5.914812	-6.233495	-3.752434
C	7.249527	-5.868235	-3.524669
C	7.541764	-4.945157	-2.511795
C	6.514318	-4.390915	-1.737106
H	8.052771	-6.299148	-4.129916
C	4.384594	-2.995474	-0.244756
C	4.818025	-1.817124	-0.900670
C	4.993390	-0.624855	-0.196165
C	4.740355	-0.612850	1.181815
C	4.364259	-1.769812	1.870863
C	4.190043	-2.952924	1.148174
N	4.819654	0.664075	1.915475
O	5.185804	1.666199	1.281321
O	4.492035	0.655300	3.113656
H	-1.630748	-4.755140	-3.156787
H	-0.307361	-3.472898	-5.961474
H	0.612468	-1.570330	-5.627641
H	1.989852	-0.328001	-2.398111
H	-0.836929	0.211431	-1.786441
H	-0.269876	0.150126	-3.461289
H	-2.403446	-2.675798	-4.620214
H	-1.845843	-1.074161	-5.125485
H	-1.809582	-2.173154	-0.916455
H	-3.015998	-2.892666	-1.998242
H	-2.618567	-0.776807	-2.915126
H	5.004015	-1.840920	-1.979025
H	3.864446	-3.860323	1.669032
H	4.195127	-1.712612	2.948081
H	5.304162	0.299482	-0.688770
H	3.852583	-5.977824	-3.172133
H	6.767831	-3.678025	-0.946891
H	8.579048	-4.654262	-2.317659
H	5.669429	-6.948529	-4.544494
H	-1.314700	-3.694244	0.828472
H	-1.526263	-6.901769	-2.091452
H	-2.098717	-8.502010	-0.282556
H	-1.908899	-5.296172	2.618905
H	-2.284397	-7.712498	2.087274
H	1.089780	1.134997	-0.370999
H	0.967551	-3.139175	0.312256
H	0.694624	-2.730200	2.766977
H	0.890228	1.535252	2.068447
H	0.663530	-0.388812	3.647560
H	0.936771	-7.594915	-1.020212
H	1.993925	-8.946557	-0.487373
H	2.431844	-7.971831	-1.937728
H	1.077583	-6.455785	1.672212
H	2.666114	-6.126698	2.442136

H	2.133665	-7.820950	2.176528
H	4.587210	-8.412725	0.768795
H	5.188337	-6.726789	0.948584
H	5.094181	-7.459616	-0.677821

[(triphos)(CO)$_2$Re(=C=C=C(*p*-C$_6$H$_4$NO$_2$)$_2$)]$^+$ allenylidene

Re	2.3216533966	-0.6332640356	0.6884345321
C	2.3473578341	-2.4859940999	0.0701967272
O	2.3737496967	-3.5852946928	-0.3216912428
C	2.5510903089	-1.1198855821	2.5605091309
O	2.7013241367	-1.3969068415	3.6856444641
C	0.3556861543	-0.6899487381	0.9238730285
C	-0.8933459944	-0.7350679675	1.1586610207
C	-2.2140729701	-0.7300836963	1.5199164047
P	2.2965578018	0.0300398913	-1.6786749034
H	2.8540891366	-1.0007150256	-2.4886268757
P	4.7345648842	-0.3974054292	0.3633468410
H	5.3664626192	-1.2682723759	-0.5734853021
H	5.6303437160	-0.6120913728	1.4499055260
P	2.4290595293	1.7181110799	1.3682685588
H	3.3107970986	1.9176366150	2.4701730016
C	3.2176873123	2.8356795075	0.0891316212
H	2.3905053617	3.3197720906	-0.4593374946
H	3.7430007981	3.6404031505	0.6305080922
C	5.2865726290	1.2909718986	-0.2520842033
H	6.1187265545	1.1334913720	-0.9576358282
H	5.7067325061	1.8322453455	0.6125585365
C	3.4503550854	1.4583864248	-2.0948306794
H	2.8472349930	2.2060537587	-2.6373434610
H	4.1897050963	1.0776563466	-2.8201811118
C	4.1817852096	2.1532006932	-0.9184737448
H	4.7314883933	2.9883561309	-1.3924531486
C	-2.5814915570	-0.1713503604	2.8400272534
C	-3.1754114774	1.0253815329	5.2889847964
C	-1.6673882398	-0.2516481399	3.9205898266
C	-3.8046755171	0.5216431738	3.0264140544
C	-4.1024080467	1.1274999899	4.2482939014
C	-1.9644601796	0.3362802780	5.1484307658
H	-0.7280155652	-0.7931982731	3.7830218032
H	-4.5056618008	0.6224912433	2.1941998423
H	-5.0281222819	1.6843220995	4.4097117421
H	-1.2840785638	0.2774204119	6.0006855477
C	-3.2457393658	-1.2312875724	0.5922173609
C	-5.1747293581	-2.1531461321	-1.2005515013
C	-3.0038163119	-1.2021713898	-0.8043412105
C	-4.4722059802	-1.7658174129	1.0639207864
C	-5.4384515903	-2.2304648948	0.1700293517
C	-3.9673713099	-1.6531180021	-1.7029841251
H	-2.0558975083	-0.7984047789	-1.1722525466
H	-4.6553361797	-1.8442597159	2.1382932190

H	-6.3882199177	-2.6501103345	0.5088831720
H	-3.8127056401	-1.6202582236	-2.7833599377
C	0.7638478815	0.3240347529	-2.6442536674
C	-1.6203701971	0.6860917271	-4.1026007213
C	0.0950309800	1.5641549845	-2.6181386403
C	0.2257854023	-0.7358034780	-3.4025822610
C	-0.9598475311	-0.5519029431	-4.1289419334
C	-1.0893792163	1.7428533534	-3.3467268607
H	0.4989227400	2.4046713687	-2.0423744153
H	0.7347882634	-1.7050246600	-3.4376812434
H	-1.3582665081	-1.3765640211	-4.7279113313
H	-1.5936065771	2.7135712245	-3.3302581658
H	-2.5388086993	0.8310457471	-4.6786683843
C	0.9711641283	2.6246252372	2.0003667734
C	-1.2813218396	3.9743181873	3.0079617837
C	1.0158400775	3.2282843418	3.2730326787
C	-0.2131137795	2.6912306663	1.2386155143
C	-1.3290903794	3.3736222578	1.7401787012
C	-0.1098187245	3.8968758759	3.7739869047
H	1.9265611155	3.1740532856	3.8788652286
H	-0.2735634789	2.1963097652	0.2635357837
H	-2.2440825056	3.4276852897	1.1425325536
H	-0.0671400328	4.3587243711	4.7647209027
H	-2.1573236226	4.4996704181	3.3992446897
N	-6.2112819422	-2.6143174730	-2.1586734198
O	-5.9307854478	-2.5496135139	-3.3636472861
O	-7.2774918221	-3.0233954727	-1.6825744763
N	-3.4745980967	1.6932806644	6.5804649543
O	-2.6145413130	1.6140708290	7.4679947268
O	-4.5562050416	2.2894587474	6.6700380089

α-phosphonioallenyl complex [(triphos)(CO)$_2$Re{C(PMe$_3$)=C=C(*p*-C$_6$H$_4$NO$_2$)$_2$}]$^+$

Re	1.5832837026	-1.0201846600	2.0520150799
C	2.1449968366	-2.8619200486	2.0087367072
O	2.5467344392	-3.9684501481	1.9961390646
C	1.5367960897	-1.0163230093	3.9806044367
O	1.5817388749	-0.9588988666	5.1513499069
C	-1.3570653524	-1.2589578977	3.1442999779
C	-2.0856949453	-0.8850177783	4.2071943596
P	2.1323866534	-0.7062250680	-0.3316989194
H	3.3567616111	-1.3956643794	-0.5881848219
P	3.8671769456	-0.3525684772	2.2359727721
H	4.8772098013	-1.3545787346	2.1251880537
H	4.2720926719	0.1789918736	3.4967584237
P	1.0469774126	1.3873488163	2.0682835978
H	0.8854015623	1.9709648023	3.3585921715
C	2.4731424616	2.4522723591	1.4457262119
H	2.0268270045	3.3693516318	1.0259486960
H	3.0603587729	2.7630231545	2.3282601124
C	4.5320611552	0.9475002839	1.0558253619

H	5.1267956637	0.4371321442	0.2793207739
H	5.2282527719	1.5964879626	1.6123699280
C	2.6694694623	1.0450184503	-0.7350814378
H	1.7669937757	1.6139638762	-1.0181706559
H	3.3053409764	0.9856857497	-1.6343657562
C	3.4157333611	1.7953384874	0.4019118364
H	3.9341926447	2.6358899366	-0.0956672078
C	-2.2649642803	-1.7730317516	5.3911626237
C	-2.7441694437	-3.5165601637	7.5330469552
C	-1.3853539282	-2.8493604991	5.6596551323
C	-3.3885560088	-1.5972288540	6.2345668955
C	-3.6319059767	-2.4628521220	7.3027870419
C	-1.6189811394	-3.7201449849	6.7246125449
H	-0.5021428927	-2.9944544607	5.0311427530
H	-4.0920910483	-0.7835795186	6.0400294408
H	-4.4994521180	-2.3449570841	7.9559313971
H	-0.9479474786	-4.5519278567	6.9507245057
C	-2.7268144074	0.4666356538	4.1880558670
C	-3.7097139523	3.0855435371	4.1169647955
C	-2.5611521525	1.3305302348	5.2971554214
C	-3.4367518403	0.9389835176	3.0640382504
C	-3.9291119924	2.2448410110	3.0206524783
C	-3.0488002776	2.6383835790	5.2670693464
H	-2.0210895305	0.9760313291	6.1795818651
H	-3.5952926671	0.2737971751	2.2098033560
H	-4.4647696857	2.6319817803	2.1522256785
H	-2.9094615256	3.3248885594	6.1053424859
C	1.2960147369	-1.2461028557	-1.8904166477
C	0.0591324401	-2.1866282082	-4.2443377961
C	0.4106021176	-0.4177052474	-2.6101446480
C	1.5567571960	-2.5495466821	-2.3656131110
C	0.9389207969	-3.0165997112	-3.5336120553
C	-0.1999653338	-0.8880969779	-3.7831984192
H	0.1977035743	0.6010884115	-2.2714101324
H	2.2652128830	-3.1961018056	-1.8342917911
H	1.1590812170	-4.0247922459	-3.8974222684
H	-0.8723847667	-0.2309003751	-4.3430981733
H	-0.4139933956	-2.5472445254	-5.1622442847
C	-0.4066823689	2.1292050964	1.2169716066
C	-2.5474397611	3.3094152128	-0.1869181685
C	-1.0797934012	1.4128600764	0.2122850418
C	-0.8232135487	3.4414044400	1.5226316750
C	-1.8900418812	4.0255576696	0.8265914149
C	-2.1400817322	2.0024732286	-0.4936702811
H	-0.7713883056	0.3848182662	0.0013186626
H	-0.3244203248	4.0090826627	2.3157743493
H	-2.2251920497	5.0327261733	1.0903828070
H	-2.6519044311	1.4388279200	-1.2810845895
H	-3.3793491691	3.7697905918	-0.7277471952
C	-0.5832737505	-1.6106330900	2.1283654089
P	-1.4952718848	-2.7672526109	1.0715965017

