Cooperativity between steric repulsion and crossed diene coordination governs the enantioselectivity in rhodium(I)/chiral, 1,4- and 1,5-diene-catalysed 1,4-addition reaction: A DFT study.

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SUPPORTING INFORMATION FILE

1. Computational details

All computations were executed on Gaussian 09 (AM64L-G09RevA.02)[1] and Gaussview 5.1W as GUI using default PBE0 functional and DGDZVP basis set. Optimizations were performed in gas phase followed by implicit solvent (1,4-dioxane) by IEFPCM treatment at 303.15K starting from structures built in Gaussview and, in certain cases, subjected to pre-optimization at HF/3-21G or PBE0/SDD. For the PBE0/DGDZVP optimizations, cutoff values for Maximum Force = 0.0001500, RMS Force = 0.0001000, Maximum Displacement = 0.001800, RMS Displacement = 0.001200 were employed. In all cases, the predicted change in energy was confirmed to be less than 1×10^{-6}. All stationary points were confirmed to reside in their respective PEHS minima by having only positive vibrational frequencies for intermediates or one negative frequency for transition states. Transition state search was performed by a two-stage relaxed PEHS scan of the key bonds broken or formed with crude step of 0.2 Å and fine step of 0.04 or 0,05 Å in the maximum region found by the crude search. The highest energy structure at the fine scan was further re-optimized with key transition state bonds frozen, followed by transition state optimization by the default Gaussian 09 algorhytm The chemical correctness of the transition states found was confirmed by visual inspection of the normal mode having the negative vibrational frequency followed by IRC. Atoms-In-Molecules (AIM) was performed by AIMAll software with default parameters on wavefunctions generated by Gaussian09.

2. Computational results

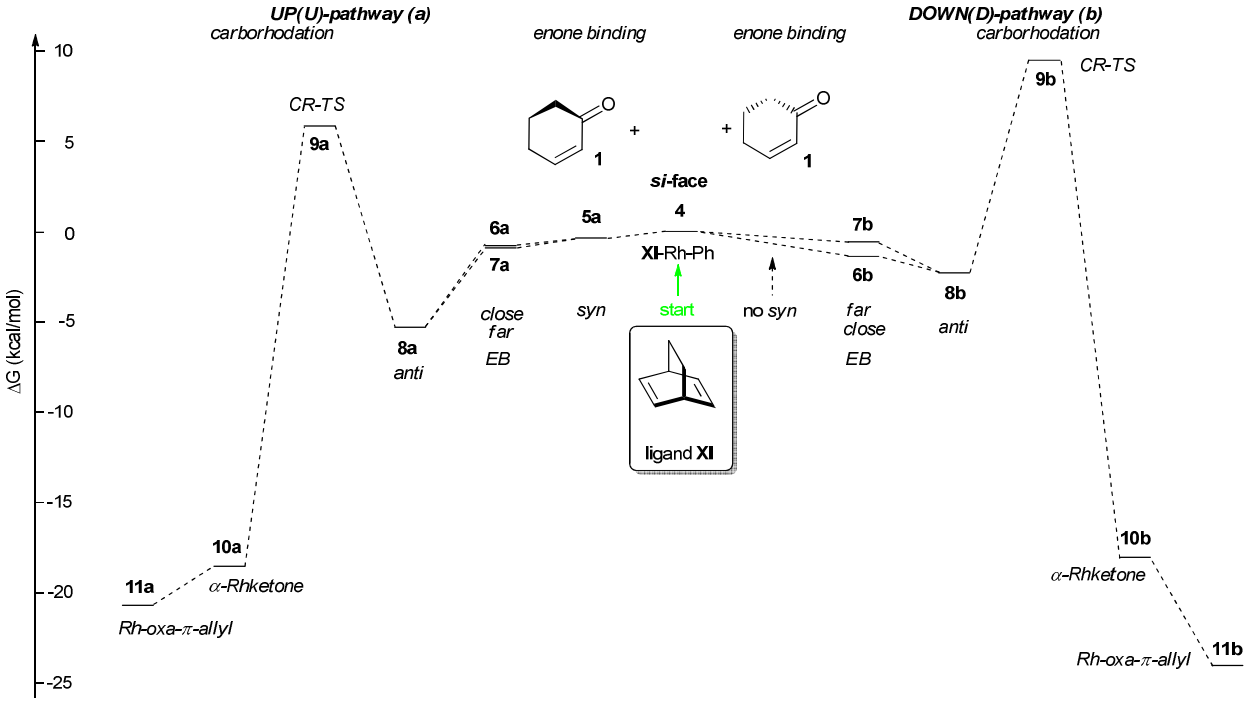
2.1. Gibbs energies summary (Table 1)

Table 1: Gibbs energies (ΔG) (kcal/mol) for the stationary points of the EB+CR steps in the enantioselective 1,4-addition mediated by Rh/chiral diene ligands (**I-X**). The corresponding achiral parent ligands (**XI-XIII**) are shown for comparison. Gibbs energies were computed at 303.15 K, in dioxane for ligands **I-IV** and **VII-XIV** and at 298.15 K, methanol for **V** and **VI**.

Ligand	Pathway	face	ΔG (kcal/mol)							
			Rh-Ph + CH	EB (*syn*)	EB (*close*)	EB (*far*)	EB (*anti*)	CR-TS	α-Rh ketone	Rh-oxa-π-allyl
XI	U	*si*	0.0 (**4**)	–0.4 (**5a**)	–1.3 (**6a**)	–1.4 (**7a**)	–5.3 (**8a**)	6.4 (**9a**)	–18.5 (**10a**)	–21.0 (**11a**)
	D	*si*	0.0 (**4**)	-	–1.3 (**6b**)	–0.6 (**7b**)	–2.6 (**8b**)	9.2 (**9b**)	–17.9 (**10b**)	–23.9 (**11b**)
I	U	*si*	0.0 (**12**)	-	2.0 (**13a**)	6.4 (**14a**)	–2.0 (**15a**)	8.6 (**16a**)	–15.9 (**17a**)	–18.0 (**18a**)
	D	*si*	0.0 (**12**)	-	–0.5 (**13b**)	0.0 (**14b**)	–0.3 (**15b**)	10.3 (**16b**)	–16.3 (**17b**)	–20.3 (**18b**)
	U	*re*	0.0 (**12**)	0.9 (**19a**)	–0.1 (**20a**)	–1.2 (**21a**)	–0.6 (**22a**)	11.7 (**23a**)	–13.2 (**24a**)	–20.4 (**25a**)
	D	*re*	0.0 (**12**)	-	–0.5 (**20b**)	–0.1 (**21b**)	1.6 (**22b**)	14.6 (**23b**)	–14.5 (**24b**)	–19.9 (**25b**)
XII	U	*si*	0.0 (**26**)	0.0 (**27a**)	–0.1 (**28a**)	0.9 (**29a**)	–3.6 (**30a**)	7.4 (**31a**)	–18.0 (**32a**)	–21.3 (**33a**)
	D	*si*	0.0 (**26**)	-	–0.3 (**28b**)	–0.9 (**29b**)	–1.6 (**30b**)	9.8 (**31b**)	–18.0 (**32b**)	–23.8 (**33b**)
II	U	*si*	0.0 (**34**)	-	4.6 (**35a**)	3.4 (**36a**)	–1.2 (**37a**)	8.9 (**38a**)	–16.1 (**39a**)	–18.2 (**40a**)
	D	*si*	0.0 (**34**)	-	4.3 (**35b**)	2.5 (**36b**)	1.4 (**37b**)	10.9 (**38b**)	–16.1 (**39b**)	–21.2 (**40b**)
	U	*re*	0.0 (**34**)	2.7 (**41a**)	1.5 (**42a**)	1.9 (**43a**)	0.5 (**44a**)	12.9 (**45a**)	–13.3 (**46a**)	–20.8 (**47a**)
	D	*re*	0.0 (**34**)	-	0.5 (**42b**)	2.5(**43b**)	3.0 (**44b**)	14.8 (**45b**)	–15.1 (**46b**)	–20.7 (**47b**)
III	U	*si*	0.0 (**48**)	-	0.1 (**50a**)	-	–2.6 (**52a**)	7.2 (**53a**)	–18.0 (**54a**)	–20.7 (**55a**)
	D	*si*	0.0 (**48**)	7.2 (**49b**)	–0.2 (**50b**)	–0.6 (**51b**)	–0.3 (**52b**)	9.6 (**53b**)	–17.6 (**54b**)	–24.0 (**55b**)
	U	*re*	0.0 (**48**)	1.7 (**56a**)	0.5 (**57a**)	1.4 (**58a**)	–1.2 (**59a**)	9.8 (**60a**)	–14.8 (**61a**)	–21.5 (**62a**)
	D	*re*	0.0 (**48**)	-	–0.3 (**57b**)	1.7 (**58b**)	1.6 (**59b**)	12.2 (**60b**)	–16.8 (**61b**)	–24.7 (**62b**)
IV	prox-U	*si*	0.0 (**63**)	-	0.2 (**65a**)	2.8 (**66a**)	–2.8 (**67a**)	7.5 (**68a**)	–14.5 (**69a**)	–19.2 (**70a**)
	prox-D	*si*	0.0 (**63**)	-	–0.1 (**65b**)	4.3 (**66b**)	0.2 (**67b**)	9.8 (**68b**)	–14.8 (**69b**)	–20.8 (**70b**)
	prox-U	*re*	0.0 (**63**)	1.7 (**71a**)	0.8 (**72a**)	1.1 (**73a**)	–0.3 (**74a**)	10.3 (**75a**)	–13.2 (**76a**)	–20.0 (**77a**)
	prox-D	*re*	0.0 (**63**)	-	–0.7 (**72b**)	3.2 (**73b**)	2.8 (**74b**)	12.8 (**75b**)	–13.7 (**76b**)	–19.8 (**77b**)
	dist-U	*si*	–0.5 (**64**)	-	–0.3 (**78a**)	8.4 (**79a**)	–0.2 (**80a**)	8.4 (**81a**)	–16.2 (**82a**)	–18.9 (**83a**)
	dist-D	*si*	–0.5 (**64**)	-	–0.3 (**78b**)	5.2 (**79b**)	2.1 (**80b**)	11.1 (**81b**)	–16.2 (**82b**)	–22.7 (**83b**)
	dist-U	*re*	–0.5 (**64**)	1.4 (**84a**)	0.4 (**85a**)	1.2 (**86a**)	0.2 (**87a**)	10.2 (**88a**)	–12.3 (**89a**)	–20.7 (**90a**)
	dist-D	*re*	–0.5 (**64**)	-	–0.5 (**85b**)	1.0 (**86b**)	3.2 (**87b**)	12.3 (**88b**)	–14.1 (**89b**)	–23.1 (**90b**)
XIII	U	*si*	0.0 (**91**)	–1.6 (**92a**)	–3.2 (**93a**)	–3.8 (**94a**)	–5.8 (**95a**)	5.5 (**96a**)	–18.4 (**97a**)	–20.7 (**98a**)
	D	*si*	0.0 (**91**)	-	–2.9 (**93b**)	–4.3 (**94b**)	–3.2 (**95b**)	8.3 (**96b**)	–18.7 (**97b**)	–23.8 (**98b**)
V	U	*si*	0.0 (**99**)	-	4.8 (**101a**)	6.0 (**102a**)	4.4 (**103a**)	14.0 (**104a**)	–11.2 (**105a**)	–12.9 (**106a**)
	D	*si*	0.0 (**99**)	8.9 (**100b**)	4.7 (**101b**)	5.2 (**102b**)	6.1 (**103b**)	16.2 (**104b**)	–11.4 (**105b**)	–17.3 (**106b**)
	U	*re*	0.0 (**99**)	4.7 (**107a**)	4.7 (**108a**)	5.7 (**109a**)	5.9 (**110a**)	17.9 (**111a**)	–7.7 (**112a**)	–14.6 (**113a**)
	D	*re*	0.0 (**99**)	6.5 (**107b**)	4.7 (**108b**)	6.1 (**109b**)	8.4 (**110b**)	20.4 (**111b**)	–9.2 (**112b**)	–15.4 (**113b**)
VI	prox-U	*si*	0.0 (**114**)	-	3.8 (**116a**)	2.0 (**117a**)	3.1 (**118a**)	11.5 (**119a**)	–14.1 (**120a**)	–12.9 (**121a**)
	prox-D	*si*	0.0 (**114**)	-	3.8 (**116b**)	2.6 (**117b**)	4.3 (**118b**)	13.8 (**119b**)	–13.9 (**120b**)	–17.3 (**121b**)
	prox-U	*re*	0.0 (**114**)	4.3 (**122a**)	4.0 (**123a**)	3.6 (**124a**)	1.6 (**125a**)	12.1 (**126a**)	–13.0 (**127a**)	–14.8 (**128a**)
	prox-D	*re*	0.0 (**114**)	5.9 (**122b**)	3.5 (**123b**)	4.1 (**124b**)	4.8 (**125b**)	15.3 (**126b**)	–12.9 (**127b**)	–16.8 (**128b**)
	dist-U	*si*	–1.3 (**115**)	-	2.4 (**129a**)	-	0.3 (**131a**)	10.4 (**132a**)	–13.9 (**133a**)	–18.0 (**134a**)
	dist-D	*si*	–1.3 (**115**)	-	2.0 (**129b**)	0.9 (**130b**)	2.8 (**131b**)	13.9 (**132b**)	–13.4 (**133b**)	–20.5 (**134b**)
	dist-U	*re*	–1.3 (**115**)	1.0 (**135a**)	1.3 (**136a**)	2.6 (**137a**)	2.1 (**138a**)	14.8 (**139a**)	–11.0 (**140a**)	–17.3 (**141a**)
	dist-D	*re*	–1.3 (**115**)	4.3 (**135b**)	1.1 (**136b**)	3.5 (**137b**)	5.5 (**138b**)	16.8 (**139b**)	–12.1 (**140b**)	–20.3 (**141b**)
XIV	U	*si*	0.0 (**142**)	5.1 (**143a**)	1.7 (**144a**)	3.0 (**145a**)	1.5 (**146a**)	9.4 (**147a**)	–15.2 (**148a**)	–20.3 (**149a**)
	D	*si*	0.0 (**142**)	-	1.6 (**144b**)	3.6 (**145b**)	4.1 (**146b**)	12.1 (**147b**)	–16.1 (**148b**)	–23.4 (**149b**)
VII	U	*si*	0.0 (**150**)	9.5 (**151a**)	5.7 (**152a**)	6.2 (**153a**)	6.0 (**154a**)	12.8 (**155a**)	–12.8 (**156a**)	–17.4 (**157a**)
	D	*si*	0.0 (**150**)	12.0 (**151b**)	4.7 (**152b**)	7.4 (**153b**)	7.6 (**154b**)	13.9 (**155b**)	–14.1 (**156b**)	–21.0 (**157b**)
	U	*re*	0.0 (**150**)	8.7 (**158a**)	5.8 (**159a**)	6.7 (**160a**)	6.5 (**161a**)	14.7 (**162a**)	–10.7 (**163a**)	–17.9 (**164a**)
	D	*re*	0.0 (**150**)	-	5.3 (**159b**)	6.2 (**160b**)	8.3 (**161b**)	17.1 (**162b**)	–12.5 (**163b**)	–22.6 (**164b**)
VIII	U	*si*	0.0 (**165**)	4.7 (**166a**)	3.4 (**167a**)	0.8 (**168a**)	–0.1 (**169a**)	9.2 (**170a**)	–14.7 (**171a**)	–20.4 (**172a**)
	D	*si*	0.0 (**165**)	5.9 (**166b**)	2.7 (**167b**)	1.6 (**168b**)	2.7 (**169b**)	11.7 (**170b**)	–16.0 (**171b**)	–23.7 (**172b**)
	U	*re*	0.0 (**165**)	-	0.8 (**174a**)	-	–1.4 (**176a**)	7.5 (**177a**)	–16.4 (**178a**)	–15.7 (**179a**)
	D	*re*	0.0 (**165**)	6.3 (**173b**)	0.8 (**174b**)	–0.3 (**175b**)	1.3 (**176b**)	9.9 (**177b**)	–15.4 (**178b**)	–18.9 (**179b**)
IX	U	*si*	0.0 (**180**)	-	5.7 (**182a**)	8.6 (**183a**)	6.2 (**184a**)	14.7 (**185a**)	–11.0 (**186a**)	–15.8 (**187a**)
	D	*si*	0.0 (**180**)	14.0 (**181b**)	5.2 (**182b**)	7.8 (**183b**)	8.7 (**184b**)	16.5 (**185b**)	–12.0 (**186b**)	–20.2 (**187b**)
	U	*re*	0.0 (**180**)	9.7 (**188a**)	6.2 (**189a**)	7.2 (**190a**)	8.2 (**191a**)	16.7 (**192a**)	–9.2 (**193a**)	–18.7 (**194a**)
	D	*re*	0.0 (**180**)	-	5.0 (**189b**)	6.9 (**190b**)	10.0 (**191b**)	18.3 (**192b**)	–11.3 (**193b**)	–19.1 (**194b**)
X	U	*si*	0.0 (**195**)	13.5 (**196a**)	8.1 (**197a**)	10.4 (**198a**)	8.8 (**199a**)	16.3 (**200a**)	–10.5 (**201a**)	–14.0 (**202a**)
	D	*si*	0.0 (**195**)	15.3 (**196b**)	7.6 (**197b**)	10.3 (**198b**)	10.0 (**199b**)	18.0 (**200b**)	–11.1 (**201b**)	–18.6 (**202b**)
	U	*re*	0.0 (**195**)	11.3 (**203a**)	9.1 (**204a**)	9.5 (**205a**)	9.5 (**206a**)	19.4 (**207a**)	–7.3 (**208a**)	–16.9 (**209a**)
	D	*re*	0.0 (**195**)	13.6 (**203b**)	8.3 (**204b**)	9.4 (**205b**)	11.3 (**206b**)	21.5 (**207b**)	–9.3 (**208b**)	–17.1 (**209b**)