C	-2.1706691834	-2.0251071490	-0.4576153461
H	-2.8119592564	-1.1707725293	-0.1932057336
H	-2.7695768484	-2.7781109023	-0.9942636945
H	-1.3543081045	-1.6830132987	-1.1116912694
C	-0.4603552809	-4.1714531211	0.5449314970
H	0.3413564718	-3.8160317588	-0.1182398591
H	-1.0888220768	-4.8939224213	0.0003841717
H	-0.0121491634	-4.6617357631	1.4209794669
C	-2.9253554875	-3.4950534437	1.9514809637
H	-3.6165162496	-2.6990016641	2.2648467453
H	-2.5767312133	-4.0247104871	2.8512540449
H	-3.4515662637	-4.2004012384	1.2893226143
N	-3.0078407585	-4.4447486197	8.6534962144
N	-4.1346250365	4.4956552548	4.0365100555
O	-4.0276248347	5.1846892873	5.0604864362
O	-4.5457978119	4.9030443102	2.9362153893
O	-4.0082450349	-4.2233553089	9.3517583164
O	-2.2118017906	-5.3824655449	8.8113899089

γ-phosphonioalkynyl complex [(triphos)(CO)$_2$Re{C≡CC(*p*-C$_6$H$_4$NO$_2$)$_2$(PMe$_3$)}]$^+$

Re	1.6217054684	-0.2472318584	1.2659037548
C	1.1850532379	-2.1032278871	0.9543069929
O	0.9271369390	-3.2357239488	0.7802423628
C	2.0385542999	-0.6222693921	3.1115363588
O	2.2979930551	-0.8472168054	4.2366031794
C	-0.3697308124	0.0381019677	1.7938466625
C	-1.5627629270	0.0361300440	2.1555657450
P	1.3029093072	0.2142998267	-1.1196437962
H	1.6828061818	-0.9215951671	-1.8949638557
P	3.9126388688	-0.5648705850	0.6012463467
H	4.3144887251	-1.8175261750	0.0475423778
H	4.9149527129	-0.4965232882	1.6159536145
P	2.3976683262	2.0451994529	1.6231976959
H	3.3820296668	2.0867656256	2.6556099027
C	3.4183785329	2.7654760732	0.2045909415
H	2.8650494541	3.6507841917	-0.1525299036
H	4.3626391880	3.1406323372	0.6349404824
C	4.6191684467	0.6262739797	-0.6778515962
H	4.8099003403	0.0541307546	-1.6015954214
H	5.6016809472	0.9710273409	-0.3150332278
C	2.4622195441	1.5047886522	-1.8339364867
H	1.8632312491	2.4209697495	-1.9770468315
H	2.7529544098	1.1619323476	-2.8413885073
C	3.7238610436	1.8475181028	-1.0038208141
H	4.3391711121	2.4745904047	-1.6779536603
C	-3.8111774573	-0.9343683268	1.6480985187
C	-5.3608799635	-2.3303448779	-0.2140486647
C	-3.4125003965	-1.0134988683	0.3010149185
C	-5.0083124456	-1.5751131380	2.0390374136

C	-5.7856937785	-2.2811551565	1.1156241329
C	-4.1882831942	-1.7014968250	-0.6366745491
H	-2.4821483298	-0.5281976977	-0.0045845271
H	-5.3642042705	-1.5170485209	3.0707285049
H	-6.7122508349	-2.7840345714	1.4012044947
H	-3.8952072303	-1.7595431161	-1.6869555694
C	-3.5956056524	1.1942184525	3.1035375857
C	-4.7030062548	3.6044259261	3.9913110587
C	-2.7728277554	2.2172684442	3.6201992679
C	-4.9860811578	1.4173634880	3.0263163773
C	-5.5442017749	2.6234088630	3.4637908432
C	-3.3199902540	3.4205331273	4.0757891048
H	-1.6878949024	2.0795979704	3.6159421534
H	-5.6463664500	0.6670317097	2.5874481976
H	-6.6163482447	2.8203567563	3.3942094694
H	-2.6940060835	4.2233606566	4.4712941509
C	-0.2889141641	0.5618018672	-1.9664538833
C	-2.7349282047	1.0681389831	-3.2633247726
C	-0.9619097916	1.7832860415	-1.7628741457
C	-0.8552131779	-0.4065195542	-2.8193755073
C	-2.0743602210	-0.1523821982	-3.4644183970
C	-2.1767495562	2.0348039744	-2.4131465356
H	-0.5368208645	2.5463513612	-1.1017367828
H	-0.3411347532	-1.3588806275	-2.9881624248
H	-2.5004254875	-0.9053714321	-4.1347420890
H	-2.6878201914	2.9896827079	-2.2579162967
H	-3.6818640767	1.2681776544	-3.7732049643
C	1.3843126818	3.4733473349	2.1684820394
C	-0.1186824761	5.7407918876	2.8742337391
C	1.9389415394	4.4583470814	3.0105778316
C	0.0633159511	3.6171935088	1.7019971679
C	-0.6786925404	4.7568149780	2.0457751785
C	1.1864435564	5.5852031058	3.3647543033
H	2.9592031484	4.3448185735	3.3932273873
H	-0.3902653764	2.8194610058	1.1046079142
H	-1.7033802877	4.8687073675	1.6787328734
H	1.6208988419	6.3430423406	4.0234638198
H	-0.7032791992	6.6244358648	3.1474259689
C	-2.9346070096	-0.1293319713	2.6353318466
P	-2.6434686002	-1.2130475567	4.2038480721
C	-1.3844169893	-0.4286979751	5.2608403472
H	-0.4722275323	-0.2445203732	4.6772657920
H	-1.1612514608	-1.1103848670	6.0970592046
H	-1.7725951529	0.5198318681	5.6612926917
C	-2.0246156931	-2.8404789206	3.6718455336
H	-1.1606956878	-2.6858176743	3.0075434335
H	-2.8142350855	-3.3788827272	3.1271264725
H	-1.7179462921	-3.4249047512	4.5532556268
C	-4.0964723881	-1.4560571122	5.3031965423
H	-3.7400495753	-1.7453847698	6.3047951968
H	-4.7596045220	-2.2454463120	4.9226424234

H	-4.6560283194	-0.5109337002	5.3861854084
N	-5.2914788391	4.8881315576	4.4438993080
N	-6.1820027188	-3.0693310847	-1.2026833770
O	-4.5100906230	5.7364874909	4.8968215069
O	-6.5177731459	5.0191187420	4.3334707669
O	-7.1973865065	-3.6385297498	-0.7805045994
O	-5.7921521143	-3.0610983693	-2.3780232656

β-phosphonium cyclopropenyl [(triphos)(CO)$_2$Re{CC(PMe$_3$)C(*p*-C$_6$H$_4$NO$_2$)$_2$}]$^+$

Re	0.7326656475	0.6412239671	1.5584266959
C	0.7346168886	-0.8336554536	2.7992150329
O	0.7377969811	-1.7543400919	3.5312638823
C	0.3759849722	1.9873029311	2.9043626016
O	0.2213221962	2.8505646620	3.6816174611
P	1.5503874496	-0.8561761113	-0.2077504850
H	2.4811229847	-1.7782111730	0.3594094360
P	3.0957417187	0.9794894795	1.9362515693
H	3.7640539553	0.1422444689	2.8766286791
H	3.5099947398	2.2311796437	2.4841936014
P	0.9892751283	2.4536024632	-0.1036857257
H	0.9324990478	3.7699324698	0.4409605293
C	2.7406457663	2.5178655922	-0.8101855713
H	2.6574423190	2.9523486311	-1.8200786072
H	3.3160514063	3.2406260847	-0.2044196414
C	4.2311351587	0.8346783608	0.4516841687
H	4.6322382144	-0.1929599059	0.4244765770
H	5.0916810638	1.5069038722	0.6030474900
C	2.6697854330	-0.0047272050	-1.4459636799
H	2.0337075919	0.3591525081	-2.2717365540
H	3.3329132066	-0.7770119802	-1.8703912193
C	3.5120065486	1.1725758945	-0.8791446999
H	4.3179473490	1.3332584772	-1.6188256373
C	-3.2006549406	2.0635078702	0.8177889863
C	-3.9009263221	3.9970381296	-1.0757336926
C	-2.7398723230	3.3943737655	0.9426232033
C	-4.0670939001	1.7490121205	-0.2452300283
C	-4.4248348893	2.7068709655	-1.1968871087
C	-3.0806218632	4.3645331149	-0.0026402813
H	-2.0899479567	3.6600993745	1.7826130809
H	-4.4465250948	0.7257789828	-0.3414488054
H	-5.0789232040	2.4783998428	-2.0411347606
H	-2.7096592413	5.3902894430	0.0574605562
C	-3.0335977405	1.2051060990	3.2316153217
C	-3.7682923491	1.4518077908	5.9364728967
C	-2.4415274795	0.3914711883	4.2290042715
C	-4.0039788204	2.1492167231	3.6431187426
C	-4.3734965738	2.2772385500	4.9850341793
C	-2.7999866325	0.5091989817	5.5737553498
H	-1.6797911139	-0.3406514525	3.9487625143
H	-4.4888342842	2.7882523944	2.9004387170
H	-5.1280026947	2.9979729615	5.3089399749

H	-2.3460130365	-0.1099555189	6.3511385923
C	0.6327073140	-2.0991998614	-1.2174942020
C	-0.7695814478	-4.0659725707	-2.6811589371
C	-0.0791092856	-1.7484140837	-2.3813395041
C	0.6385138287	-3.4467315835	-0.7970990568
C	-0.0615057745	-4.4221114808	-1.5225126227
C	-0.7698292156	-2.7290115795	-3.1099625508
H	-0.0906973568	-0.7133990250	-2.7360294142
H	1.2106563583	-3.7423699790	0.0900073145
H	-0.0351605204	-5.4651040583	-1.1917248189
H	-1.3004707770	-2.4464029822	-4.0246066511
H	-1.3014770020	-4.8289868587	-3.2570679833
C	-0.0460765620	2.6761691169	-1.6083604729
C	-1.5427187044	2.9853015788	-3.9729218263
C	0.1239110515	3.8222075694	-2.4144315740
C	-0.9840210640	1.6994625631	-1.9830169620
C	-1.7205280573	1.8511484419	-3.1687242442
C	-0.6252294491	3.9762959580	-3.5871495744
H	0.8301747642	4.6073861601	-2.1210416050
H	-1.1580448696	0.8427868062	-1.3241821616
H	-2.4532507512	1.0893952842	-3.4526004171
H	-0.4992440541	4.8765100900	-4.1958058759
H	-2.1312929904	3.1114021381	-4.8858230658
C	-2.6998189159	1.0132372159	1.7723037246
P	-3.2295009230	-1.9573485883	1.2586255604
C	-2.1250533329	-3.2664906645	1.8901686836
H	-1.2684980718	-3.3737328625	1.2066241589
H	-2.6705100246	-4.2224112666	1.9413465386
H	-1.7569009529	-2.9933817163	2.8900010175
C	-3.7665282938	-2.4893195736	-0.4077837759
H	-2.8868698169	-2.5638932553	-1.0667157965
H	-4.4669291820	-1.7489391200	-0.8229782353
H	-4.2660145366	-3.4697615156	-0.3505455404
C	-4.7116923079	-1.8867148836	2.3197155977
H	-5.2280215309	-2.8590885001	2.3128448111
H	-5.3931600066	-1.1067982272	1.9471388890
H	-4.4122145124	-1.6288452483	3.3469023602
N	-4.1674145841	1.5660290247	7.3553634311
N	-4.1694151064	4.9780011192	-2.1454343359
O	-3.6340776345	0.7850505025	8.1586386872
O	-5.0096066628	2.4295333980	7.6422636989
O	-4.8137227968	4.5839843517	-3.1309844780
O	-3.7103767296	6.1203976522	-2.0000896567
C	-1.3244031039	0.3266500666	1.3732744349
C	-2.4610712589	-0.3885057889	1.2653371053