2.2. Complete reaction profiles, thermodynamic quantities for stationary points therein and additional discussion thereof.

BOD-Rh pathway (Ligand XI) (kcal/mol, 303.15K, 1,4-dioxane)

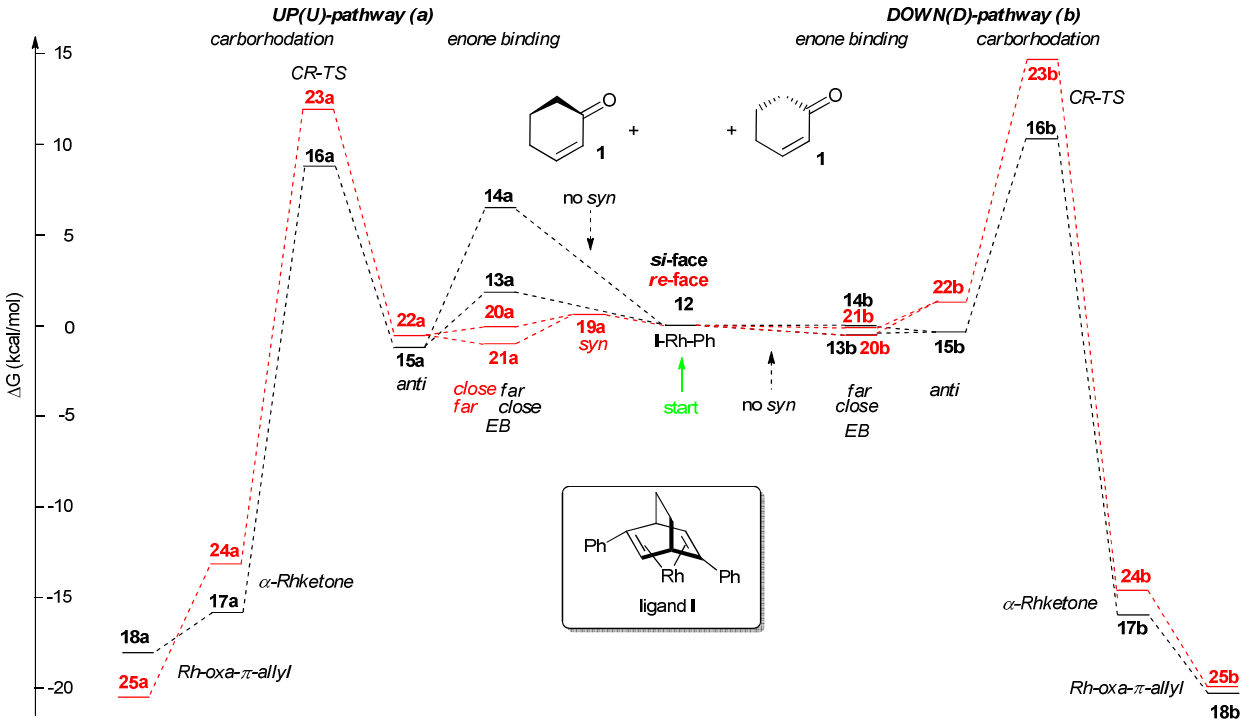


si-face

	4+1	5a	6a	7a	8a	9a	10a	11a	6b	7b	8b	9b	10b	11b
ΔG	0.0	–0.4	–1.3	–1.4	–5.3	6.4	–18.5	–21.0	–1.3	–0.6	–2.6	9.2	–17.9	–23.9
ΔH	0.0	–13.9	–14.6	–14.4	–18.6	–8.6	–33.6	–35.7	–14.6	–13.1	–15.9	-5.8	–32.8	–38.6
–TΔS	0.0	13.5	13.3	12.9	13.3	15.0	15.1	14.7	13.3	12.5	13.3	15.1	14.9	14.7

The calculated profile for 1,4-addition reaction with ligand **XI** (BOD) (**4**-**11**), shows that the starting Rh-Ph intermediate **4** is symmetrical with respect of the two halves of the BOD ligand as a consequence of Ph ring being perpendicular to the C=C bonds but unsymmetrical with respect to Rh-alkene coordination due to the strong trans-effect of the Ph group (Rh- C(diene) distances of 2.078 and 2.313Å for the proximal and distal C=C bonds, respectively). For both U- and D- pathways, 14 EB conformers were found, out 16 possible. For the D-pathway, no *syn*- conformer could be found. As expected for the achiral **4**, all structures resulting from attacks at *si*- and *re*-face of CH have the same energies (within ~0.03 kcal/mol), being enantiomers. Only structures for *si*-attack are presented here. In EB intermediates, C_α-Rh distance is 2.210-2.265 Å and C_β-Rh - 2.216-2.299 Å. In both pathways, *anti*- is the most stable EB orientation (**8a**, –5.3 kcal/mol for U- and **8b**, –2.6 kcal/mol for D-). Collapse of TSs **9** lead to α-rhodioketones **10** and then proceeds further to Rh-oxa-π-allyl (enolate) intermediates **11** via a conformational, low barrier twist of the cyclohexenone moiety to relieve the torsional strain of the nearly-eclipsing Ph and [(diene)Rh]. For structures **8**→**9**→**10**, C_1-C_β-C_α-Rh dihedral angle changes –19°→–18°→–35° in U-pathway (**a**) *vs.* –28°→–24°→–58° in D-pathway (**b**). The Rh-oxa-π-allyl intermediate (**11a**) produced by U-pathway are less-stable than the product of D-pathway (**11b**) (–21.0 *vs.* –29.3 kcal.mol).

(S)-PhBOD-Rh pathway (Ligand I) (kcal/mol, 303.15K, 1,4-dioxane)



si-face

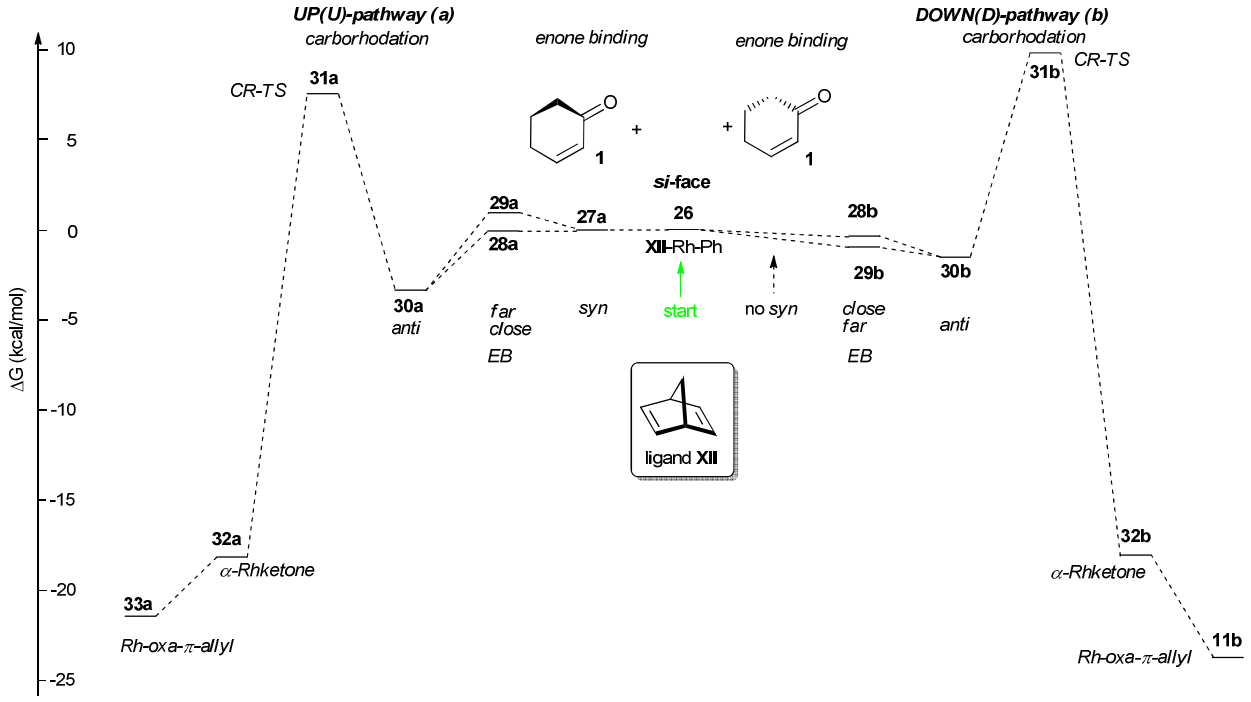
	12+1	13a	14a	15a	16a	17a	18a	13b	14b	15b	16b	17b	18b
ΔG	0.0	2.0	6.4	–2.0	8.6	–15.9	–18.0	–0.5	0.0	–0.3	10.3	–16.3	–20.3
ΔH	0.0	–11.9	–8.1	–16.8	–7.6	–30.7	–32.9	–14.9	–14.4	–14.3	–5.2	–31.2	–35.8
–TΔS	0.0	13.9	14.5	14.8	16.2	14.9	14.9	14.3	14.3	14.0	15.5	14.8	15.5

re-face

	12+1	19a	20a	21a	22a	23a	24a	25a	20b	21b	22b	23b	24b	25b
ΔG	0.0	0.9	–0.1	–1.2	–0.6	11.7	–13.2	–20.4	–0.5	–0.1	1.6	14.6	–14.5	–19.9
ΔH	0.0	–13.4	–14.2	–15.1	–15.2	–4.7	–29.8	–34.8	–14.8	–14.2	–12.6	–0.6	–31.2	–35.1
–TΔS	0.0	14.3	14.0	13.9	14.6	16.4	16.6	14.5	14.3	14.1	14.1	15.2	16.7	15.3

The calculated profile for 1,4-addition reaction with ligand **I** (PhBOD) (**12**-**25**), shows that the starting Rh-Ph intermediate **12** is unsymmetrical (10° deviation) with respect of the two halves of the ligand as well as unsymmetrical with respect to Rh-alkene coordination due to the strong trans-effect of the Ph group (Rh- C(Ph-diene) distances of 2.126 and 2.298Å for the proximal and distal C=C bonds, respectively). Total of 13 EB conformers were found, out of 16 possible. Only one *syn*-conformer was found, in the U/*re*-pathway. In EB intermediates, C_α-Rh distance is 2.210-2.287 Å and C_β-Rh - 2.226-2.321 Å. The most favorable EB intermediates occur in *anti* (**15a**; –2.0 kcal/mol), *close* (**14b**,–0.5 kcal/mol), *far* (**20a**, –1.2 kcal/mol) and *close* (**20b**, –0.5 kcal/mol) for U/*si*-, D/*si*-, U/*re*- and D/*re*-pathways, respectively. Collapse of TSs **16** and **23** leads to α-rhodioketones **17** and **24**, which then proceed further to Rh-oxa-π-allyl (enolate) intermediates **18** and **25**. For *si*-attack structures **16**→**17**→**18**, C_1-C_β-C_α-Rh dihedral angle change –16°→–12°→–86° in U-pathway (**a**) *vs.* –28°→–23°→–60° in D-pathway (**b**). For *re*-attack structures **23**→**24**→**25**, C_1-C_β-C_α-Rh dihedral angle change 13°→8°→1° in U-pathway (**a**) *vs.* 26°→18°→39° in D-pathway (**b**). The Rh-oxa-π-allyl intermediates (**18a** and **25a**) produced by U-pathways and D-pathways (**18b** and **25b**) show approximately equal stability (–18.0 and –20.4 *vs.* –20.3 and –19.9 kcal.mol).