[(triphos)(CO)$_2$Re{C=C=CH(*p*-C$_6$H$_4$NO$_2$)}]*

Re	2.0146824891	-0.1211762620	2.3698721901
C	1.8720757695	-1.8709174011	3.2038785210
O	1.7799128876	-2.9219742388	3.7064808791

C	2.2608174664	0.6794867792	4.1415148793
O	2.4118196928	1.1494946290	5.1980296554
C	-1.2104961620	0.2009102403	2.5693770711
C	-2.5561141916	0.3521888176	2.6053666390
P	1.9680247533	-1.1379993273	0.1349350613
H	2.6767493998	-2.3736077533	0.0952703246
P	4.4372164442	-0.2659413731	2.0397032620
H	5.1654267471	-1.4292862086	2.4237295702
H	5.2154938493	0.6885405649	2.7560202520
P	2.2464535886	2.0526988043	1.2323744698
H	2.7007832501	3.0977890031	2.0877434906
C	3.5924656667	2.0949606033	-0.0733405821
H	3.2508299102	2.7520722177	-0.8903032368
H	4.4547252977	2.6109094125	0.3838074626
C	5.0429459327	-0.0264073985	0.2785359238
H	5.2548264506	-1.0266017904	-0.1367023664
H	6.0072247279	0.5058213622	0.3205229588
C	2.8920449710	-0.1589343917	-1.1664478170
H	2.1378535299	0.4623689003	-1.6790749230
H	3.2642421005	-0.8778206449	-1.9155278995
C	4.0548790916	0.7293923211	-0.6488489323
H	4.6467244580	0.9834976596	-1.5477894407
C	-3.4928654461	-0.4219686505	3.3980023604
C	-5.3645707507	-1.8817275372	4.8538328628
C	-3.0690611182	-1.4548017783	4.2766606523
C	-4.8799646852	-0.1417918236	3.2786656866
C	-5.8218613795	-0.8700267463	4.0025259946
C	-4.0033021708	-2.1845701438	5.0061038176
H	-2.0006123394	-1.6690295940	4.3698923202
H	-5.2114979518	0.6547089041	2.6049504483
H	-6.8945225408	-0.6799540660	3.9267461153
H	-3.7140578687	-2.9850679293	5.6901224586
C	0.4065527791	-1.6604341676	-0.6507242566
C	-2.0070885562	-2.4698639720	-1.8329978089
C	-0.6269064223	-0.7229976776	-0.8550577745
C	0.2219812041	-3.0046239763	-1.0308265075
C	-0.9863238240	-3.4055615356	-1.6167968313
C	-1.8247836229	-1.1306861441	-1.4548240221
H	-0.5033042191	0.3178696163	-0.5385148456
H	1.0152589614	-3.7411419194	-0.8662254133
H	-1.1273297962	-4.4514156337	-1.9043053381
H	-2.6226874010	-0.4006545388	-1.6210263497
H	-2.9481027199	-2.7852076376	-2.2932620446
C	0.7628528845	2.8706453706	0.5185298877
C	-1.6011713920	4.0755852736	-0.4278692176
C	0.5129941027	2.9586259482	-0.8640745293
C	-0.1872864016	3.3855364788	1.4257752756
C	-1.3582665200	3.9901933821	0.9518045133
C	-0.6654080019	3.5592761691	-1.3336115784
H	1.2346575864	2.5761032120	-1.5928307174
H	-0.0097346612	3.3232855442	2.5045146144

H	-2.0784102084	4.4053641758	1.6635294371
H	-0.8433573395	3.6306253049	-2.4106138113
H	-2.5142232425	4.5525489884	-0.7959332037
C	0.0565162470	0.0950405720	2.4752325226
N	-6.3623262791	-2.6702596616	5.6246448638
O	-7.5547905554	-2.3821830835	5.4583623755
O	-5.9244262506	-3.5552285668	6.3712666541
H	-3.0060361193	1.1325761974	1.9690286603

α-phosphonioallenyl complex [(triphos)$(CO)_2$Re{C(PMe_3)=C=CH(*p*-$C_6H_4NO_2$)}]$^+$

Re	1.8866965690	-0.9223920572	2.1783503421
C	2.7146333532	-2.6239236114	2.4769282431
O	3.3103561150	-3.6276284439	2.6626487494
C	1.5446925211	-0.7068714436	4.0691831340
O	1.3174898028	-0.5889059692	5.2150254090
C	-1.3056803297	-1.0277474286	2.0592759817
C	-2.4591255279	-0.3646147434	2.1042823098
P	2.3384462395	-1.1123811066	-0.2141848394
H	3.4442170375	-1.9733009167	-0.4833380397
P	4.0538166802	0.0638022019	2.3462440102
H	5.1681947206	-0.7458672144	2.7144540860
H	4.2305428840	1.0803482850	3.3354417152
P	1.3197943288	1.4680129980	1.7924603907
H	1.5097025122	2.1864103334	3.0084931783
C	2.5639235644	2.3690512576	0.6856577058
H	1.9654173971	2.9459990949	-0.0387973433
H	3.0816150223	3.1124464072	1.3159434764
C	4.7202737588	0.9356021807	0.8290072719
H	5.3309942094	0.2110642653	0.2631275130
H	5.4026584024	1.7366396603	1.1586814278
C	2.9585127358	0.4683317785	-1.0202847874
H	2.0927775283	0.9194788933	-1.5364751764
H	3.6717060639	0.1769000445	-1.8097573308
C	3.6051838551	1.5155328086	-0.0781976165
H	4.1153198374	2.2299073777	-0.7519633503
C	-3.1742647515	0.0216226525	3.3294719109
C	-4.6242948896	0.7597150950	5.6069755737
C	-2.6335643037	-0.1770815551	4.6244792119
C	-4.4579129261	0.6069705658	3.2146203946
C	-5.1875705227	0.9751325476	4.3451832044
C	-3.3533008923	0.1896182630	5.7612826944
H	-1.6326953621	-0.6063991876	4.7336793544
H	-4.8851679942	0.7707607328	2.2198899822
H	-6.1809545392	1.4237669866	4.2762231138
H	-2.9559239349	0.0507510564	6.7692026682
C	1.1722721144	-1.7894222536	-1.4579723390
C	-0.6201457575	-2.8132771247	-3.3703022802
C	-0.1619438575	-1.3322372403	-1.4964151864
C	1.5968436753	-2.7695241680	-2.3781283250
C	0.7014321034	-3.2801977597	-3.3284112444

C	-1.0492544081	-1.8388405167	-2.4558378345
H	-0.5080304074	-0.5908644719	-0.7693630378
H	2.6289488635	-3.1359180678	-2.3538952655
H	1.0399040937	-4.0404684750	-4.0385318141
H	-2.0809121611	-1.4747987864	-2.4875092370
H	-1.3161960138	-3.2093472563	-4.1154968028
C	-0.2799059791	2.2386107699	1.3081718827
C	-2.7242169408	3.4406798772	0.6004359834
C	-0.7097213448	2.2398904332	-0.0339866458
C	-1.0860681264	2.8419948398	2.2921662403
C	-2.3037384428	3.4381553546	1.9376951827
C	-1.9254563995	2.8415945031	-0.3854313711
H	-0.0937957335	1.7849112688	-0.8180409656
H	-0.7661174085	2.8496344175	3.3394312457
H	-2.9205095910	3.9070456543	2.7099699465
H	-2.2440007322	2.8513996894	-1.4323074123
H	-3.6690576913	3.9177479056	0.3237452827
C	-0.1765934689	-1.7105967276	2.0394760724
P	-0.5376803980	-3.4760335601	2.2000933839
C	-2.3164787588	-3.8504925717	1.9910170989
H	-2.9092929420	-3.2889278146	2.7277968291
H	-2.4816818328	-4.9300699604	2.1321878714
H	-2.6415702849	-3.5598453505	0.9809104932
C	0.3427720079	-4.5184655926	0.9863310324
H	0.1387926165	-4.1501068946	-0.0303573527
H	-0.0143733119	-5.5561729339	1.0814004072
H	1.4244434446	-4.4937565324	1.1765234421
C	-0.0896576608	-4.0736898382	3.8688427773
H	-0.6317107306	-3.4801751529	4.6208357008
H	0.9913306496	-3.9673871934	4.0339521498
H	-0.3702820063	-5.1341172798	3.9688169855
N	-5.3882345690	1.1500643082	6.8088840805
O	-6.5030756504	1.6638646418	6.6316516021
O	-4.8616130264	0.9375749835	7.9116602327
H	-2.9356377352	-0.0804637281	1.1551487313

γ-phosphonioalkynyl complex [(triphos)(CO)$_2$Re{C≡CCH(*p*-C$_6$H$_4$NO$_2$)(PMe$_3$)}]$^+$

Re	1.8854832540	-0.3029905028	1.3263395018
C	1.7516230978	-2.2110055152	1.0644413733
O	1.6461270550	-3.3728191200	0.9171211689
C	2.3079060363	-0.5586256838	3.1932184302
O	2.5183235714	-0.7226411508	4.3383102055
C	-0.1081807932	-0.2785540745	1.8765702524
C	-1.2781019323	-0.3101285642	2.2967540585
P	1.4527920732	0.0387861170	-1.0571169777
H	2.1024071060	-0.9705710323	-1.8291614408
P	4.1925750924	-0.1764865328	0.6637350495
H	4.9162357377	-1.3395347333	0.2623715585
H	5.1361847689	0.2826077066	1.6337882970
P	2.1824399985	2.1176655315	1.5942623286