NBD-Rh pathway (Ligand XII) (kcal/mol, 303.15K, 1,4-dioxane)

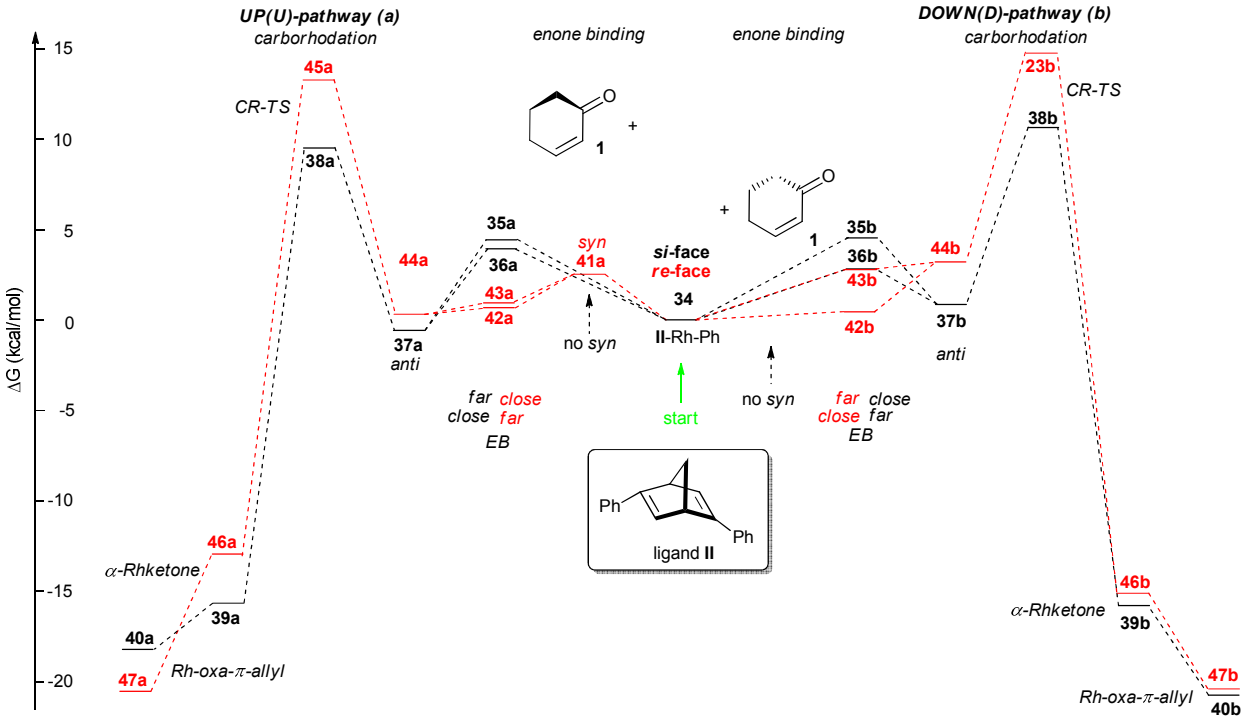


si-face

	26+1	27a	28a	29a	30a	31a	32a	33a	28b	29b	30b	31b	32b	33b
ΔG	0.0	0.0	–0.1	0.9	–3.6	7.4	–18.0	–21.3	–0.3	–0.9	–1.6	9.8	–18.0	–23.8
ΔH	0.0	–13.2	–13.1	–12.1	–17.3	–7.6	–33.1	–35.8	–13.2	–13.5	–14.6	-4.9	–32.6	–38.6
–TΔS	0.0	13.2	13.0	13.0	13.6	15.0	15.1	14.6	12.9	12.6	13.0	14.6	14.6	14.8

The calculated profile for 1,4-addition reaction with ligand **XII** (NBD) (**26-33**), shows that the starting Rh-Ph intermediate **26** is symmetrical with respect of the two halves of NBD ligand as a consequence of Ph ring being perpendicular to the C=C bonds but unsymmetrical with respect to Rh-alkene coordination due to the strong trans-effect of the Ph group (Rh- C(diene) distances of 2.076 and 2.285Å for the proximal and distal C=C bonds, respectively). Only structures for *si*-attack are presented here. For both U- and D- pathways, 7 EB conformers were found, out 8 possible. For the D-pathway, no *syn*- conformer could be found. In EB intermediates, C_α-Rh distance is 2.222-2.274 Å and C_β-Rh - 2.237-2.311 Å. In both pathways, *anti*- is the most stable EB orientation (**30a**, –3.6 kcal/mol for U- and **30b**, –1.6 kcal/mol for D-). Collapse of TSs **31** lead to α-rhodioketones **32** and then proceeds further to Rh-oxa-π-allyl (enolate) intermediates **33** via a conformational, low barrier twist of the cyclohexenone moiety to relieve the torsional strain of the nearly-eclipsing Ph and [(diene)Rh]. For structures **31→32→33**, C_1-C_β-C_α-Rh dihedral angle changes –19°→–18°→–33° in U-pathway (**a**) *vs.* –27°→–24°→–56° in D-pathway (**b**). The Rh-oxa-π-allyl intermediate (**33a**) produced by U-pathway is less-stable than the product of D-pathway (**11b**) (–21.3 *vs.* –23.8 kcal.mol).

(S)-PhNBD-Rh pathway (Ligand II) (303.15K, 1,4-dioxane)



si-face

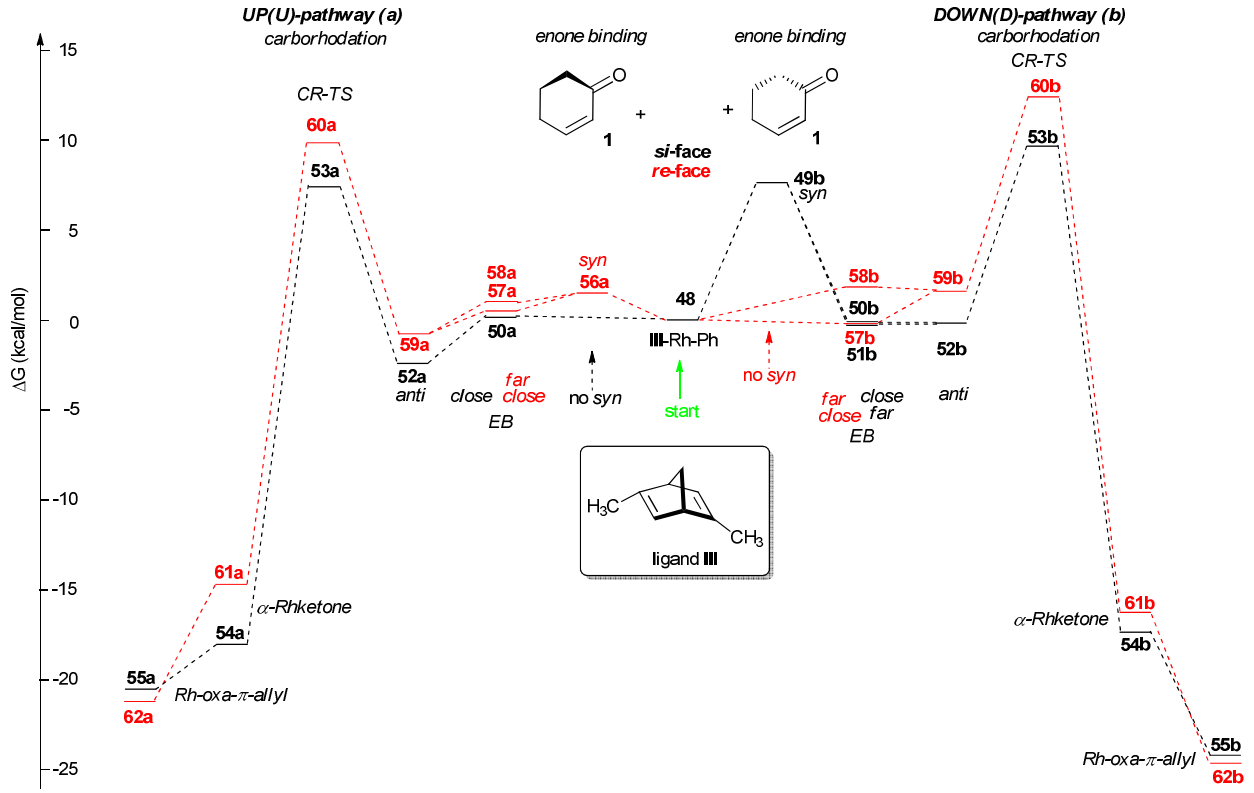
	34+1	35a	36a	37a	38a	39a	40a	35b	36b	37b	38b	39b	40b
ΔG	0.0	4.6	3.4	–1.2	8.9	–16.1	–18.2	4.3	2.5	1.4	10.9	–16.1	–21.2
ΔH	0.0	–10.8	–10.6	–16.2	–7.7	–32.6	–33.7	–10.9	–12.5	–13.6	–5.2	–31.7	–36.9
–TΔS	0.0	15.4	13.9	15.0	16.5	16.5	15.5	15.2	15.0	15.0	16.1	15.6	15.7

re-face

	34+1	41a	42a	43a	44a	45a	46a	47a	42b	43b	44b	45b	46b	47b
ΔG	0.0	2.7	1.5	1.9	0.5	12.9	–13.3	–20.8	0.5	2.5	3.0	14.8	–15.1	–20.7
ΔH	0.0	–12.2	–12.8	–12.6	–14.7	–4.4	–29.7	–36.1	–13.4	–11.9	–12.1	-2.0	–31.1	–36.4
–TΔS	0.0	14.9	14.3	14.6	15.2	17.3	16.4	15.3	14.0	14.4	15.2	16.8	16.0	15.7

The calculated profile for 1,4-addition reaction with ligand **II** (PhNBD) (**34**-**47**), shows that the starting Rh-Ph intermediate **34** is unsymmetrical (72° deviation) with respect of the two halves of the ligand as well as unsymmetrical with respect to Rh-alkene coordination due to the strong trans-effect of the Ph group (Rh- C(Ph-diene) distances of 2.123 and 2.259Å for the proximal and distal C=C bonds, respectively). Total of 13 EB conformers were found, out of 16 possible. Only one *syn*-conformer was found, in the U/*re*-pathway. In EB intermediates, C_α-Rh distance is 2.251-2.302 Å and C_β-Rh - 2.259-2.360 Å. The most favorable EB intermediates occur in *anti* (**37a**; –1.2 kcal/mol), *anti* (**37b**, 1.4 kcal/mol), *anti* (**44a**, 0.5 kcal/mol) and *close* (**42b**, 0.5 kcal/mol) for U/*si*-, D/*si*-, U/*re*- and D/*re*-pathways, respectively. Collapse of TSs **38** and **45** leads to α-rhodioketones **39** and **46**, which then proceed further to Rh-oxa-π-allyl (enolate) intermediates **40** and **47**. For *si*-attack structures **38**→**39**→**40**, C_1-C_β-C_α-Rh dihedral angle change –17°→–19°→–84° in U-pathway (**a**) *vs.* –27°→–30°→–61° in D-pathway (**b**). For *re*-attack structures **45**→**46**→**47**, C_1-C_β-C_α-Rh dihedral angle change 12°→13°→3° in U-pathway (**a**) *vs.* 23°→21°→38° in D-pathway (**b**). The Rh-oxa-π-allyl intermediates (**40a** and **47a**) produced by U-pathways are on average less-stable than the product of D-pathways (**40b** and **47b**) (–18.2 and –20.8 *vs.* –21.2 and –20.7 kcal.mol).