H	3.0355639361	2.4352864050	2.6924933695
C	3.1826436675	2.9362696628	0.2094633389
H	2.6058039029	3.8204959997	-0.1104973262
H	4.1167688334	3.3173724629	0.6570704836
C	4.5845276467	0.9762335553	-0.7723619440
H	4.7008878036	0.3546818728	-1.6768218210
H	5.5666667509	1.4402152139	-0.5830094785
C	2.2596611049	1.5652360506	-1.7788563459
H	1.4947198421	2.3613464523	-1.7924535376
H	2.5025132578	1.3451880189	-2.8320783857
C	3.5205283662	2.0747929648	-1.0319941840
H	4.0034399660	2.7784828026	-1.7367940376
C	-3.7607506304	-0.6198960358	1.8730429910
C	-5.8559004162	-0.9425976234	0.0692593653
C	-3.5170851592	-1.1553465073	0.5951173552
C	-5.0716175679	-0.2431248354	2.2309199170
C	-6.1291835635	-0.4005775419	1.3294876699
C	-4.5671871742	-1.3246150183	-0.3124174197
H	-2.4894039809	-1.3979823136	0.3072130429
H	-5.2656277447	0.2034340945	3.2129146267
H	-7.1518079213	-0.1037526959	1.5728333410
H	-4.4019874415	-1.7269856302	-1.3134181950
C	-0.1788756636	-0.0420027954	-1.8983401922
C	-2.6696665975	-0.2265239545	-3.1992777422
C	-1.0998521564	1.0218204583	-1.8237385021
C	-0.5225591884	-1.2041325497	-2.6180780733
C	-1.7635435384	-1.2951135129	-3.2636589708
C	-2.3356948998	0.9295473517	-2.4771885754
H	-0.8558127427	1.9298765990	-1.2620973072
H	0.1848505838	-2.0377554074	-2.6856307277
H	-2.0146798203	-2.1973135132	-3.8298058643
H	-3.0398322510	1.7654668474	-2.4257879164
H	-3.6348831287	-0.2941463126	-3.7106137417
C	0.8395204505	3.3231117785	1.9369953222
C	-1.1901611816	5.2170629604	2.3820482836
C	1.1273904405	4.5280061315	2.6110615815
C	-0.4752066398	3.0647151089	1.5046577947
C	-1.4835478252	4.0148179187	1.7234185913
C	0.1148684846	5.4702029992	2.8312527061
H	2.1423905356	4.7307534396	2.9701259151
H	-0.7120589586	2.1038202561	1.0392706367
H	-2.5043574802	3.8099801511	1.3850281075
H	0.3446903001	6.4016571028	3.3571985588
H	-1.9791573734	5.9554825995	2.5538102691
C	-2.6076324303	-0.4412139374	2.8622101999
P	-2.4943116412	-1.9492676792	3.9890778055
C	-1.2478070393	-1.6201212288	5.2729512100
H	-0.3033688585	-1.3304447208	4.7877005684
H	-1.0929683015	-2.5221726960	5.8851661197
H	-1.5919772323	-0.7986806687	5.9209026282
C	-1.9805282597	-3.3802280336	2.9942704445

H	-1.0369856220	-3.1313672218	2.4847399098
H	-2.7539582740	-3.6035449304	2.2433020469
H	-1.8375026860	-4.2554543573	3.6463129750
C	-4.0780529189	-2.3459321427	4.8125860051
H	-3.9645770560	-3.2489481652	5.4331159086
H	-4.8563988707	-2.5204625285	4.0544231857
H	-4.3857981282	-1.5074920249	5.4566101268
N	-6.9652309072	-1.0908824691	-0.9044042355
O	-8.1013871548	-0.7832805843	-0.5188390978
O	-6.6723201979	-1.5093898750	-2.0339614566
H	-2.8616522560	0.3900084403	3.5554155978

γ-phosphonium cyclopropenyl [(triphos)(CO)$_2$Re{CC(PMe$_3$)CH (*p*-C$_6$H$_4$NO$_2$)}]$^+$

Re	0.9013412474	0.3322031868	1.6291228934
C	0.9799748139	-1.2480029296	2.7297868483
O	1.0116070422	-2.2194038016	3.3934766096
C	0.5346898342	1.4939117151	3.1435524697
O	0.3884132065	2.2339204749	4.0388357375
P	1.6822267508	-0.9503363176	-0.2949449558
H	2.7053298579	-1.8639526206	0.1014303477
P	3.2584002447	0.7867908664	1.8813624316
H	4.0842234493	-0.0938700044	2.6416149883
H	3.6401266382	1.9949630526	2.5403803348
P	0.9418910073	2.3414267142	0.2190523297
H	0.9979193780	3.5568221363	0.9613320017
C	2.5438697368	2.5353846356	-0.7709129053
H	2.2580265542	2.9365506581	-1.7578160290
H	3.1433783440	3.3192786699	-0.2755964187
C	4.2585136154	0.9100908184	0.2928408519
H	4.7687870845	-0.0561696303	0.1392904286
H	5.0502663326	1.6625058019	0.4418083617
C	2.6313294311	0.0617436171	-1.5491837578
H	1.9081587751	0.4254972676	-2.3002270426
H	3.3187900061	-0.6219129503	-2.0749841588
C	3.4145363589	1.2671476396	-0.9584557414
H	4.1524866628	1.5394516631	-1.7362361505
C	-3.0683303608	1.2673474520	2.6875845311
C	-4.1512373608	2.4234551482	5.0003031986
C	-2.7650347022	0.7468442943	3.9672081289
C	-3.9191512833	2.3927410975	2.6066728541
C	-4.4641020332	2.9747384721	3.7532249447
C	-3.3010885805	1.3180953894	5.1233433920
H	-2.0882432726	-0.1099976286	4.0542900925
H	-4.1613240984	2.8113655322	1.6236572896
H	-5.1294977831	3.8397449202	3.7069490639
H	-3.0773119449	0.9325775932	6.1206731048
C	0.7152096696	-2.1476428486	-1.3075451667
C	-0.7724612105	-4.0482534417	-2.7664080970
C	-0.1171726286	-1.7385599517	-2.3674231250

C	0.7944990327	-3.5193824809	-0.9854603135
C	0.0527106092	-4.4632029382	-1.7097845900
C	-0.8526578793	-2.6863360702	-3.0946586182
H	-0.1864264349	-0.6821807068	-2.6454234771
H	1.4528906850	-3.8553732860	-0.1763255015
H	0.1362424045	-5.5256861656	-1.4609162783
H	-1.4797234064	-2.3595657500	-3.9299357772
H	-1.3379862054	-4.7861266055	-3.3431828278
C	-0.3638933599	2.8071852922	-0.9867727858
C	-2.2916761254	3.5180736203	-2.9075713543
C	-0.5177751648	4.1541268789	-1.3744561896
C	-1.1928467932	1.8232630528	-1.5565247895
C	-2.1492182405	2.1784068765	-2.5190809007
C	-1.4796129682	4.5057461936	-2.3301160400
H	0.1064436777	4.9334655382	-0.9235964077
H	-1.1059096736	0.7853680254	-1.2183823169
H	-2.7930169071	1.4095144169	-2.9575762298
H	-1.5988093575	5.5541433137	-2.6192053240
H	-3.0423622705	3.7961896224	-3.6531068381
C	-2.5402953041	0.6601711433	1.4310254663
P	-3.0146761604	-2.3612065749	1.4459570783
C	-1.8457454247	-3.6925554249	1.8763414704
H	-1.1247052288	-3.8171124016	1.0536693366
H	-2.3949910182	-4.6349318030	2.0284101133
H	-1.2995537212	-3.4261762691	2.7935647703
C	-3.8287706166	-2.8317014914	-0.1246297362
H	-3.0666715832	-2.9380464506	-0.9123594274
H	-4.5400698893	-2.0424996076	-0.4129879292
H	-4.3723844507	-3.7825268701	-0.0047853202
C	-4.3325401166	-2.3091472114	2.7110983045
H	-4.8826669039	-3.2632388353	2.7234694308
H	-5.0270594778	-1.4876749500	2.4779023036
H	-3.8921512031	-2.1208049280	3.7011069943
N	-4.7372107481	3.0197987441	6.2181959191
O	-4.4586942615	2.4869361399	7.3037850000
O	-5.4703866557	4.0099110077	6.0716615531
C	-1.1395664288	-0.0316616322	1.3824429899
C	-2.2341513680	-0.8125844198	1.3329155821
H	-2.8761712214	1.1835147144	0.5220745953

α-phosphonioallenyl complex [(triphos)(CO)$_2$Re{C(PMePh$_2$)=C=CPh(*p*-C$_6$H$_4$NO$_2$)}]$^+$ (6)

Re	1.829364	-1.005892	1.952043
C	2.297330	-2.859757	2.115316
O	2.721195	-3.957091	2.214157
C	1.864499	-0.805875	3.873872
O	1.926549	-0.659514	5.036754
C	-1.335971	-0.479464	2.425926
C	-2.341034	0.287987	2.878946
P	1.913597	-1.172453	-0.498017

H	2.644499	-2.322413	-0.921086
P	4.179541	-0.576400	1.840275
H	5.082235	-1.679388	1.897216
H	4.744090	0.179541	2.914096
P	1.882870	1.468852	1.798369
H	2.679064	1.931333	2.889384
C	2.915118	2.123138	0.356637
H	2.197122	2.616826	-0.321015
H	3.558815	2.924553	0.758168
C	4.844244	0.370469	0.359077
H	5.367729	-0.348994	-0.293536
H	5.605573	1.082393	0.719051
C	2.899428	0.186997	-1.347739
H	2.167005	0.799956	-1.901222
H	3.535120	-0.297051	-2.108599
C	3.760630	1.115435	-0.457806
H	4.323177	1.741245	-1.177755
C	-2.471314	0.439583	4.367039
C	-2.702385	0.643371	7.174331
C	-1.388207	0.893236	5.145696
C	-3.674576	0.087123	5.017254
C	-3.787206	0.190303	6.408714
C	-1.502666	0.992288	6.539234
H	-0.458495	1.182448	4.647936
H	-4.519466	-0.277853	4.424939
H	-4.726479	-0.085972	6.898350
H	-0.653021	1.351115	7.128569
C	-3.322857	0.941365	1.982356
C	-5.153713	2.215401	0.276096
C	-4.211273	1.928797	2.472804
C	-3.386069	0.614253	0.605429
C	-4.290361	1.242857	-0.246472
C	-5.125132	2.563912	1.629604
H	-4.173263	2.212952	3.526806
H	-2.712134	-0.149805	0.208409
H	-4.356600	0.997083	-1.309036
H	-5.810641	3.331362	1.996368
C	0.476895	-1.366935	-1.640408
C	-1.726876	-1.658218	-3.382888
C	-0.456289	-0.322443	-1.796428
C	0.295597	-2.558106	-2.372048
C	-0.803380	-2.703049	-3.233410
C	-1.545051	-0.463973	-2.667569
H	-0.327655	0.617160	-1.248724
H	1.022428	-3.373242	-2.282197
H	-0.926695	-3.630917	-3.800249
H	-2.250674	0.363869	-2.790341
H	-2.575808	-1.767067	-4.064008
C	0.581304	2.760759	1.904459
C	-1.299655	4.848656	1.927954
C	-0.531974	2.722555	1.044299

C	0.735546	3.844689	2.792161
C	-0.205850	4.882365	2.803681
C	-1.463768	3.767021	1.050291
H	-0.689795	1.861091	0.387922
H	1.593774	3.883159	3.472077
H	-0.080417	5.719752	3.496724
H	-2.329142	3.724026	0.382547
H	-2.030840	5.662448	1.935360
C	-0.370151	-1.320032	2.092524
P	-1.050422	-3.012870	2.189814
C	-0.406967	-4.157567	0.913044
H	-0.451238	-3.660681	-0.067809
H	-1.050528	-5.050220	0.888387
H	0.628100	-4.451716	1.128795
N	-6.101662	2.891644	-0.626748
O	-6.848031	3.750655	-0.133156
O	-6.083281	2.559137	-1.823982
H	-2.794671	0.727439	8.261578
C	-5.644465	-3.122374	1.530226
C	-4.772493	-2.963831	0.442106
C	-3.387570	-2.929433	0.645957
C	-2.863498	-3.055406	1.951760
C	-3.740499	-3.216286	3.041922
C	-5.125892	-3.248037	2.826559
H	-6.725635	-3.150362	1.366128
H	-5.172620	-2.864991	-0.571370
H	-2.722813	-2.801502	-0.214559
H	-3.344341	-3.320776	4.056321
H	-5.800832	-3.377725	3.678055
C	-0.266766	-4.785989	6.394090
C	-0.550974	-3.421352	6.239902
C	-0.754218	-2.881626	4.963314
C	-0.680248	-3.715899	3.827643
C	-0.392540	-5.087718	3.984249
C	-0.185413	-5.614965	5.265303
H	-0.106235	-5.203924	7.392241
H	-0.612186	-2.765572	7.113375
H	-0.967547	-1.813809	4.856348
H	-0.327771	-5.750488	3.116695
H	0.040499	-6.679131	5.379704