(S)-MeNBD-Rh pathway (Ligand III) (kcal/mol, 303.15K, 1,4-dioxane)



si-face

	48+1	50a	52a	53a	54a	55a	49b	50b	51b	52b	53b	54b	55b
ΔG	0.0	0.1	–2.6	7.2	–18.0	–20.7	7.2	–0.2	–0.6	–0.3	9.6	–17.6	–24.0
ΔH	0.0	–13.3	–16.7	–8.2	–33.3	–35.5	–6.3	–13.4	–14.0	–14.2	–5.6	–32.4	–38.6
–TΔS	0.0	13.3	14.1	15.4	15.3	14.8	13.6	13.2	13.6	13.9	15.2	14.8	14.6

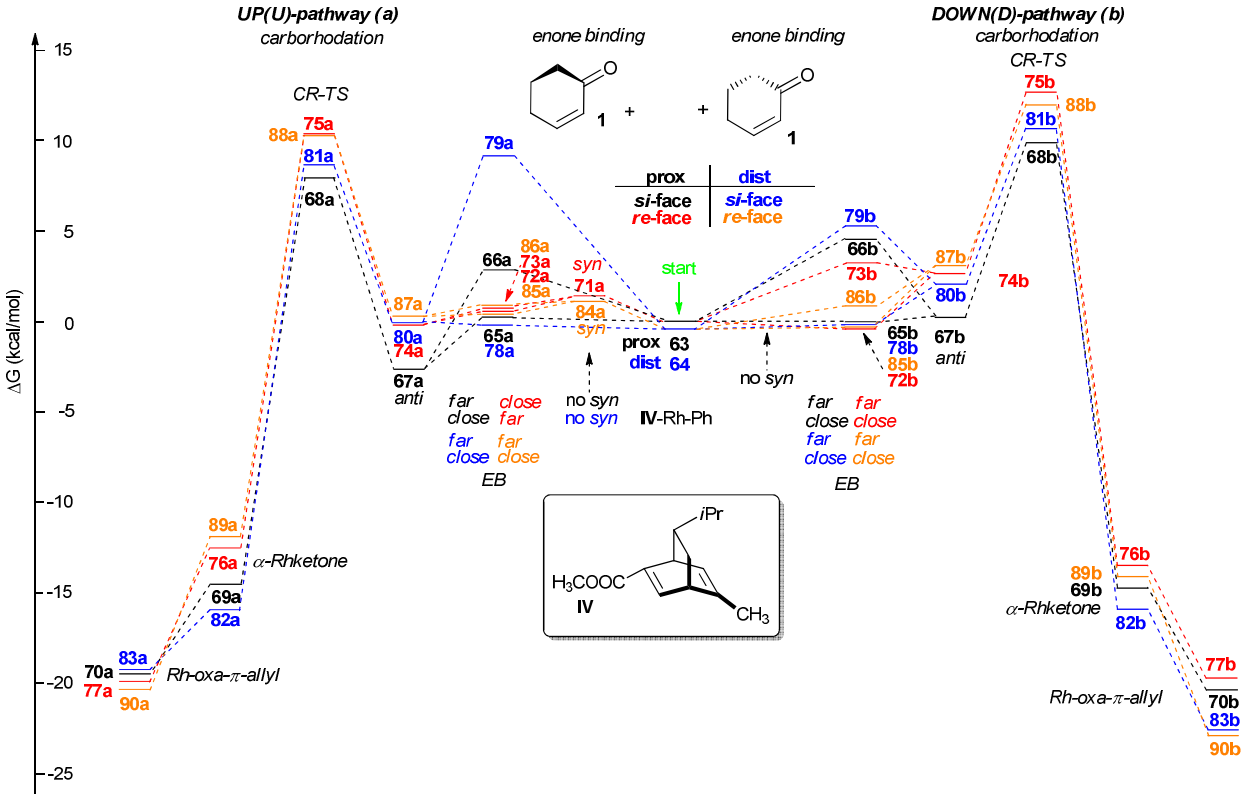
re-face

	48+1	56a	57a	58a	59a	60a	61a	62a	57b	58b	59b	60b	61b	62b
ΔG	0.0	1.7	0.5	1.4	–1.2	9.8	–14.8	–21.5	–0.3	1.7	1.6	12.2	–16.8	–24.7
ΔH	0.0	–12.1	–12.8	–12.8	–15.1	–5.5	–29.9	–36.5	–13.6	–11.3	–12.1	–3.0	–30.9	–39.3
–TΔS	0.0	13.8	13.3	13.3	13.9	15.3	15.1	15.0	13.3	13.0	13.7	15.2	14.1	14.5

The calculated profile for 1,4-addition reaction with ligand **III** (MeNBD) (**48-62**), shows that the starting Rh-Ph intermediate **48** is unsymmetrical (23° deviation) with respect of the two halves of the ligand as well as unsymmetrical with respect to Rh-alkene coordination due to the strong trans-effect of the Ph group (Rh- C(Me-diene) distances of 2.096 and 2.270Å for the proximal and distal C=C bonds, respectively). Total of 13 EB conformers were found, out of 16 possible. Two *syn*-conformers were found, in the D/*si*- and U/*re*-pathways; U/*si*-pathway far intermediate was not found. In EB intermediates, C_α-Rh distance is 2.232-2.314 Å and C_β-Rh - 2.243-2.322 Å. The most favorable EB intermediates occur in *anti* (**52a**; –2.6 kcal/mol), *far* (**51b**, 1.4 kcal/mol), *anti* (**59a**, –1.2 kcal/mol) and *close* (**57b**, –0.3 kcal/mol) for U/*si*-, D/*si*-, U/*re*- and D/*re*-pathways, respectively. Collapse of TSs **53** and **60** leads to α-rhodioketones **54** and **61**, which then proceed further to Rh-oxa-π-allyl (enolate) intermediates **55** and **62**. For *si*-attack structures **53**→**54**→**55**, C_1-C_β-C_α-Rh dihedral angle change –18°→–21°→–27° in U-pathway (**a**) *vs.* –28°→–32°→–56° in D-pathway (**b**). For *re*-attack structures **60**→**61**→**62**, C_1-C_β-C_α-Rh dihedral angle change 14°→14°→37° in U-pathway (**a**) *vs.* 24°→22°→59° in D-pathway (**b**). The Rh-oxa-π-allyl

intermediates (**40a** and **47a**) produced by U-pathways are considerably less-stable than the product of D-pathways (**40b** and **47b**) (–18.0 and –21.5 *vs.* –24.0 and –24.7 kcal.mol).

(S)- Ligand IV-Rh pathway (kcal/mol, 303.15K, 1,4-dioxane)



Prox-si-face

	63+1	65a	66a	67a	68a	69a	70a	65b	66b	67b	68b	69b	70b
ΔG	0.0	0.2	2.8	–2.8	7.5	–14.5	–19.2	–0.1	4.3	0.2	9.8	–14.8	–20.8
ΔH	0.0	–13.7	–11.0	–16.9	–8.3	–30.4	–34.3	–13.8	–9.5	–14.1	–5.7	–29.9	–36.5
–TΔS	0.0	14.0	13.8	14.1	15.8	15.9	15.1	13.7	13.8	14.3	15.6	15.1	15.7

Prox-re-face

	63+1	71a	72a	73a	74a	75a	76a	77a	72b	73b	74b	75b	76b	77b
ΔG	0.0	1.7	0.8	1.1	–0.3	10.3	–13.2	–20.0	–0.7	3.2	2.8	12.8	–13.7	–19.8
ΔH	0.0	–13.0	–13.1	–11.3	–14.8	–5.7	–28.0	–35.2	–13.8	–10.5	–11.6	–3.1	–29.1	–34.8
–TΔS	0.0	14.7	13.9	12.4	14.5	16.0	14.8	15.2	13.1	13.6	14.3	15.9	15.4	14.9

Dist-si-face

	64+1	78a	79a	80a	81a	82a	83a	78b	79b	80b	81b	82b	83b
ΔG	–0.5	–0.3	8.4	–0.2	8.4	–16.2	–18.9	–0.3	5.2	2.1	11.1	–16.2	–22.7
ΔH	–0.2	–13.9	–5.7	–14.3	–6.9	–32.4	–33.9	–14.0	–8.2	–11.5	–4.1	–31.9	–37.5
–TΔS	–0.3	13.6	14.0	14.1	15.3	16.1	15.0	13.7	13.3	13.6	15.2	15.7	14.9

Dist-re-face

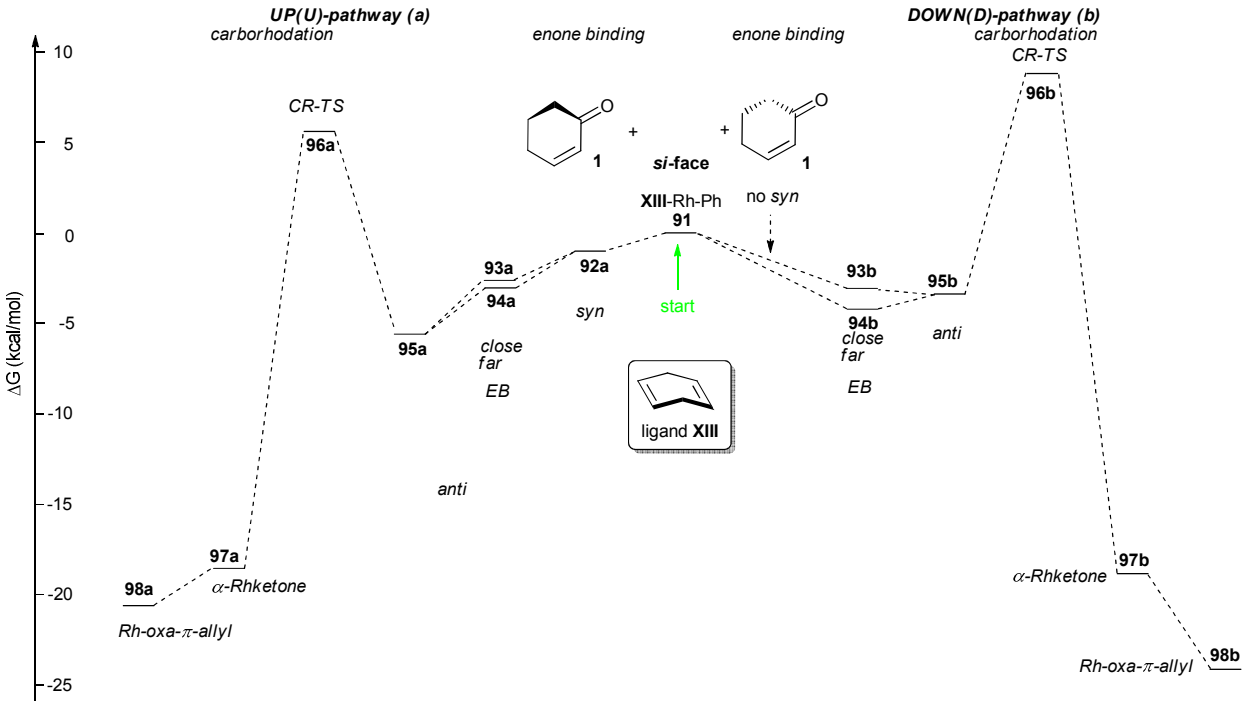
	64+1	84a	85a	86a	87a	88a	89a	90a	85b	86b	87b	88b	89b	90b
ΔG	–0.5	1.4	0.4	1.2	0.2	10.2	–12.3	–20.7	–0.5	1.0	3.2	12.3	–14.1	–23.1
□H	–0.2	–12.6	–13.7	–12.1	–13.3	–5.9	–27.1	–35.8	–14.1	–12.3	–10.1	–3.3	–28.2	–38.4
–TΔS	–0.3	13.9	14.1	13.4	13.5	16.2	14.8	15.1	13.6	13.3	13.3	15.6	14.1	15.3

The calculated profile for 1,4-addition reaction with ligand **IV** (**63**-**90**) comprises of two sections due to the C_1-symmetry leading to the appearance of two Rh-Ph intermediates, one having Ph(Rh) oriented towards the methyl ester substituent of the ligand (proximal; **63**) and the other oriented towards the methyl substituent on the ligand (distal, **64**). Structure **64** is 0.5 kcal/mol more stable than **63**, (the standard). Both Rh-Ph intermediates are unsymmetrical (82° deviation for **63** and 58° for **64**) with respect of the two halves of the ligand as well as unsymmetrical with respect to Rh-alkene coordination due to the strong trans-effect of the Ph group (Rh- C(Me-diene) distances of 2.355 Å for **63** and 2.121 Å for **64**; Rh- C(COOMe-diene) distances of 2.093 Å for **63** and 2.270 Å for **64**, respectively).

*1. Pathway commencing with **63***.Total of 13 EB conformers were found, out of 16 possible. Only one *syn*-conformer was found, in the U/*re*-pathway. In EB intermediates, C_α-Rh distance is 2.221-2.289 Å and C_β-Rh - 2.222-2.337 Å. The most favorable EB intermediates occur in *anti* (**67a**; –2.8 kcal/mol), *close* (**65b**, –0.1 kcal/mol), *anti* (**74a**, –0.3 kcal/mol) and *close* (**72b**, –0.7 kcal/mol) for U/*si*-, D/*si*-, U/*re*- and D/*re*-pathways, respectively. Collapse of TSs **68** and **75** leads to α-rhodioketones **69** and **76**, which then proceed further to Rh-oxa-π-allyl (enolate) intermediates **70** and **77**. For *si*-attack structures **68→69→70**, C_1-C_β-C_α-Rh dihedral angle change –19°→–20°→–88° in U-pathway (**a**) *vs.* –29°→–30°→–71° in D-pathway (**b**). For *re*-attack structures **75→76→77**, C_1-C_β-C_α-Rh dihedral angle change 14°→8°→1° in U-pathway (**a**) *vs.* 22°→20°→40° in D-pathway (**b**). The Rh-oxa-π-allyl intermediates (**70a** and **77a**) produced by U-pathways are less-stable than the product of D-pathways (**70b** and **77b**) (–19.2 and –13.2 *vs.* –20.8 and –19.8 kcal.mol).