γ-phosphonioalkynyl complex [(triphos)(CO)$_2$Re{C≡CPh(*p*-C$_6$H$_4$NO$_2$)(PMePh$_2$)}]$^+$ (5)

Re	-4.315530	3.806255	4.592732
C	-3.937995	4.197524	2.743347
O	-3.698601	4.428024	1.615216
C	-2.500164	4.244018	5.096249
O	-1.398790	4.509906	5.402335
C	-3.663563	1.866931	4.220855
C	-3.172774	0.770815	3.889409

P	-6.668246	3.393753	4.042286
H	-7.116048	4.244859	2.986594
P	-5.065410	6.048634	5.016787
H	-5.105009	7.002362	3.955151
H	-4.303804	6.845639	5.926742
P	-4.885821	3.487007	6.960355
H	-3.938695	4.115634	7.820501
C	-6.456167	4.393912	7.503791
H	-7.040231	3.673474	8.101036
H	-6.147315	5.195347	8.197298
C	-6.791653	6.263106	5.729150
H	-7.457645	6.582030	4.908904
H	-6.766993	7.093443	6.454384
C	-7.870175	3.926923	5.389612
H	-8.155722	3.009641	5.934132
H	-8.785549	4.286770	4.889309
C	-7.363767	4.988456	6.397974
H	-8.270408	5.328498	6.934816
C	-3.570792	-1.085886	2.280362
C	-2.329144	-1.510573	4.510466
C	-1.840724	-3.353637	6.606742
C	-1.540360	-2.663295	4.292217
C	-2.857432	-1.296019	5.795951
C	-2.620762	-2.211172	6.830788
C	-1.297763	-3.572682	5.332627
H	-1.095059	-2.858630	3.313772
H	-3.450619	-0.395782	5.978254
H	-3.049404	-2.017092	7.818632
H	-0.682309	-4.457121	5.140337
C	-7.423984	1.824406	3.459535
C	-8.681931	-0.570625	2.687593
C	-8.559309	1.855314	2.623517
C	-6.908189	0.585982	3.888123
C	-7.543637	-0.605226	3.506362
C	-9.183738	0.661496	2.239544
H	-8.954824	2.813023	2.266614
H	-5.990520	0.557912	4.483928
H	-7.133992	-1.565132	3.836294
H	-10.060751	0.693733	1.586022
H	-9.171836	-1.501171	2.385988
C	-4.994936	1.881874	7.854791
C	-5.188484	-0.551057	9.266505
C	-4.086996	1.584386	8.889900
C	-5.994345	0.943795	7.525344
C	-6.092099	-0.262804	8.231098
C	-4.184474	0.373184	9.590581
H	-3.305096	2.303207	9.157008
H	-6.700858	1.147497	6.713344
H	-6.877922	-0.978822	7.971564
H	-3.479748	0.159676	10.400089
H	-5.274352	-1.488077	9.824711

C	-2.656616	-0.499650	3.392183
P	-0.979506	0.041833	2.520490
C	-1.405716	1.310697	1.280513
H	-0.489392	1.627644	0.760607
H	-1.894831	2.164551	1.770346
H	-2.094951	0.877445	0.541597
C	-5.283987	-2.048931	0.281220
C	-4.339474	-0.199342	1.492705
H	-4.301369	0.870404	1.713482
C	-3.701233	-2.471556	2.047344
H	-3.159754	-3.189241	2.665313
C	-4.557041	-2.957710	1.052570
H	-4.678962	-4.028225	0.872974
C	-5.188217	-0.669715	0.487633
H	-5.795572	0.006629	-0.117947
C	1.169404	-3.300568	0.114540
C	-0.066921	-2.796133	-0.316439
C	-0.709303	-1.783960	0.407789
C	-0.111612	-1.267321	1.580803
C	1.135964	-1.772301	2.007007
C	1.768447	-2.783771	1.272775
H	1.666566	-4.091551	-0.454385
H	-0.536551	-3.190702	-1.222290
H	-1.676213	-1.409773	0.058983
H	1.614594	-1.371860	2.905032
H	2.737101	-3.166483	1.607596
C	2.025677	1.934377	5.498753
C	1.619282	2.637950	4.356979
C	0.694300	2.073198	3.470010
C	0.165654	0.788548	3.720491
C	0.571964	0.084428	4.876780
C	1.497701	0.660772	5.755138
H	2.751021	2.377370	6.187209
H	2.020153	3.634623	4.152003
H	0.390483	2.644574	2.590047
H	0.170638	-0.907877	5.092955
H	1.806508	0.105989	6.646087
H	-1.653259	-4.065485	7.416029
N	-6.205322	-2.559953	-0.758594
O	-6.849703	-1.722333	-1.405956
O	-6.268462	-3.788599	-0.907022

β-phosphonium cyclopropenyl[(triphos)$(CO)_2$Re{CC(PMe_3)CPh(*p*-$C_6H_4NO_2$)}]$^+$

C	1.7398482344	-0.2722966154	2.3214696548
C	1.3525465349	-1.4309009877	3.0134677485
C	0.9512334603	-2.5690101569	2.2982462460
C	0.9422775433	-2.5554329076	0.8951066183
C	1.3061834924	-1.3895814967	0.1981047706
C	1.7078072651	-0.2476248512	0.9208048638
P	1.2045480984	-1.3216106741	-1.6368589731

C	-0.2541157685	-0.1597945840	-1.9155038429
C	-1.5960393919	-0.8326360535	-2.3146977677
C	-1.9495302176	-2.0870445308	-1.4643230960
P	-1.1378235673	-3.6787109154	-2.0241447202
C	-1.7327152141	-4.9564453502	-0.8269864207
C	-1.9826256664	-4.6999320757	0.5346315828
C	-2.4487936220	-5.7265054656	1.3721116852
C	-2.6640596581	-7.0156558452	0.8637610259
C	-2.4115293037	-7.2783637253	-0.4926298786
C	-1.9475399583	-6.2572306389	-1.3327611895
Re	1.0768033872	-3.3426654671	-3.0382772270
C	2.3685207531	-4.4285181173	-1.7821752637
C	2.8850807066	-5.3456390694	-0.9445639731
P	2.7827107095	-6.8512246518	-0.0469185132
C	0.7847124715	-4.9287861045	-4.0955738343
O	0.5665823477	-5.9034301659	-4.7184035626
C	2.6281045050	-2.7746743658	-4.0461504835
O	3.5156058396	-2.3512160104	-4.6850454572
P	-0.2367851965	-2.0001469692	-4.5486254581
C	-1.7079348435	-1.0721279136	-3.8407992500
C	1.1672649027	-6.9918498920	0.7938805634
C	3.9429552574	-4.4515176401	-1.5344797000
C	4.8581686894	-5.0094968988	-2.6012592315
C	4.3545487777	-5.7440591600	-3.6966321523
C	5.2147603373	-6.3005312456	-4.6521028467
C	6.6043563702	-6.1496208416	-4.5354886682
C	7.1218905375	-5.4337968853	-3.4471183138
C	6.2613193160	-4.8707399670	-2.4945425012
H	7.2752506148	-6.5854787538	-5.2817302371
C	4.4642513641	-3.2887263711	-0.7333789918
C	5.0340804676	-2.1765830174	-1.4023452095
C	5.4168651875	-1.0301942518	-0.7025865197
C	5.2360417640	-0.9944966740	0.6861686147
C	4.7178823306	-2.0897438659	1.3853086212
C	4.3338912697	-3.2249154103	0.6692014380
N	5.5499319284	0.2425887529	1.4197790883
O	6.0540379846	1.1786625564	0.7785650215
O	5.2660798382	0.2776354082	2.6304440023
H	-2.0403135434	-4.0388381069	-3.0709275956
H	-0.8348520931	-2.6166211795	-5.6876665133
H	0.4396512638	-0.9549801356	-5.2479764074
H	2.2692932104	-0.4141740961	-1.9052922661
H	-0.3831521629	0.4194432591	-0.9858814689
H	0.0433057365	0.5613363347	-2.6981311104
H	-2.6206445473	-1.6475284054	-4.0713700184
H	-1.7985130821	-0.1093010595	-4.3703277299
H	-1.6548076768	-1.9079136602	-0.4158252042
H	-3.0396412857	-2.2550610302	-1.4699743553
H	-2.3807729844	-0.0917159054	-2.0741570453
H	5.1669976568	-2.2119314642	-2.4878240915
H	3.9095968484	-4.0775884014	1.2073494427

H	4.6063006898	-2.0232937319	2.4693117445
H	5.8402502243	-0.1589462200	-1.2082246772
H	3.2761320054	-5.8791362233	-3.8042750768
H	6.6867168525	-4.3092580970	-1.6563870098
H	8.2039460351	-5.3083144403	-3.3363595212
H	4.7942295091	-6.8572961343	-5.4958709838
H	-1.8285225705	-3.7003191806	0.9522884446
H	-1.7640750422	-6.4715315037	-2.3921997198
H	-2.5867973157	-8.2780306407	-0.9023340549
H	-2.6557766341	-5.5103076135	2.4248432517
H	-3.0380720930	-7.8095305540	1.5167613224
H	2.0141604561	0.6620127697	0.3917469367
H	0.6862709224	-3.4587501663	0.3321924773
H	0.6569269427	-3.4772850134	2.8349663914
H	2.0838574534	0.6087842951	2.8707336339
H	1.3730182352	-1.4457989563	4.1071089667
H	0.3734770114	-6.9268389749	0.0334025411
H	1.0410242463	-6.1683816876	1.5122896003
H	1.0910001895	-7.9626786486	1.3071405911
C	6.2337653319	-6.9319059931	3.0297756521
C	4.9163312166	-7.1260930109	3.4684978198
C	3.8566361193	-7.1124472795	2.5502441838
C	4.1182740128	-6.9019870343	1.1811535742
C	5.4468543238	-6.7108523820	0.7384952550
C	6.4954607177	-6.7263503408	1.6658499520
H	7.0568888315	-6.9408276606	3.7501629534
H	4.7089338776	-7.2892492556	4.5300918814
H	2.8344586572	-7.2655826013	2.9085898774
H	5.6624456002	-6.5444336291	-0.3220208175
H	7.5221983024	-6.5742944040	1.3200982179
C	3.1854947048	-10.5337260384	-2.8145805737
C	3.8896732447	-10.4986990884	-1.6031967242
C	3.7815595200	-9.3865010315	-0.7580525199
C	2.9619814988	-8.3042483329	-1.1342793239
C	2.2540094496	-8.3385178932	-2.3528263706
C	2.3666041222	-9.4563727383	-3.1870303012
H	3.2811334708	-11.4006761714	-3.4752343513
H	4.5334731986	-11.3352396852	-1.3158800976
H	4.3417521972	-9.3570579496	0.1811539791
H	1.6356344054	-7.4896069740	-2.6616184412
H	1.8251929637	-9.4783141592	-4.1374085249