*2. Pathway commencing with **64***.Total of 13 EB conformers were found, out of 16 possible. Only one *syn*-conformer was found, in the U/*re*-pathway. In EB intermediates, C_α-Rh distance is 2.206-2.289 Å and C_β-Rh - 2.230-2.386 Å. The most favorable EB intermediates occur in *close* (**78a**; –0.3 kcal/mol), *close* (**78b**, –0.3 kcal/mol), *anti* (**87a**, 0.2 kcal/mol) and *close* (**85b**, –0.5 kcal/mol) for U/*si*-, D/*si*-, U/*re*- and D/*re*-pathways, respectively. Collapse of TSs **81** and **88** leads to α-rhodioketones **82** and **89**, which then proceed further to Rh-oxa-π-allyl (enolate) intermediates **83** and **90**. For *si*-attack structures **81→82→83**, C_1-C_β-C_α-Rh dihedral angle change –18°→–20°→–83° in U-pathway (**a**) *vs.* –29°→–31°→–55° in D-pathway (**b**). For *re*-attack structures **88→89→90**, C_1-C_β-C_α-Rh dihedral angle change 17°→11°→4° in U-pathway (**a**) *vs.* 27°→23°→63° in D-pathway (**b**). The Rh-oxa-π-allyl intermediates (**83a** and **90a**) produced by U-pathways are less-stable than the product of D-pathways (**83b** and **90b**) (–18.9 and –20.7 *vs.* –22.7 and –23.1 kcal.mol).

CHD-Rh pathway (Ligand XIII) (kcal/mol, 303.15K, 1,4-dioxane)

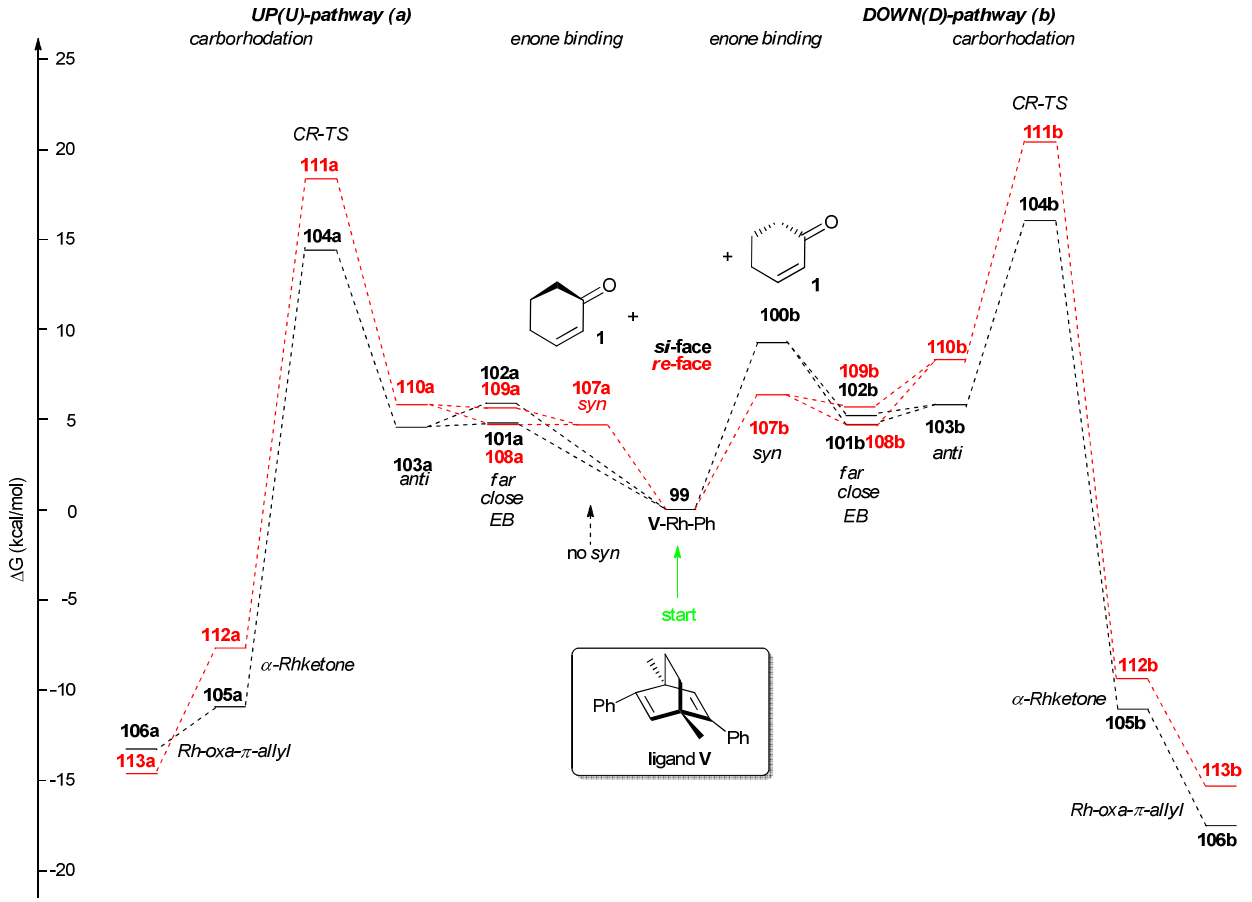


si-face

	91+1	**92a**	**93a**	**94a**	**95a**	**96a**	**97a**	**98a**	**93b**	**94b**	**95b**	**96b**	**97b**	**98b**
ΔG	0.0	–1.6	–3.2	–3.8	–5.8	5.5	–18.4	–20.7	–2.9	–4.3	–3.2	8.3	–18.7	–23.8
ΔH	0.0	–15.5	–16.7	–17.2	–20.2	–10.2	–34.6	–36.6	–16.8	–17.7	–17.4	–7.4	–34.1	–39.6
–TΔS	0.0	13.9	13.5	13.4	14.4	15.7	16.3	15.8	13.9	13.4	14.2	15.7	15.4	15.8

The calculated profile for 1,4-addition reaction with ligand **XIII** (CHD) (**91**-**98**), shows that the starting Rh-Ph intermediate **91** is symmetrical with respect of the two halves of CHD ligand as a consequence of Ph ring being coplanar to the C=C bonds but unsymmetrical with respect to Rh-alkene coordination due to the strong trans-effect of the Ph group (Rh- C(diene) distances of 2.094 and 2.373Å for the proximal and distal C=C bonds, respectively). Only structures for *si*-attack are presented here. For both U- and D- pathways, 7 EB conformers were found, out 8 possible. For the D-pathway, no *syn*- conformer could be found. In EB intermediates, C_α-Rh distance is 2.192-2.265 Å and C_β-Rh - 2.221-2.294 Å. The most favorable EB intermediates occur in *anti* (**95a**; –0.3 kcal/mol) and *far* (**94b**, –0.3 kcal/mol) for U- and D-pathways, respectively. Collapse of TSs **96** lead to α-rhodioketones **97**, which then proceeds further to Rh-oxa-π-allyl (enolate) intermediates **98** via a conformational, low barrier twist of the cyclohexenone moiety to relieve the torsional strain of the nearly-eclipsing Ph and [(diene)Rh]. For structures **96→97→98**, C_1-C_β-C_α-Rh dihedral angle changes –18°→–18°→–36° in U-pathway (**a**) *vs.* –27°→–24°→–58° in D-pathway (**b**). The Rh-oxa-π-allyl intermediate (**98a**) produced by U-pathway is considerably less-stable than the product of D-pathway (**98b**) (–18.4 *vs.* –23.8 kcal.mol).

(S)-Ligand V (Ph-substituted Carnell ligand)-Rh pathway (kcal/mol, 298.15K, methanol)



si-face

	99+1	101a	102a	103a	104a	105a	106a	100b	101b	102b	103b	104b	105b	106b
ΔG	0.0	4.8	6.0	4.4	14.0	–11.2	–12.9	8.9	4.7	5.2	6.1	16.2	–11.4	–17.3
ΔH	0.0	–9.4	–7.8	–9.9	–1.8	–25.9	–27.7	–5.0	–9.6	–8.7	–7.9	0.4	–26.1	–32.0
–TΔS	0.0	14.2	13.8	14.3	15.8	14.8	14.8	13.9	14.3	14.0	13.9	15.8	14.7	14.7

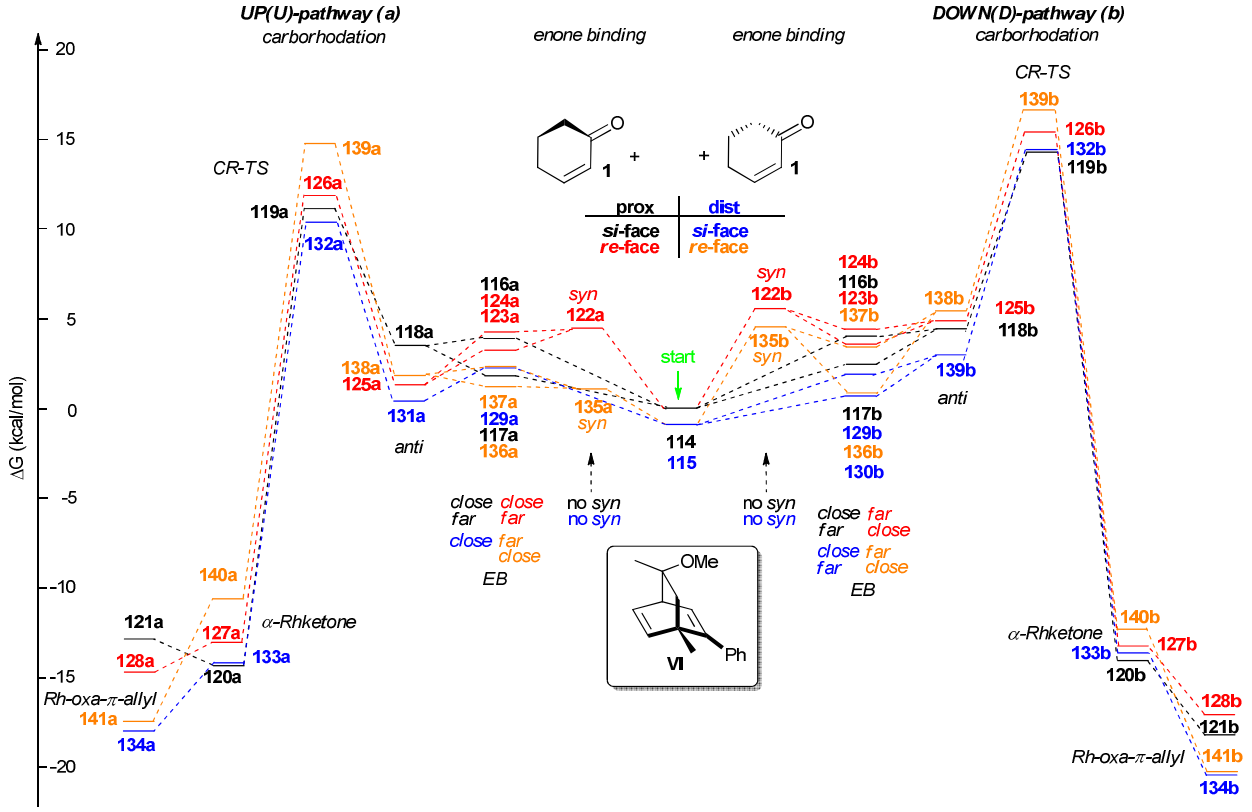
re-face

	99+1	107a	108a	109a	110a	111a	112a	113a	107b	108b	109b	110b	111b	112b	113b
ΔG	0.0	4.7	4.7	5.7	5.9	17.9	–7.7	–14.6	6.5	4.7	6.1	8.4	20.4	–9.2	–15.4
ΔH	0.0	–9.5	–9.3	–8.6	–8.4	2.3	–23.4	–30.0	–7.4	–9.8	–8.3	–5.9	4.9	–24.9	–30.8
–TΔS	0.0	14.2	14.0	14.3	14.3	15.4	15.8	15.4	14.0	14.5	14.3	14.3	15.4	15.7	15.4

The calculated profile for 1,4-addition reaction with ligand **V** (**99**-**113**), shows that the starting Rh-Ph intermediate **99** is slightly unsymmetrical (5° deviation) with respect of the two halves of the ligand as well as unsymmetrical with respect to Rh-alkene coordination due to the strong trans-effect of the Ph group (Rh- C(Ph-diene) distances of 2.107 and 2.295Å for the proximal and distal C=C bonds, respectively). Total of 15 EB conformers were found, out of 16 possible. Only one *syn*-conformer was not found, in the U/*si*-pathway. In EB intermediates, C_α-Rh distance is 2.225-2.345 Å and C_β-Rh - 2.232-2.328 Å. The most favorable EB intermediates occur in *anti* (**103a**; 4.4 kcal/mol), *close* (**101b**, 4.7 kcal/mol), *syn* and *close* (**107a** and **108a**, 4.7 kcal/mol) and *close* (**108b**, 4.7 kcal/mol) for U/*si*-, D/*si*-, U/*re*- and D/*re*-pathways, respectively. Collapse of TSs **104** and **111** leads to α-rhodioketones **105** and **112**, which then proceed further to Rh-oxa-π-allyl (enolate) intermediates **106** and **113**. For *si*-attack structures **104**→**105**→**106**, C_1-C_β-C_α-Rh dihedral angle change –19°→–22°→–35° in U-pathway (**a**) *vs.* –28°→–31°→–59° in

D-pathway (**b**). For *re*-attack structures **111**→**112**→**113**, C_1-C_β-C_α-Rh dihedral angle change 3°→3°→6° in U-pathway (**a**) *vs.* 5°→16°→42° in D-pathway (**b**). The Rh-oxa-π-allyl intermediates (**106a** and **113a**) produced by U-pathways less-stable than the product of D-pathways (**106b** and **113b**) (–12.9 and –14.6 *vs.* –17.3 and –15.4 kcal.mol).