Transition state for the formation of α-phosphonioallenyl complex [(triphos)$(CO)_2$Re{C(PMe_3)=C=CPh(*p*-$C_6H_4NO_2$)}]$^+$

Re	0.3722062697	1.6620237605	1.7968216778
C	-0.5989193814	2.5089471962	3.2415516737
O	-1.1876934469	3.0179824098	4.1182978307

C	-1.2685769754	1.4743991206	0.7915701331
O	-2.2574406148	1.3592926047	0.1688900480
C	-0.0808090220	-0.9369604019	3.7515565200
C	-0.2725624310	-1.7054486507	4.8616556550
P	2.5134003303	2.0964066855	2.9286680491
H	2.4872893366	3.3998727103	3.5093685101
P	0.8749903090	3.7850827817	0.7541206315
H	0.4255192050	4.9990696781	1.3510801882
H	0.3379801577	4.0131250299	-0.5481468810
P	1.6850704186	0.7426003552	-0.0630626654
H	0.9795016355	0.6228335605	-1.2966514706
C	3.0811761104	1.8803265040	-0.6397209193
H	3.9101954718	1.2248398667	-0.9550343031
H	2.7281163196	2.3998471696	-1.5481309449
C	2.6910857855	4.1787179105	0.4779705756
H	3.0261713430	4.8281847888	1.3046547096
H	2.7767260242	4.7763529207	-0.4444868129
C	3.9605729237	2.3062240916	1.7663369922
H	4.4189630271	1.3143392261	1.6091896363
H	4.7127993834	2.9289364885	2.2787070212
C	3.5966623595	2.9231617287	0.3851412788
H	4.5548435895	3.2863365129	-0.0307677239
C	0.7913705610	-2.6122089863	5.3514754002
C	2.8220029041	-4.3551607651	6.2692177006
C	1.7124000520	-3.1911991773	4.4482133450
C	0.9234940903	-2.9109854977	6.7290217419
C	1.9324686143	-3.7684134452	7.1806121122
C	2.7069304195	-4.0618275718	4.9008651117
H	1.6173906287	-2.9650051715	3.3821893810
H	0.2402159301	-2.4526097329	7.4491380736
H	2.0216594188	-3.9827105124	8.2499824791
H	3.3895549324	-4.5302699560	4.1840135360
H	3.5987325917	-5.0403490746	6.6222286747
C	-1.5804436891	-1.6550998943	5.5680980684
C	-4.0875831600	-1.6081232596	6.8125878420
C	-2.3460804880	-0.4641051819	5.6060794433
C	-2.1143640036	-2.8222018808	6.1718255623
C	-3.3664480047	-2.8052709443	6.7886164916
C	-3.5938423246	-0.4342412814	6.2305784387
H	-1.9424737718	0.4466935033	5.1546466753
H	-1.5499490345	-3.7573924086	6.1333016587
H	-3.7984865492	-3.6980207094	7.2463875137
H	-4.1935589585	0.4771172580	6.2830291528
C	3.1288138996	1.1723430209	4.3890021161
C	3.8928213913	-0.2393975747	6.6969682673
C	4.1325272719	0.1889734065	4.3158690380
C	2.5081882751	1.4434979293	5.6263084030
C	2.8920902747	0.7409111302	6.7739083983
C	4.5114750228	-0.5121872797	5.4700461920
H	4.6313904938	-0.0352091432	3.3677898248
H	1.7235047023	2.2054450853	5.6955611284

H	2.4105316112	0.9636077795	7.7308332109
H	5.2957752589	-1.2723261441	5.4077870596
H	4.1909029978	-0.7892181733	7.5942824298
C	2.4826409937	-0.9100719619	-0.0254326222
C	3.8836823462	-3.3494193445	0.0106427493
C	2.8805251575	-1.4787421173	1.1998080521
C	2.7734379754	-1.5817627538	-1.2320508496
C	3.4662643160	-2.7993584919	-1.2111488570
C	3.5904777517	-2.6890125796	1.2126991281
H	2.6094197971	-0.9892246050	2.1405854168
H	2.4607953717	-1.1543081808	-2.1914451241
H	3.6830296403	-3.3171491992	-2.1502892889
H	3.9107490654	-3.1159039835	2.1683593552
H	4.4333164885	-4.2953317809	0.0238290177
C	0.0529219046	-0.1320422604	2.7569388218
P	-1.1632870575	-2.0013097669	1.2243935414
C	-1.3665954067	-2.0411660313	-0.6210719280
H	-1.7910289351	-1.0849416529	-0.9637825709
H	-2.0420804694	-2.8592939499	-0.9260242849
H	-0.3855905545	-2.1908148461	-1.0989547534
C	-2.9091865017	-1.9312427204	1.8278675316
H	-3.3659383268	-0.9798670103	1.5146500244
H	-2.9209176700	-1.9779687025	2.9274578831
H	-3.5046476675	-2.7674093251	1.4234741795
C	-0.6589678468	-3.7395939470	1.6127465402
H	-1.3949243662	-4.4618154665	1.2199662996
H	0.3252792165	-3.9475600651	1.1646272385
H	-0.5813706499	-3.8704982788	2.7028888711
N	-5.4156985062	-1.5851506822	7.4689681578
O	-6.0338745803	-0.5108307272	7.4579028391
O	-5.8129622011	-2.6427951656	7.9794020696

Transition state for the formation of γ-phosphonioalkynyl complex [(triphos)$(CO)_2$Re{C≡CCPh(*p*-$C_6H_4NO_2$)(PMe_3)}]$^+$

Re	0.2862486731	3.0793224530	1.5536075776
C	0.9423923562	2.0758636515	3.0761251423
O	1.3363094183	1.4483366165	3.9844719065
C	-0.8494320927	4.2105755590	2.6447290492
O	-1.5369166143	4.8975990750	3.2988180342
C	-1.2089346193	1.7089415152	1.4391439370
C	-2.1141577161	0.8328253526	1.4940269991
P	1.7650175299	1.7871213974	0.0840393343
H	2.7160970705	0.9661224524	0.7570061030
P	2.1463220141	4.6287578487	1.6897789848
H	3.3373274787	4.1682459011	2.3267652318
H	2.0205703400	5.8524851813	2.4113473460
P	-0.2872320133	4.4507382959	-0.4150037289
H	-0.2851427173	5.8368741144	-0.0706319406
C	1.0746604364	4.4659807978	-1.7053834103
H	0.8595302571	3.6405163619	-2.4065957405

H	0.9841697815	5.4021992129	-2.2810878289
C	2.8233798812	5.2546801720	0.0516805517
H	3.9118795386	5.3909539317	0.1617007702
H	2.3970527005	6.2568448491	-0.1250131586
C	2.9554069502	2.8591690998	-0.9149586983
H	3.1057437364	2.3500767593	-1.8815725168
H	3.9290587111	2.8409167951	-0.3935852411
C	2.5222580542	4.3283049083	-1.1550094025
H	3.1782892396	4.6923047154	-1.9677149346
C	-2.7738840401	-1.5561573988	1.2884930164
C	-2.0816999455	-4.2382864028	0.7277132514
C	-1.5604785568	-1.8667586970	0.6393220709
C	-3.6306471685	-2.6190023128	1.6627203747
C	-3.2870825928	-3.9449286728	1.3865401798
C	-1.2222861102	-3.1959136239	0.3572871980
H	-0.8953522772	-1.0507890415	0.3426888483
H	-4.5634194358	-2.3995132111	2.1930624234
H	-3.9583882144	-4.7542904218	1.6890733336
H	-0.2826671253	-3.4135146395	-0.1592221872
H	-1.8153101047	-5.2770451893	0.5106030079
C	-4.5284765943	0.3524080750	1.2944994549
C	-7.0893000131	1.3445720065	0.7474434545
C	-4.9287799871	1.6265860137	1.7661073085
C	-5.4426122992	-0.3962914909	0.5180267169
C	-6.7225420467	0.0963880097	0.2418947265
C	-6.2053908704	2.1226581506	1.5075742207
H	-4.2125747895	2.2308327736	2.3318057851
H	-5.1439002569	-1.3597989769	0.0996077947
H	-7.4380517752	-0.4652442393	-0.3628270593
H	-6.5339457682	3.0988770944	1.8709781999
C	1.1469966308	0.5626724237	-1.1362178674
C	0.2960310277	-1.2432332841	-3.1171021158
C	-0.0846108584	0.7579596589	-1.7913948946
C	1.9415838546	-0.5547835292	-1.4682238055
C	1.5147395303	-1.4537825037	-2.4543665305
C	-0.5024416841	-0.1401042253	-2.7835183084
H	-0.7296929070	1.5967048513	-1.5117158570
H	2.8950512618	-0.7252947007	-0.9561050848
H	2.1363876849	-2.3186012783	-2.7054125247
H	-1.4593750685	0.0198293979	-3.2891955830
H	-0.0338482217	-1.9442430591	-3.8894885624
C	-1.8447184061	4.3765153119	-1.3877527262
C	-4.2572341554	4.2912834372	-2.8309516945
C	-2.0699015122	5.2809786948	-2.4472226882
C	-2.8386626301	3.4399327102	-1.0481908124
C	-4.0402366629	3.3993650800	-1.7722355748
C	-3.2708505823	5.2336366283	-3.1648033280
H	-1.3173347218	6.0324739927	-2.7092064470
H	-2.6721565358	2.7538130203	-0.2117521949
H	-4.8100842063	2.6718680190	-1.4966565159
H	-3.4406193764	5.9409001830	-3.9820111818

H	-5.1963314292	4.2625216141	-3.3911333445
C	-3.1274942806	-0.1264502200	1.5476098471
P	-3.3097428507	-0.3813227073	4.1843778944
C	-3.2295566402	1.2782065196	4.9890113106
H	-2.4855997269	1.9007703771	4.4662894420
H	-2.9470609881	1.1980595440	6.0521471782
H	-4.2127012382	1.7688594065	4.9157665506
C	-1.7188653646	-1.1894938612	4.6469714991
H	-0.8828114136	-0.6303416629	4.1981696796
H	-1.7034229956	-2.2180295759	4.2540767485
H	-1.5862393107	-1.2171288957	5.7411531376
C	-4.5866625037	-1.2934526493	5.1705571107
H	-4.3541197915	-1.2704143064	6.2488090404
H	-4.6292036016	-2.3426946869	4.8391774443
H	-5.5750746031	-0.8362633407	5.0080784584
N	-8.4427486836	1.8713440988	0.4543527802
O	-8.7239985593	2.9900163023	0.9088692547
O	-9.1931642796	1.1573162047	-0.2264257573

Transition state for the formation of α-phosphonioallenyl complex [(triphos)$(CO)_2$Re{C(PMe_3)=C=C(*p*-$C_6H_4NO_2)_2$}]$^+$