(5R,8S)- Ligand VI (Ph-substituted Darses ligand)-Rh pathway (kcal/mol, 298.15K, methanol)



Prox-si-face

	114+1	116a	117a	118a	119a	120a	121a	116b	117b	118b	119b	120b	121b
ΔG	0.0	3.8	2.0	3.1	11.5	–14.1	–12.9	3.8	2.6	4.3	13.8	–13.9	–17.3
ΔH	0.0	–9.5	–11.6	–12.3	–3.2	–28.8	–27.9	–9.6	–10.0	–9.1	–0.6	–28.3	–32.2
–TΔS	0.0	13.3	13.6	15.3	14.7	14.7	14.9	13.5	12.6	13.4	14.5	14.4	14.9

Prox-re-face

	114+1	122a	123a	124a	125a	126a	127a	128a	122b	123b	124b	125b	126b	127b	128b
ΔG	0.0	4.3	4.0	3.6	1.6	12.1	–13.0	–14.8	5.9	3.5	4.1	4.8	15.3	–12.9	–16.8
ΔH	0.0	–9.5	–9.3	–9.3	–11.3	–2.3	–27.9	–30.1	–7.7	–9.8	–8.9	–8.6	0.3	–27.5	–31.4
–TΔS	0.0	13.9	13.2	12.9	12.9	14.4	14.9	15.3	13.6	13.3	13.0	13.4	14.9	14.6	14.6

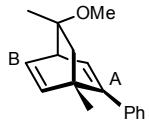
Dist-si-face

	115+1	129a	131a	132a	133a	134a	129b	130b	131b	132b	133b	134b
ΔG	–1.3	2.4	0.3	10.4	–13.9	–18.0	2.0	0.9	2.8	13.9	–13.4	–20.5
ΔH	–1.1	–11.1	–13.1	–4.3	–28.7	–32.0	–11.5	–11.7	–10.3	–1.3	–27.3	–34.8
–TΔS	–0.1	13.5	13.4	14.7	14.8	14.0	13.5	12.5	13.1	15.2	13.9	14.3

Dist-re-face

	115+1	135a	136a	137a	138a	139a	140a	141a	135b	136b	137b	138b	139b	140b	141b
ΔG	–1.3	1.0	1.3	2.6	2.1	14.8	–11.0	–17.3	4.3	1.1	3.5	5.5	16.8	–12.1	–20.3
ΔH	–1.1	–12.1	–11.7	–10.7	–10.5	–0.8	–25.9	–31.6	–9.1	–11.9	–9.7	–7.9	2.0	–26.5	–34.5
–TΔS	–0.1	13.1	13.0	13.3	12.7	15.6	14.8	14.3	13.4	13.0	13.2	13.4	14.8	14.4	14.3

The calculated profile for 1,4-addition reaction with ligand **VI** (**114**-**141**) comprises of two sections due to the C_1-symmetry leading to the appearance of two Rh-Ph intermediates, one having Ph(Rh) oriented towards the phenyl substituent of the ligand (proximal; **114**) and the other oriented towards the unsubstittued double bond (distal, **115**).

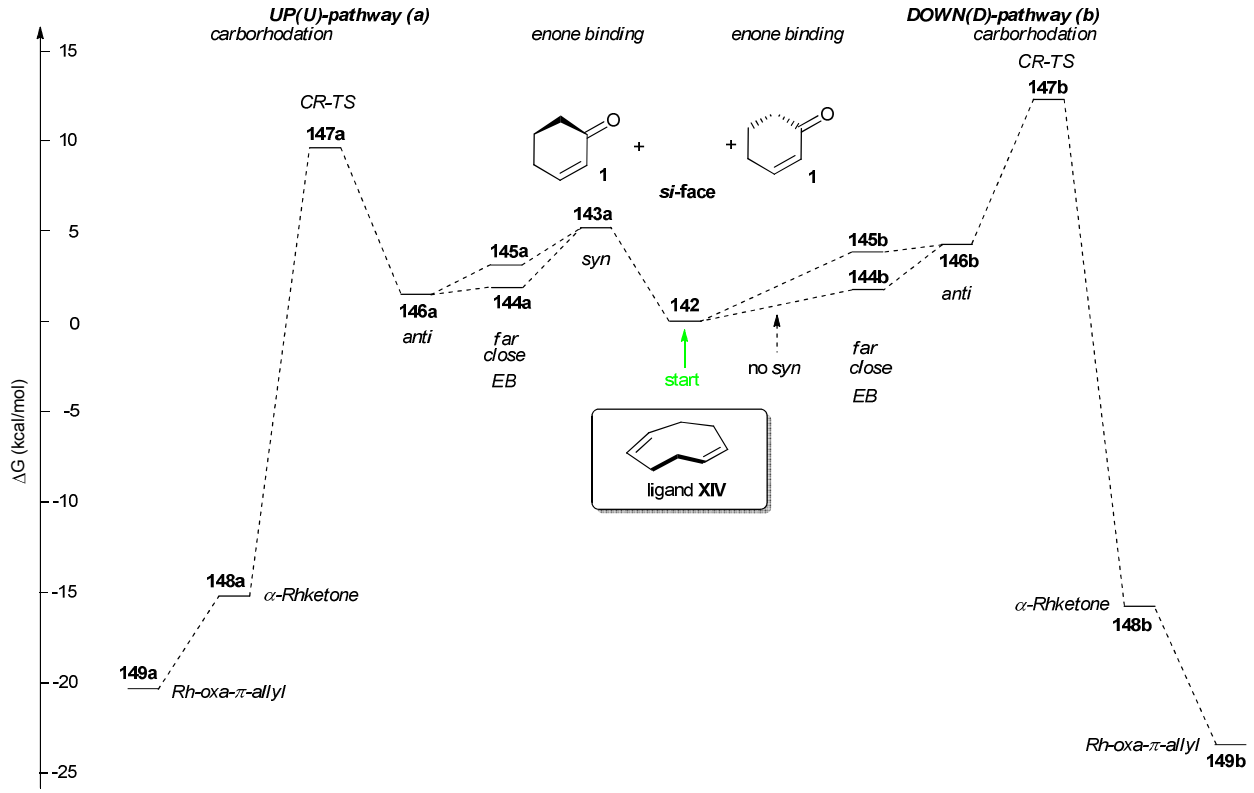


Structure **114** is 1.3 kcal/mol more stable than **115** (the standard). The Rh-Ph intermediates are almost symmetrical (4° deviation for **114** and 1° for **115**) with respect of the two halves of the ligand. They are unsymmetrical with respect to Rh-alkene coordination due to the strong trans-effect of the Ph group. Rh-C(A) distances are 2.106 Å for **114** and 2.309 Å for **115**; Rh- C(B) distances are 2.082 Å for **114** and 2.309 Å for **115**, respectively).

*1. Pathway commencing with **114***.Total of 14 EB conformers were found, out of 16 possible. Only two *syn*-conformers were found, in the U/*re*- and D/*re*-pathways. In EB intermediates, C_α-Rh distance is 2.208-2.291 Å and C_β-Rh - 2.221-2.316 Å. The most favorable EB intermediates occur in *far* (**117a**; 2.0 kcal/mol), *far* (**117b**, 2.6 kcal/mol), *anti* (**125a**, 1.6 kcal/mol) and *far* (**124b**, –0.7 kcal/mol) for U/*si*-, D/*si*-, U/*re*- and D/*re*-pathways, respectively. Collapse of TSs **119** and **126** leads to α-rhodioketones **120** and **127**, which then proceed further to Rh-oxa-π-allyl (enolate) intermediates **121** and **128**. For *si*-attack structures **119→120→121**, C_1-C_β-C_α-Rh dihedral angle change –22°→–20°→–36° in U-pathway (**a**) *vs.* –29°→–29°→–60° in D-pathway (**b**). For *re*-attack structures **126→127→128**, C_1-C_β-C_α-Rh dihedral angle change 19°→10°→7° in U-pathway (**a**) *vs.* 28°→22°→60° in D-pathway (**b**). The Rh-oxa-π-allyl intermediates (**121a** and **128a**) produced by U-pathways are considerably less-stable than the product of D-pathways (**121b** and **128b**) (–12.9 and –14.8 *vs.* –17.3 and –16.8 kcal.mol). The Rh-oxa-π-allyl intermediate **121a** is also less stable than the corresponding α-rhodioketone (**120a**, –14.1 kcal/mol).

*2. Pathway commencing with **115***. Total of 13 EB conformers were found, out of 16 possible. Only two *syn*-conformers were found, in the U/*re*- and D/*re*-pathways. In addition, there is no *far* conformation in U/*si*-pathway. In EB intermediates, C_α-Rh distance is 2.224-2.301 Å and C_β-Rh - 2.222-2.338 Å. The most favorable EB intermediates occur in *close* (**131a**; 0.3 kcal/mol), *far* (**131b**, 0.9 kcal/mol), *syn* (**135a**, 1.0 kcal/mol) and *close* (**136b**, 1.1 kcal/mol) for U/*si*-, D/*si*-, U/*re*- and D/*re*-pathways, respectively. Collapse of TSs **132** and **139** leads to α-rhodioketones **133** and **140**, which then proceed further to Rh-oxa-π-allyl (enolate) intermediates **134** and **141**. For *si*-attack structures **132→133→134**, C_1-C_β-C_α-Rh dihedral angle change –21°→–19°→–37° in U-pathway (**a**) *vs.* –29°→–28°→–59° in D-pathway (**b**). For *re*-attack structures **139→140→141**, C_1-C_β-C_α-Rh dihedral angle change 12°→13°→36° in U-pathway (**a**) *vs.* 21°→21°→58° in D-pathway (**b**). The Rh-oxa-π-allyl intermediates (**134a** and **141a**) produced by U-pathways are less-stable than the product of D-pathways (**134b** and **141b**) (–18.0 and –17.3 *vs.* –20.5 and –20.3 kcal.mol).

COD-Rh pathway (Ligand XIV) (kcal/mol, 303.15K, 1,4-dioxane)

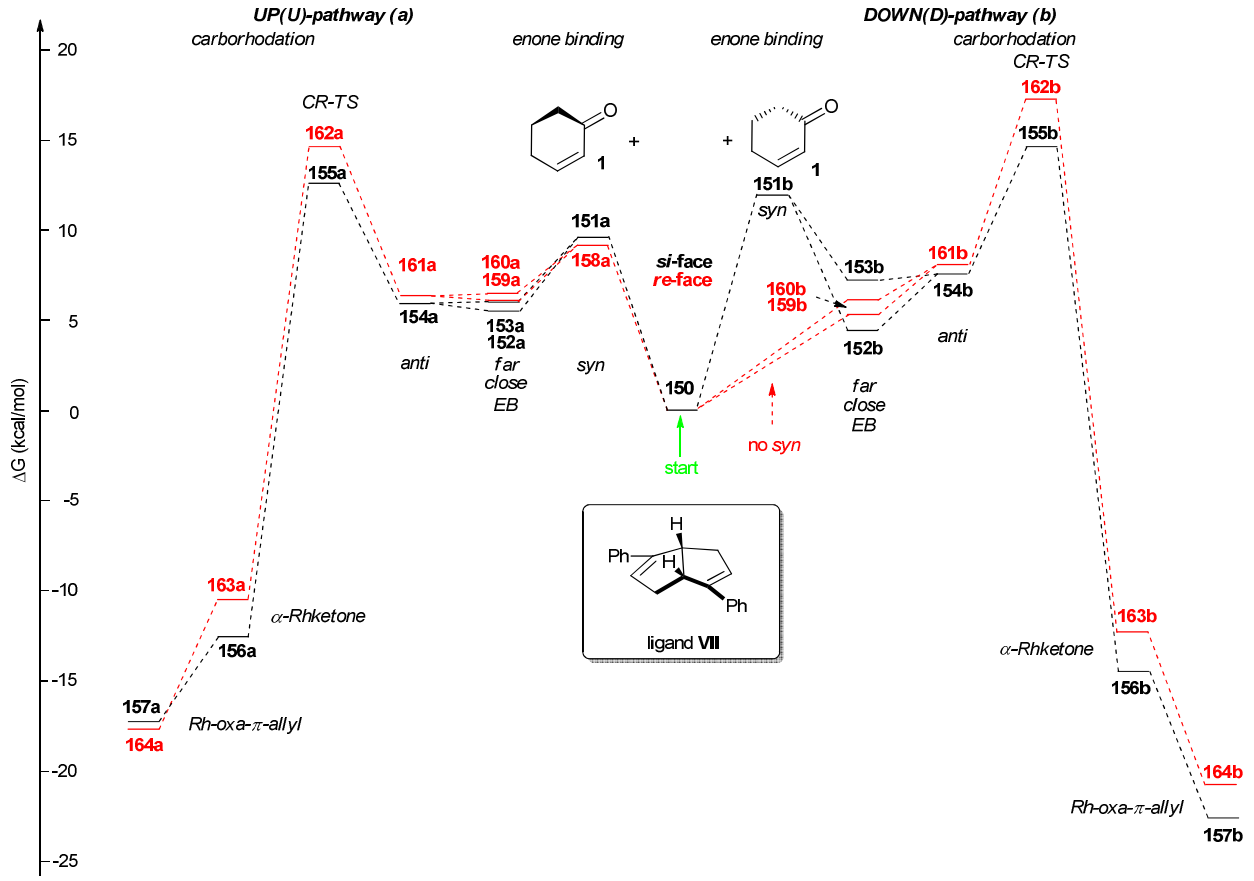


si-face

	142+1	143a	144a	145a	146a	147a	148a	149a	144b	145b	146b	147b	148b	149b
ΔG	0.0	5.1	1.7	3.0	1.5	9.4	–15.2	–20.3	1.6	3.6	4.1	12.1	–16.1	–23.4
ΔH	0.0	–9.5	–12.0	–10.3	–13.0	–5.8	–30.3	–35.3	–12.6	–10.0	–9.9	-3.3	–30.9	–38.5
–TΔS	0.0	14.5	13.7	13.3	14.5	15.2	15.1	15.0	14.3	13.6	14.0	15.4	14.8	15.1

The calculated profile for 1,4-addition reaction with ligand **XIV** (COD) (**142-149**), shows that the starting Rh-Ph intermediate **91** is unsymmetrical (22° deviation) with respect of the two halves of the ligand as well as unsymmetrical with respect to Rh-alkene coordination due to the strong trans-effect of the Ph group (Rh- C(down) distances of 2.091 and 2.235Å for the proximal and distal C=C bonds, respectively). Only structures for *si*-attack are presented here. For both U- and D- pathways, 7 EB conformers were found, out 8 possible. For the D-pathway, no *syn*- conformer could be found. In EB intermediates, C_α-Rh distance is 2.250-2.291 Å and C_β-Rh - 2.257-2.354 Å. The most favorable EB intermediates occur in *anti* (**146a**; 1.5 kcal/mol) and *close* (**144b**, 1.6 kcal/mol) for U- and D-pathways, respectively. Collapse of TSs **147** lead to α-rhodioketones **148**, which then proceeds further to Rh-oxa-π-allyl (enolate) intermediates **149** via a conformational, low barrier twist of the cyclohexenone moiety to relieve the torsional strain of the nearly-eclipsing Ph and [(diene)Rh]. For structures **147→148→149**, C_1-C_β-C_α-Rh dihedral angle changes –18°→–19°→–39° in U-pathway (**a**) *vs.* –27°→–27°→–60° in D-pathway (**b**). The Rh-oxa-π-allyl intermediate (**98a**) produced by U-pathway is less-stable than the product of D-pathway (**98b**) (–20.3 *vs.* –23.4 kcal.mol).