Re	1.9248760000	-0.5486690000	2.2116130000
C	2.0221210000	-2.3756580000	2.8369120000
O	2.1137550000	-3.4790250000	3.2251290000
C	2.0817200000	0.0568610000	4.0469540000
O	2.1489880000	0.4191180000	5.1582330000
C	-1.2598730000	-0.1372890000	2.8725260000
C	-2.4563300000	0.3483980000	3.3169580000
P	1.8706090000	-1.2658180000	-0.1406670000
H	2.5882580000	-2.4833690000	-0.3351140000
P	4.3298300000	-0.4784050000	1.8791230000
H	5.1157890000	-1.6280600000	2.1820680000
H	5.0514360000	0.4557550000	2.6796540000
P	2.1161740000	1.7786760000	1.3979300000
H	2.7091750000	2.5921700000	2.4060630000
C	3.3763300000	2.0135550000	0.0138750000
H	2.9069400000	2.6724020000	-0.7355700000
H	4.2154020000	2.5897710000	0.4403960000
C	4.9454910000	-0.0539340000	0.1603490000
H	5.1968340000	-1.0005090000	-0.3484980000
H	5.8874190000	0.5105030000	0.2581210000
C	2.8112760000	-0.1375790000	-1.3114920000
H	2.0546450000	0.5048820000	-1.7949050000
H	3.2321790000	-0.7725980000	-2.1093340000
C	3.9225780000	0.7442070000	-0.6886900000
H	4.5011620000	1.1270290000	-1.5506450000
C	-2.9120070000	0.0815350000	4.7023610000
C	-3.7902330000	-0.5431060000	7.2835920000
C	-1.9840440000	-0.0857550000	5.7599480000
C	-4.2939800000	-0.0754370000	4.9808070000

C	-4.7364320000	-0.3930250000	6.2659010000
C	-2.4178170000	-0.3913190000	7.0504460000
H	-0.9162690000	0.0416260000	5.5597160000
H	-5.0247460000	0.0243460000	4.1736080000
H	-5.7949390000	-0.5323460000	6.4967480000
H	-1.7215550000	-0.5120470000	7.8834100000
C	-3.3015720000	1.1501080000	2.4021170000
C	-4.7436590000	2.7704670000	0.6387380000
C	-4.1015470000	2.2143440000	2.8883290000
C	-3.2679430000	0.9093100000	1.0084290000
C	-3.9888780000	1.7088720000	0.1253590000
C	-4.8179300000	3.0303980000	2.0105620000
H	-4.1305240000	2.4253660000	3.9603390000
H	-2.6652750000	0.0779700000	0.6335590000
H	-3.9811040000	1.5433280000	-0.9544500000
H	-5.4184910000	3.8719200000	2.3632730000
C	0.3665680000	-1.6847660000	-1.1018990000
C	-1.9160380000	-2.2871810000	-2.6364410000
C	-0.6899560000	-0.7559420000	-1.1939210000
C	0.2703210000	-2.9170390000	-1.7794060000
C	-0.8698560000	-3.2166050000	-2.5398500000
C	-1.8201900000	-1.0563940000	-1.9670640000
H	-0.6318120000	0.1982020000	-0.6586050000
H	1.0862320000	-3.6453340000	-1.7171900000
H	-0.9350440000	-4.1754410000	-3.0629790000
H	-2.6316390000	-0.3265040000	-2.0501210000
H	-2.8007410000	-2.5179990000	-3.2367690000
C	0.7064290000	2.8826130000	0.9774500000
C	-1.4595480000	4.6000250000	0.4367150000
C	0.2096130000	3.0083010000	-0.3341040000
C	0.1006480000	3.6132350000	2.0192960000
C	-0.9766460000	4.4663580000	1.7471340000
C	-0.8662170000	3.8675900000	-0.6016560000
H	0.6654960000	2.4538740000	-1.1621400000
H	0.4789080000	3.5300030000	3.0441340000
H	-1.4293470000	5.0396610000	2.5615730000
H	-1.2355170000	3.9701120000	-1.6264670000
H	-2.2909610000	5.2781380000	0.2241620000
C	-0.0901300000	-0.4956880000	2.4817330000
P	-1.3231660000	-3.0695250000	2.2957610000
C	-3.0986470000	-2.9391820000	1.7853200000
H	-3.5578210000	-2.0516200000	2.2482690000
H	-3.6708400000	-3.8316290000	2.0917500000
H	-3.1542070000	-2.8323530000	0.6906530000
C	-0.7975240000	-4.6608850000	1.4926600000
H	-0.7992510000	-4.5447450000	0.3978630000
H	-1.4760060000	-5.4863660000	1.7698570000
H	0.2222990000	-4.9138090000	1.8221350000
C	-1.4387730000	-3.5618790000	4.0780580000
H	-1.8281290000	-2.7219850000	4.6720390000
H	-0.4341060000	-3.8140920000	4.4517650000

H	-2.0989460000	-4.4364330000	4.2088160000
N	-4.2554120000	-0.8814080000	8.6497420000
N	-5.4496460000	3.6638130000	-0.3040510000
O	-6.0992650000	4.6016060000	0.1792810000
O	-5.3259100000	3.4199920000	-1.5146910000
O	-5.4777920000	-0.9896930000	8.8193420000
O	-3.3874080000	-1.0341290000	9.5202150000

Transition state for the formation of γ-phosphonioalkynyl complex [(triphos)$(CO)_2$Re{C≡CC(*p*-$C_6H_4NO_2$)$_2$(PMe_3)}]$^+$

Re	1.6100300000	-0.1726740000	1.2182770000
C	1.2641890000	-2.0190370000	0.7651910000
O	1.0748830000	-3.1405260000	0.4758440000
C	2.1121880000	-0.6637880000	3.0293280000
O	2.3955620000	-0.9633560000	4.1271120000
C	-0.3196770000	0.0107390000	1.7864490000
C	-1.5439600000	-0.0145800000	2.0793490000
P	1.0671640000	0.4507570000	-1.0946220000
H	1.4201350000	-0.5745670000	-2.0213560000
P	3.8915080000	-0.2907190000	0.3950520000
H	4.4156490000	-1.5010240000	-0.1422950000
H	4.9349800000	-0.0491360000	1.3341680000
P	2.3571430000	2.1207560000	1.6996610000
H	3.4360150000	2.0610330000	2.6343100000
C	3.2595850000	2.9498950000	0.2504970000
H	2.7181590000	3.8829660000	0.0438370000
H	4.2560210000	3.2418840000	0.6108380000
C	4.3298600000	0.9206370000	-0.9744790000
H	4.3028610000	0.3713390000	-1.9271520000
H	5.3750210000	1.2353800000	-0.8296420000
C	2.0570740000	1.8864570000	-1.7630280000
H	1.4145620000	2.7754640000	-1.6821030000
H	2.2226530000	1.7105840000	-2.8357760000
C	3.4108060000	2.1606130000	-1.0679260000
H	3.9436380000	2.8515100000	-1.7485670000
C	-3.7146740000	-1.0927680000	1.5718380000
C	-5.1667630000	-3.0528540000	0.1992900000
C	-3.0956480000	-1.8757500000	0.5664080000
C	-5.0832630000	-1.3215200000	1.8778450000
C	-5.8154140000	-2.2961770000	1.1950350000
C	-3.8157290000	-2.8556360000	-0.1234900000
H	-2.0443780000	-1.6960730000	0.3257280000
H	-5.5744350000	-0.7398900000	2.6732830000
H	-6.8694760000	-2.4925310000	1.4164830000
H	-3.3573710000	-3.4730610000	-0.9028500000
C	-3.5428500000	1.2042690000	2.7841620000
C	-4.4995140000	3.7209220000	3.5371640000
C	-2.9116470000	1.9278240000	3.8166630000
C	-4.6701050000	1.7693110000	2.1424630000
C	-5.1510820000	3.0320460000	2.5156480000

C	-3.3893400000	3.1774060000	4.2099410000
H	-2.0091990000	1.5064290000	4.2881970000
H	-5.1523310000	1.2419310000	1.3171700000
H	-6.0086900000	3.4991500000	2.0200160000
H	-2.9067040000	3.7557860000	5.0016830000
C	-0.6580730000	0.7402360000	-1.6479980000
C	-3.3438000000	1.1066490000	-2.4245420000
C	-1.3995580000	1.8423950000	-1.1685890000
C	-1.2768680000	-0.1773420000	-2.5210340000
C	-2.6140630000	0.0070950000	-2.9019360000
C	-2.7314630000	2.0240520000	-1.5625880000
H	-0.9432850000	2.5638820000	-0.4843890000
H	-0.7160300000	-1.0379690000	-2.9069480000
H	-3.0800670000	-0.7119190000	-3.5800140000
H	-3.2915090000	2.8883610000	-1.1883760000
H	-4.3815760000	1.2508640000	-2.7270880000
C	1.4354070000	3.5148720000	2.4619510000
C	0.0968220000	5.7731650000	3.4794600000
C	2.1432830000	4.5069640000	3.1838210000
C	0.0503880000	3.6485220000	2.2753910000
C	-0.6095030000	4.7799670000	2.7772170000
C	1.4743610000	5.6300330000	3.6906090000
H	3.2214040000	4.4082350000	3.3498680000
H	-0.5087280000	2.8607340000	1.7598470000
H	-1.6865470000	4.8802290000	2.6331310000
H	2.0318010000	6.3929590000	4.2554510000
H	-0.4275760000	6.6515240000	3.8748520000
C	-2.9100650000	-0.0676700000	2.3025480000
P	-2.9994760000	-1.4288550000	4.6035920000
C	-1.4974980000	-1.1426150000	5.6358680000
H	-0.6101270000	-1.0717330000	4.9915450000
H	-1.3533040000	-1.9572850000	6.3619790000
H	-1.6009620000	-0.1890390000	6.1866580000
C	-2.9171980000	-3.2231600000	4.1559370000
H	-2.0387860000	-3.4007520000	3.5106480000
H	-3.8201970000	-3.5022720000	3.5960940000
H	-2.8408180000	-3.8589350000	5.0491770000
C	-4.3949790000	-1.3329130000	5.8073910000
H	-4.2369140000	-2.0022040000	6.6680660000
H	-5.3299770000	-1.6235670000	5.3069570000
H	-4.4907930000	-0.2956590000	6.1763400000
N	-4.9448210000	5.0936360000	3.8848060000
N	-5.9363890000	-4.1004630000	-0.5268540000
O	-4.2243470000	5.7423310000	4.6584280000
O	-5.9906160000	5.4991190000	3.3664700000
O	-7.1158570000	-4.2836750000	-0.1979870000
O	-5.3471260000	-4.7160450000	-1.4151830000

Transition state for the formation of α-phosphonioallenyl complex [(triphos)$(CO)_2$Re{C($PMePh_2$)=C=CPh(*p*-$C_6H_4NO_2$)}]$^+$

Re	2.0801109793	-1.0596965942	1.6530424126
C	2.3756745211	-2.8977461914	1.1131940357
O	2.6257418578	-3.9981583097	0.7865041277
C	2.5397666862	-1.5242814920	3.4728930151
O	2.8094556560	-1.8027278595	4.5788867755
C	-0.9932972180	-1.3879995406	2.7939776384
C	-2.1350241138	-1.2841505456	3.5459355816
P	1.6674801836	-0.4157662084	-0.6931506696
H	2.4136685865	-1.2721317683	-1.5565663456
P	4.3782325314	-0.5128017876	1.1133855747
H	5.2121737614	-1.5223359646	0.5482001540
H	5.2202427385	-0.1643757083	2.2124234470
P	2.1443157043	1.3177913373	2.2979878099
H	3.1039498640	1.4901123231	3.3410674035
C	2.8865180165	2.4810122501	1.0071679642
H	2.0773070540	3.1776852621	0.7267535407
H	3.6567836458	3.0869205474	1.5155762562
C	4.6905791525	0.9247737712	-0.0588534645
H	5.0118197278	0.5025355887	-1.0262285837
H	5.5444818875	1.5052685681	0.3285520149
C	2.3780866453	1.2470362279	-1.1941820119
H	1.5242974528	1.9448535642	-1.2516014343
H	2.7601246452	1.1388732796	-2.2232251768
C	3.4698277002	1.8531262604	-0.2810005836
H	3.8678204093	2.7125508229	-0.8546964114
C	-2.2742285595	-2.0234838256	4.8238976498
C	-2.5381070837	-3.4858665119	7.2338620572
C	-1.1341039315	-2.3538948502	5.6014433454
C	-3.5504738510	-2.4580373368	5.2758396389
C	-3.6760575709	-3.1842963603	6.4634955788
C	-1.2676852528	-3.0683498246	6.7956015184
H	-0.1432267243	-2.0246374993	5.2670050061
H	-4.4395971753	-2.2466795173	4.6698025937
H	-4.6669358577	-3.5220815829	6.7891821785
H	-0.3756156947	-3.2974799266	7.3920276411
C	-3.2229174942	-0.3855060615	3.0913020211
C	-5.2047757526	1.3876936856	2.2247822424
C	-3.9940811813	0.3480347247	4.0273079163
C	-3.4751466606	-0.2033017173	1.7097948779
C	-4.4657100378	0.6733643383	1.2728692031
C	-4.9835685970	1.2378417850	3.5987715754
H	-3.7910190483	0.2392658802	5.0967812590
H	-2.8993798242	-0.7829383064	0.9832252005
H	-4.6898296236	0.8143732183	0.2129041346
H	-5.5774972490	1.8264800831	4.3022389249
C	0.0895057853	-0.4481608279	-1.6408522127
C	-2.2804704083	-0.4417455344	-3.1682614068
C	-0.9845178798	0.3948660263	-1.2851897143
C	-0.0360452781	-1.2881304802	-2.7684298793
C	-1.2172580983	-1.2850192115	-3.5255279752
C	-2.1583074651	0.4000211875	-2.0493428752

H	-0.9028145930	1.0593266500	-0.4175492969
H	0.7936254313	-1.9382838889	-3.0683711943
H	-1.2994884780	-1.9349621376	-4.4036017280
H	-2.9795266346	1.0694945108	-1.7753465749
H	-3.1961205338	-0.4310498323	-3.7673538011
C	0.7801085202	2.2992091294	3.0113311731
C	-1.2860479506	3.8951696934	4.0329927741
C	-0.5333465166	2.1596051500	2.5173785290
C	1.0501078654	3.2296868603	4.0317194180
C	0.0159699364	4.0234995364	4.5402823464
C	-1.5597612513	2.9659033296	3.0225925796
H	-0.7553168149	1.3945517206	1.7687234204
H	2.0661519136	3.3299863782	4.4329604142
H	0.2286429158	4.7399032048	5.3368654262
H	-2.5775168093	2.8534717891	2.6369796312
H	-2.0918090725	4.5165846552	4.4332996871
C	0.1233985108	-1.4134513967	2.1643839271
P	-0.9049774745	-3.7686349196	1.0033699707
C	-0.3711860716	-4.5624843714	-0.5928341446
H	-0.4027066979	-3.8264496624	-1.4090451296
H	-1.0147810455	-5.4163715800	-0.8542605701
H	0.6648590172	-4.9058716641	-0.4658300153
N	-6.2378274862	2.3410653406	1.7606415250
O	-6.8890669719	2.9587490540	2.6240848830
O	-6.3743421856	2.4640059813	0.5321670645
H	-2.6383414977	-4.0457387159	8.1686259040
C	-0.5897909840	-7.2886341081	4.0295590055
C	-1.3162101163	-7.4543565475	2.8384751550
C	-1.4155681369	-6.3993228948	1.9250710508
C	-0.7867276733	-5.1665297262	2.1936318721
C	-0.0589303355	-5.0063220637	3.3869146799
C	0.0370635734	-6.0652409383	4.3033327775
H	-0.5177857394	-8.1136997716	4.7463245365
H	-1.8110938240	-8.4062149149	2.6264809786
H	-2.0021304567	-6.5316022941	1.0112647499
H	0.4229447747	-4.0483547926	3.6047138217
H	0.5995482953	-5.9320907355	5.2342165158
C	-5.4762592483	-3.1054397046	0.4165474568
C	-4.9882234861	-3.5567659460	1.6501577824
C	-3.6172206472	-3.7849797576	1.8315301058
C	-2.7133810590	-3.5658639265	0.7688189163
C	-3.2145790350	-3.1001352494	-0.4677352134
C	-4.5850778823	-2.8801983179	-0.6427361137
H	-6.5472486834	-2.9339312762	0.2758157782
H	-5.6809837438	-3.7424271249	2.4759022490
H	-3.2489973647	-4.1572304737	2.7927631464
H	-2.5340836080	-2.9116900870	-1.3037338547
H	-4.9601103098	-2.5334760503	-1.6113343947

Transition state for the formation of γ-phosphonioalkynyl complex [(triphos)$(CO)_2$Re{C≡CCPh(*p*-$C_6H_4NO_2$)($PMePh_2$)}]$^+$

Re	-4.6023330000	3.9529470000	4.4020060000
C	-4.6285350000	4.3729060000	2.5077400000
O	-4.6448520000	4.6311270000	1.3659930000
C	-2.7677790000	4.5416140000	4.6239410000
O	-1.6657670000	4.9007350000	4.7835990000
C	-3.8892270000	2.1056250000	3.9736420000
C	-3.3594130000	0.9997300000	3.6740060000
P	-7.0177110000	3.4512770000	4.3163210000
H	-7.6945240000	4.4123380000	3.5053050000
P	-5.4137560000	6.1592850000	5.0058740000
H	-5.7267700000	7.1180020000	3.9946830000
H	-4.5421970000	6.9903430000	5.7754000000
P	-4.7043960000	3.4920440000	6.8119490000
H	-3.5844150000	3.9654570000	7.5569590000
C	-6.0706680000	4.4459950000	7.6979180000
H	-6.4293740000	3.8020030000	8.5162900000
H	-5.5997680000	5.3241480000	8.1715490000
C	-6.9834420000	6.2103190000	6.0391190000
H	-7.8242330000	6.4308490000	5.3595260000
H	-6.9072570000	7.0625820000	6.7332420000
C	-7.8745520000	3.7715860000	5.9552940000
H	-7.8548090000	2.8183990000	6.5129620000
H	-8.9343260000	3.9925580000	5.7439200000
C	-7.2680120000	4.9060580000	6.8266700000
H	-8.0620910000	5.1744390000	7.5480000000
C	-3.5585550000	-0.9500870000	2.2061650000
C	-2.0672500000	-1.0198610000	4.3304770000
C	-0.5830080000	-2.4398740000	6.2757090000
C	-1.3702400000	-2.2058110000	3.9877640000
C	-1.9932330000	-0.5596400000	5.6675700000
C	-1.2649950000	-1.2655250000	6.6288060000
C	-0.6354120000	-2.9033480000	4.9508000000
H	-1.3761190000	-2.5643260000	2.9545050000
H	-2.5308330000	0.3524820000	5.9408100000
H	-1.2331350000	-0.8988460000	7.6603540000
H	-0.0938150000	-3.8093570000	4.6620160000
C	-7.8061470000	1.9111490000	3.6968600000
C	-8.9974600000	-0.4479110000	2.7341840000
C	-9.2117490000	1.7903730000	3.6598930000
C	-7.0032440000	0.8529390000	3.2339240000
C	-7.6025080000	-0.3239030000	2.7575350000
C	-9.8005980000	0.6138260000	3.1810120000
H	-9.8520900000	2.6144290000	3.9921370000
H	-5.9139970000	0.9578450000	3.2384130000
H	-6.9699910000	-1.1406450000	2.3988600000
H	-10.8906870000	0.5295170000	3.1499030000
H	-9.4623110000	-1.3646380000	2.3595330000
C	-4.8058630000	1.7921750000	7.5012570000
C	-5.0356280000	-0.7810200000	8.6218720000
C	-4.2376890000	1.5112990000	8.7620630000

C	-5.4770690000	0.7704690000	6.8017120000
C	-5.5957120000	-0.5077970000	7.3656600000
C	-4.3525040000	0.2293070000	9.3164930000
H	-3.6997980000	2.2922150000	9.3114540000
H	-5.8862400000	0.9634400000	5.8051160000
H	-6.1195200000	-1.2938410000	6.8132510000
H	-3.9047590000	0.0207730000	10.2927290000
H	-5.1237570000	-1.7808450000	9.0566670000
C	-2.8630480000	-0.2549480000	3.3357460000
P	-0.5891430000	0.3143440000	1.8043220000
C	-5.0165460000	-2.1658880000	0.1492000000
C	-3.9338360000	-0.2159280000	1.0535870000
H	-3.6377870000	0.8354390000	0.9730670000
C	-3.9532380000	-2.3051700000	2.3047910000
H	-3.7128750000	-2.8796400000	3.2024120000
C	-4.6842080000	-2.9162450000	1.2795220000
H	-5.0034140000	-3.9598700000	1.3415110000
C	-4.6496150000	-0.8173750000	0.0201430000
H	-4.9305690000	-0.2705780000	-0.8834300000
H	-0.0090080000	-2.9899110000	7.0278760000
N	-5.7852620000	-2.8091700000	-0.9377960000
O	-6.0206950000	-2.1251730000	-1.9427890000
O	-6.1395300000	-3.9847260000	-0.7631140000
C	0.5895770000	1.0575620000	3.0217510000
H	1.5936980000	1.2026290000	2.5942210000
H	0.1906410000	2.0376140000	3.3279380000
H	0.6483990000	0.4150150000	3.9138580000
C	1.3087670000	-3.6067720000	0.1640830000
C	1.9868070000	-2.8780560000	1.1514480000
C	1.4531500000	-1.6770500000	1.6413430000
C	0.2294770000	-1.1816750000	1.1415820000
C	-0.4562150000	-1.9327650000	0.1553470000
C	0.0857720000	-3.1279930000	-0.3339950000
H	1.7290260000	-4.5429570000	-0.2150440000
H	2.9411520000	-3.2432320000	1.5427680000
H	2.0011090000	-1.1238770000	2.4091500000
H	-1.4154510000	-1.5742640000	-0.2354480000
H	-0.4519220000	-3.6913370000	-1.1024680000
C	-0.8605300000	3.4214250000	-1.6582640000
C	-1.4224730000	3.6830950000	-0.3978470000
C	-1.3185380000	2.7371220000	0.6301110000
C	-0.6365770000	1.5177940000	0.4138940000
C	-0.0776520000	1.2610670000	-0.8565520000
C	-0.1893310000	2.2108160000	-1.8817190000
H	-0.9475970000	4.1566010000	-2.4638070000
H	-1.9568420000	4.6202200000	-0.2154170000
H	-1.7722560000	2.9474830000	1.6055770000
H	0.4521210000	0.3228710000	-1.0428590000
H	0.2546890000	2.0008850000	-2.8610570000