(R)-Ph-bicyclo[3.3.0]octadiene (Ligand VII) -Rh pathway (kcal/mol, 303.15K, dioxane)



si-face

	150+1	151a	152a	153a	154a	155a	156a	157a	151b	152b	153b	154b	155b	156b	157b
ΔG	0.0	9.5	5.7	6.2	6.0	12.8	–12.8	–17.4	12.0	4.7	7.4	7.6	13.9	–14.1	–21.0
ΔH	0.0	–4.8	–9.1	–8.3	–9.0	–4.3	–29.8	–33.3	–2.7	–9.9	–7.8	–7.3	–3.1	–30.9	–37.3
–TΔS	0.0	14.3	14.8	14.5	15.0	17.1	16.9	15.8	14.8	14.6	15.2	14.9	17.1	16.8	16.3

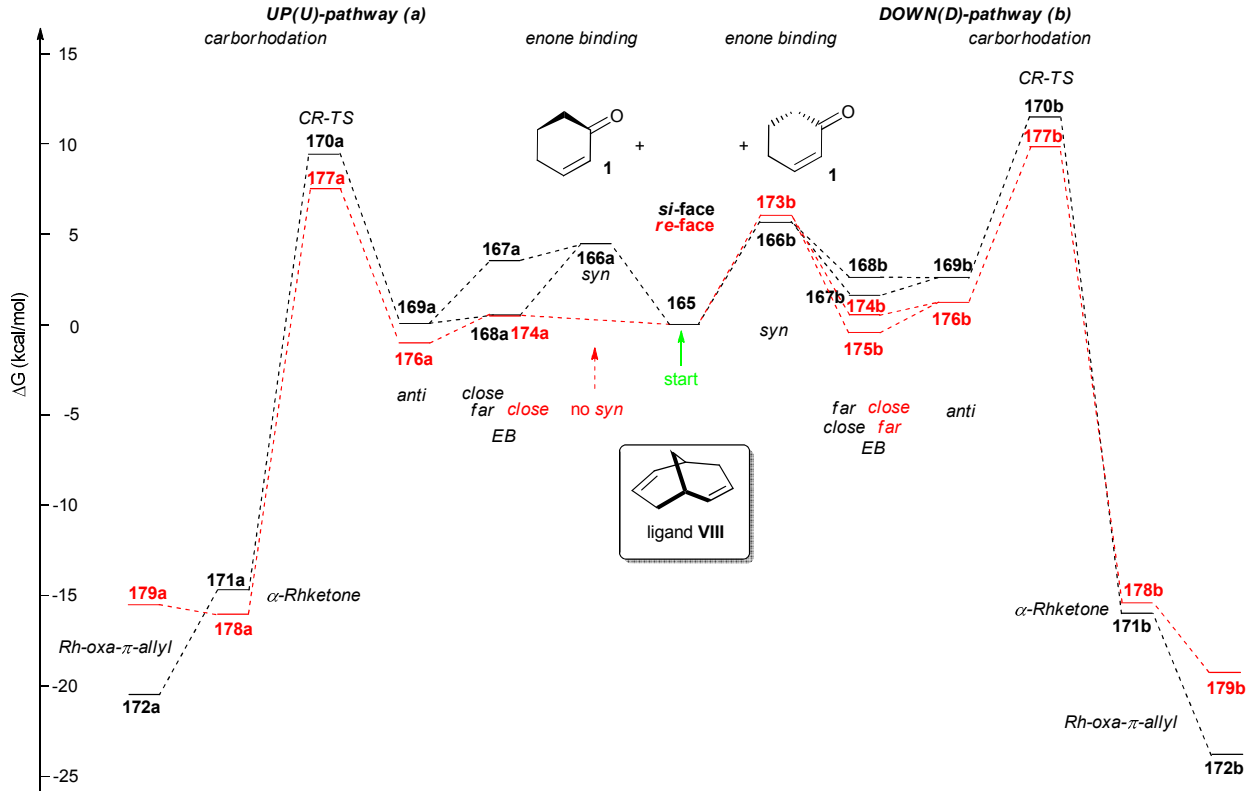
re-face

	150+1	158a	159a	160a	161a	162a	163a	164a	159b	160b	161b	162b	163b	164b
ΔG	0.0	8.7	5.8	6.7	6.5	14.7	–10.7	–17.9	5.3	6.2	8.3	17.1	–12.5	–22.6
ΔH	0.0	–6.4	–8.9	–7.8	–8.4	–2.3	–28.3	–33.2	–9.8	–8.4	–6.2	0.1	–30.0	–38.9
–TΔS	0.0	15.1	14.7	14.5	14.6	17.1	17.6	15.3	15.1	14.6	14.5	17.0	17.5	16.3

The calculated profile for 1,4-addition reaction with ligand **VII** (**150**-**164**), shows that the starting Rh-Ph intermediate **150** is unsymmetrical (24° deviation) with respect of the two halves of the ligand as well as unsymmetrical with respect to Rh-alkene coordination due to the strong trans-effect of the Ph group (Rh- C(Ph-diene) distances of 2.107 and 2.260Å for the proximal and distal C=C bonds, respectively). Total of 15 EB conformers were found, out of 16 possible. One *syn*-conformer was not found, in the D/*re*-pathway. In EB intermediates, C_α-Rh distance is 2.273-2.370 Å and C_β-Rh - 2.305-2.407 Å. The most favorable EB intermediates occur in *anti* (**154a**; 6.0 kcal/mol), *close* (**152b**, 4.7 kcal/mol), *anti* (**161a**, 4.7 kcal/mol) and *close* (**159b**, 5.3 kcal/mol) for U/*si*-, D/*si*-, U/*re*- and D/*re*-pathways, respectively. Collapse of TSs **155** and **162** leads to α-rhodioketones **156** and **163**, which then proceed further to Rh-oxa-π-allyl (enolate) intermediates **157** and **164**. For *si*-attack structures **155**→**156**→**157**, C_1-C_β-C_α-Rh dihedral angle change –14°→–20°→–37° in U-pathway (**a**) *vs.* –

27°→–32°→–58° in D-pathway (**b**). For *re*-attack structures **162→163→164**, C_1-C_β-C_α-Rh dihedral angle change 8°→8°→–5° in U-pathway (**a**) *vs.* 17°→21°→63° in D-pathway (**b**). The Rh-oxa-π-allyl intermediates (**157a** and **164a**) produced by U-pathways are considerably less-stable than the product of D-pathways (**157b** and **164b**) (–17.4 and –17.9 *vs.* –21.0 and –22.6 kcal.mol).

(R)-BND (Ligand VIII) - Rh pathway (kcal/mol, 303.15K, dioxane)



si-face

	165+1	166a	167a	168a	169a	170a	171a	172a	166b	167b	168b	169b	170b	171b	172b
ΔG	0.0	4.7	3.4	0.8	–0.1	9.2	–14.7	–20.4	5.9	2.7	1.6	2.7	11.7	–16.0	–23.7
ΔH	0.0	–10.0	–11.4	–12.9	–14.5	–6.3	–30.5	–35.8	–9.7	–11.6	–11.9	–11.3	–3.8	–31.2	–38.9
–TΔS	0.0	14.7	14.8	13.6	14.3	15.5	15.8	15.4	15.7	14.3	13.5	14.0	15.4	15.2	15.2

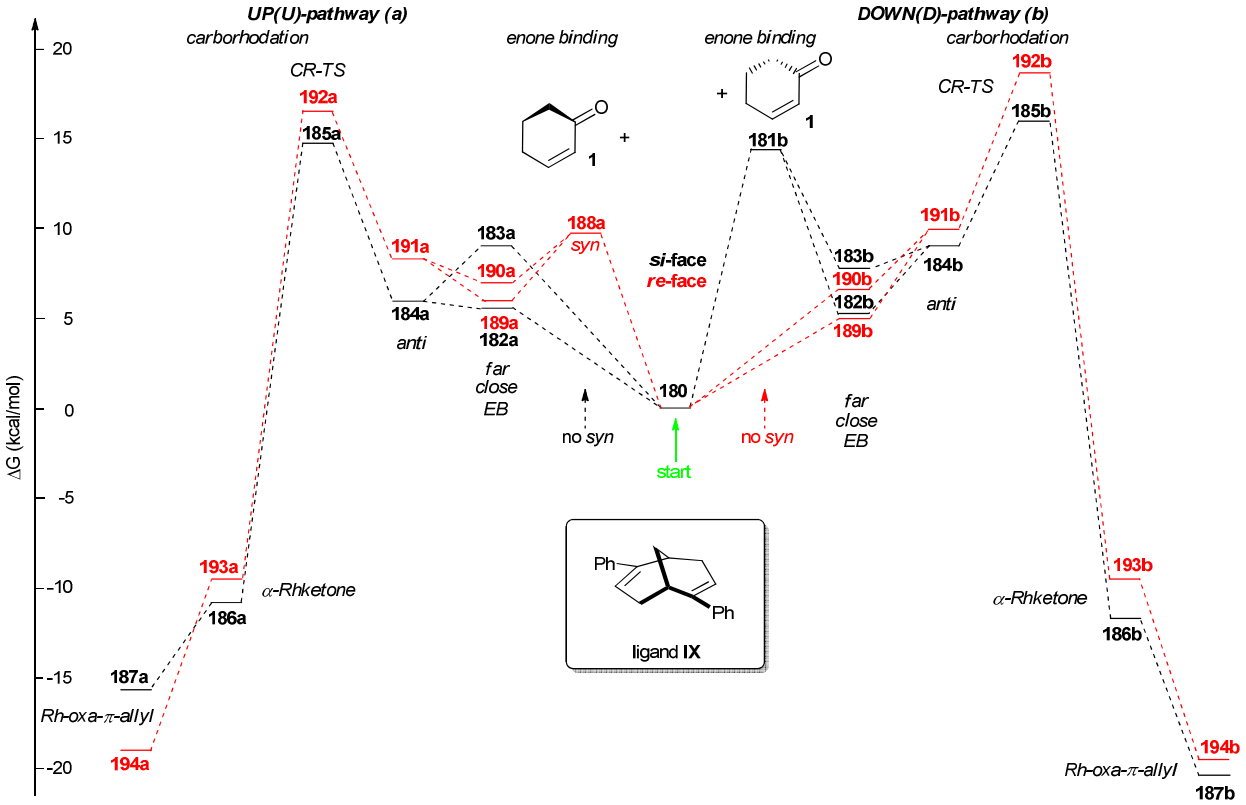
re-face

	165+1	174a	176a	177a	178a	179a	173b	174b	175b	176b	177b	178b	179b
ΔG	0.0	0.8	–1.4	7.5	–16.4	–15.7	6.3	0.8	–0.3	1.3	9.9	–15.4	–18.9
ΔH	0.0	–13.4	–15.5	–8.0	–32.5	–30.6	–7.2	–13.5	–14.5	–12.8	–5.7	–30.8	–33.9
–TΔS	0.0	14.2	14.1	15.5	16.1	14.9	13.5	14.4	14.1	14.1	15.6	15.3	15.0

The calculated profile for 1,4-addition reaction with ligand **VII** (**165-179**), shows that the starting Rh-Ph intermediate **150** is unsymmetrical (81° deviation) with respect of the two halves of the ligand as well as unsymmetrical with respect to Rh-alkene coordination due to the strong trans-effect of the Ph group. The Rh-C(down) distances were 2.099 and 2.256 Å for the proximal and distal C=C bonds, and the Rh-C(up) distances were 2.106 and 2.313Å for the proximal and distal C=C bonds, respectively. Total of 14 EB conformers were found, out of 16 possible. The *syn*- and *far*-conformers was not found in the U/*re*-pathway. In EB intermediates, C_α-Rh distance is 2.218-2.310 Å and C_β-Rh - 2.244-2.338 Å. The most favorable EB intermediates occur in *anti* (**169a**; –0.1 kcal/mol), *far* (**168b**, 2.7 kcal/mol), *anti* (**176a**, –1.4 kcal/mol) and *far* (**175b**, –0.3 kcal/mol) for U/*si*-, D/*si*-,

U/*re*- and D/*re*-pathways, respectively. Collapse of TSs **170** and **177** leads to α-rhodioketones **171** and **178**, which then proceed further to Rh-oxa-π-allyl (enolate) intermediates **172** and **179**. For *si*-attack structures **170→171→172**, C_1-C_β-C_α-Rh dihedral angle change –14°→–20°→–37° in U-pathway (**a**) *vs.* –27°→–32°→–58° in D-pathway (**b**). For *re*-attack structures **177→178→179**, C_1-C_β-C_α-Rh dihedral angle change 8°→8°→–5° in U-pathway (**a**) *vs.* 17°→21°→63° in D-pathway (**b**). The Rh-oxa-π-allyl intermediates (**172a** and **179a**) produced by U-pathways are considerably more stable than the product of D-pathways (**172b** and **179b**) (–20.4 and –15.7 *vs.* –23.7 and –18.9 kcal.mol). The Rh-oxa-π-allyl intermediate **179a** is also less stable than the corresponding α-rhodioketone (**178a**, –16.4 kcal/mol).

(R)-PhBND-Rh pathway (Ligand IX) (kcal/mol, 303.15K, dioxane)



si -face

	180+1	182a	183a	184a	185a	186a	187a	181b	182b	183b	184b	185b	186b	187b
ΔG	0.0	5.7	8.6	6.2	14.7	–11.0	–15.8	14.0	5.2	7.8	8.7	16.5	–12.0	–20.2
ΔH	0.0	–9.1	–6.3	–7.6	–2.5	–28.0	–31.4	–0.9	–9.7	–6.6	–5.1	–0.6	–28.5	–36.0
–TΔS	0.0	14.7	14.9	13.8	17.2	17.1	15.6	15.0	14.9	14.4	13.8	17.1	16.5	15.8

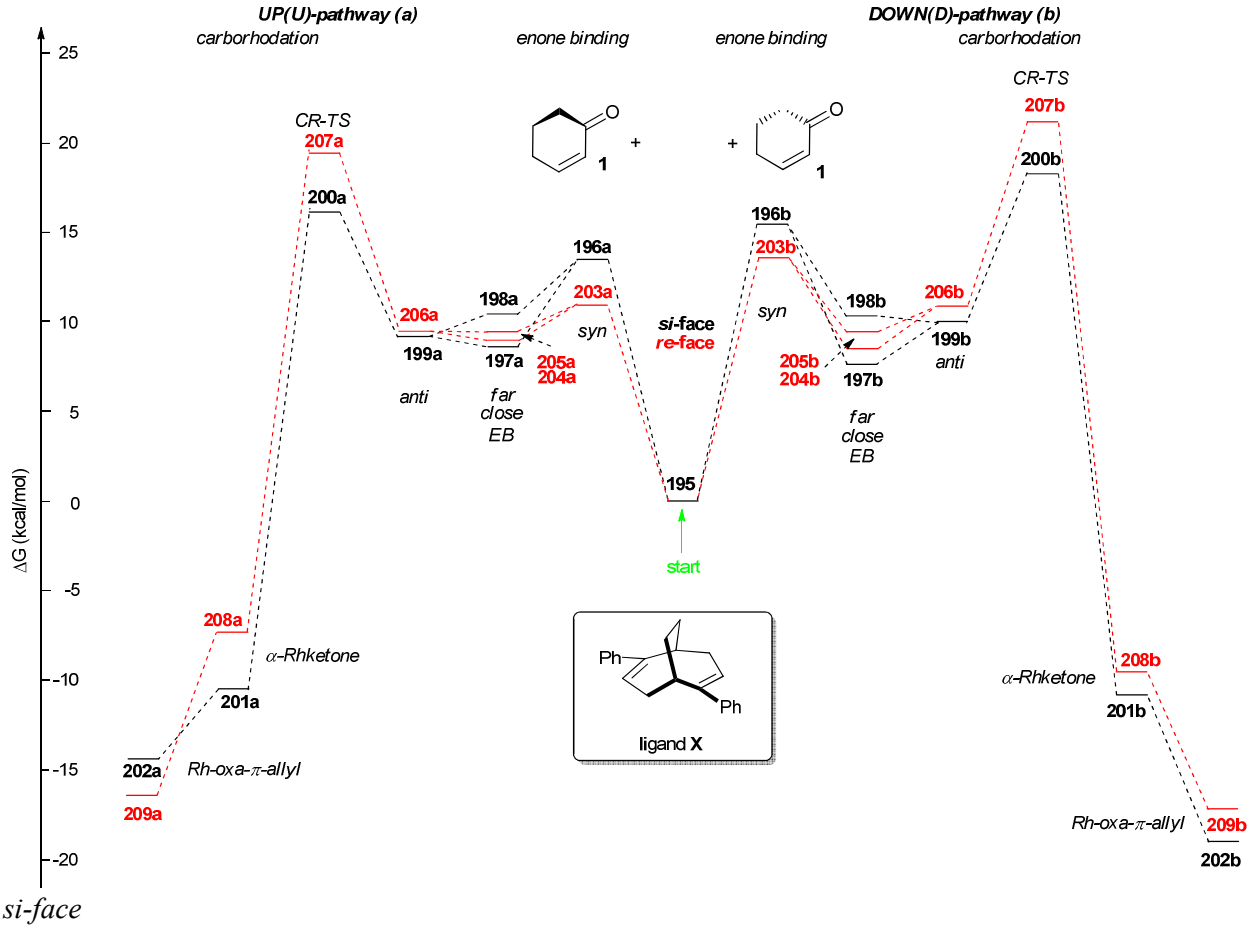
re -face

	180+1	188a	189a	190a	191a	192a	193a	194a	189b	190b	191b	192b	193b	194b
ΔG	0.0	9.7	6.2	7.2	8.2	16.7	–9.2	–18.7	5.0	6.9	10.0	18.3	–11.3	–19.1
ΔH	0.0	–5.6	–8.5	–7.2	–7.2	–0.2	–26.2	–33.5	–9.5	–8.0	–4.6	2.3	–28.5	–35.4
–TΔS	0.0	15.2	14.7	14.5	15.4	16.9	17.0	14.8	14.5	15.0	14.6	16.0	17.2	16.2

The calculated profile for 1,4-addition reaction with ligand **IX** (**180**-**194**), shows that the starting Rh-Ph intermediate **180** is unsymmetrical (22° deviation) with respect of the two halves of the ligand as well as unsymmetrical with respect to Rh-alkene coordination due to the strong trans-effect of the Ph group (Rh-C(Ph-diene) distances of 2.139

and 2.277Å for the proximal and distal C=C bonds, respectively). Total of 14 EB conformers were found, out of 16 possible. Two *syn*-conformer was found, in the D/*re*- and U/*si*-pathways. In EB intermediates, C_α-Rh distance is 2.244-2.404 Å and C_β-Rh - 2.264-2.436 Å. The most favorable EB intermediates occur in *close* (**182a**; 5.7 kcal/mol), *close* (**182b**, 5.2 kcal/mol), *close* (**189a**, 6.2 kcal/mol) and *close* (**189b**, 5.0 kcal/mol) for U/*si*-, D/*si*-, U/*re*- and D/*re*-pathways, respectively. Collapse of TSs **185** and **192** leads to α-rhodioketones **186** and **193**, which then proceed further to Rh-oxa-π-allyl (enolate) intermediates **187** and **194**. For *si*-attack structures **185→186→187**, C_1-C_β-C_α-Rh dihedral angle change –13°→–20°→–37° in U-pathway (**a**) *vs.* –26°→–33°→–59° in D-pathway (**b**). For *re*-attack structures **192→193→194**, C_1-C_β-C_α-Rh dihedral angle change 6°→7°→–5° in U-pathway (**a**) *vs.* 18°→19°→65° in D-pathway (**b**). The Rh-oxa-π-allyl intermediates (**187a** and **194a**) produced by U-pathways are slightly less-stable than the product of D-pathways (**187b** and **184b**) (–15.8 and –18.7 *vs.* –20.2 and –19.1 kcal.mol).

(S)-PhBDD-Rh pathway (Ligand X) (kcal/mol, 303.15K, dioxane)



si-face

	195+1	196a	197a	198a	199a	200a	201a	202a	196b	197b	198b	199b	200b	201b	202b
ΔG	0.0	13.5	8.1	10.4	8.8	16.3	–10.5	–14.0	15.3	7.6	10.3	10.0	18.0	–11.1	–18.6
ΔH	0.0	–2.0	–8.5	–5.0	–7.1	–1.8	–28.2	–30.6	0.0	–8.9	–6.0	–5.2	–0.1	–28.9	–35.4
–TΔS	0.0	15.5	16.6	15.4	16.0	18.2	17.8	16.5	15.4	16.5	16.3	15.2	18.1	17.8	16.8

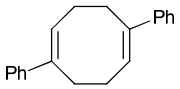
re-face

	195+1	203a	204a	205a	206a	207a	208a	209a	203b	204b	205b	206b	207b	208b	209b
ΔG	0.0	11.3	9.1	9.5	9.5	19.4	–7.3	–16.9	13.6	8.3	9.4	11.3	21.5	–9.3	–17.1
ΔH	0.0	–4.5	–7.4	–6.7	–7.2	0.8	–25.2	–34.3	–2.3	–8.8	–7.1	–4.6	3.3	–27.2	–34.2
–TΔS	0.0	15.8	16.5	16.2	16.7	18.6	18.0	17.4	15.8	17.2	16.5	15.9	18.1	17.8	17.0

The calculated profile for 1,4-addition reaction with ligand **IX** (**195-209**), shows that the starting Rh-Ph intermediate **195** is unsymmetrical (88° deviation) with respect of the two halves of the ligand as well as unsymmetrical with respect to Rh-alkene coordination due to the strong trans-effect of the Ph group (Rh-C(Ph-diene) distances of 2.146 and 2.262Å for the proximal and distal C=C bonds, respectively). All of the 16 possible conformers were found. In EB intermediates, C_α-Rh distance is 2.270-2.422 Å and C_β-Rh - 2.278-2.453 Å. The most favorable EB intermediates occur in *close* (**197a**; 8.1 kcal/mol), *close* (**197b**, 7.6 kcal/mol), *close* (**204a**, 9.1 kcal/mol) and *close* (**204b**, 8.3 kcal/mol) for U/*si*-, D/*si*-, U/*re*- and D/*re*-pathways, respectively. Collapse of TSs **200** and **207** leads to α-rhodioketones **201** and **208**, which then proceed further to Rh-oxa-π-allyl (enolate) intermediates **202** and **209**. For *si*-attack structures **200**→**201**→**202**, C_1-C_β-C_α-Rh dihedral angle change –13°→–20°→–38° in U-pathway (**a**) *vs.* –26°→–33°→–59° in D-pathway (**b**). For *re*-attack structures **207**→**208**→**209**, C_1-C_β-C_α-Rh dihedral angle change 0°→–3°→–5° in U-pathway (**a**) *vs.* 8°→17°→42° in D-pathway (**b**). The Rh-oxa-π-allyl intermediates (**202a** and **209a**) produced by U-pathways are slightly less-stable than the product of D-pathways (**202b** and **209b**) (–14.0 and –16.9 *vs.* –18.6 and –17.1 kcal.mol).

Ligand XV-XX-Rh pathways (kcal/mol, 303.15K, dioxane).

Only the enantioselectivity-determining stationary points were calculated for U/*si*- and U/*re*-pathways. Ligand **XV**: 1,5-cyclooctadiene:



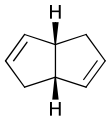
$XV_{2,6}$

	Rh-Ph 210+1	EB-*si*-*anti* 211a	CR-TS-*si* 212a	EB-*re*-anti 213a	CR-TS-*re* 214a
ΔG	0.0	8.5	15.6	7.9	18.4
ΔH	0.0	–5.6	–0.3	–6.6	2.2
–TΔS	0.0	14.1	16.0	14.5	16.2

$XV_{3,7}$

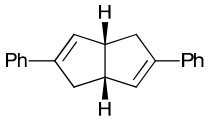
	Rh-Ph 215+1	EB-*si*-*anti* 216a	CR-TS-*si* 217a	EB-*re*-anti 218a	CR-TS-*re* 219a
ΔG	0.0	8.8	21.2	8.8	18.3
ΔH	0.0	–5.9	5.0	–5.1	2.4
–TΔS	0.0	14.7	16.2	13.8	16.0

Ligand **XVI**: (*R*,*R*)-Bicyclo[3.3.0]-2,6-octadiene:



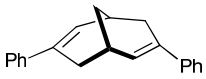
	Rh-Ph 220+1	EB-*si*-*anti* 221a	CR-TS-*si* 222a	EB-*re*-anti 223a	CR-TS-*re* 224a
ΔG	0.0	0.5	9.8	–1.5	7.7
ΔH	0.0	–13.9	–5.9	–15.6	–7.9
–TΔS	0.0	14.3	15.6	14.1	15.6

Ligand **XVII**: (*R*,*R*)-3,7-diphenylbicyclo[3.3.0]-2,6-octadiene:



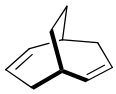
	Rh-Ph 225+1	**EB-*si*-*anti* 226a**	**CR-TS-*si* 227a**	**EB-*re*-anti 228a**	**CR-TS-*re* 229a**
ΔG	0.0	6.5	20.7	6.0	15.1
ΔH	0.0	–9.1	3.8	–9.1	–1.4
–TΔS	0.0	15.6	16.9	15.1	16.5

Ligand **XVIII**: (*R*,*R*)-3,7-diphenylbicyclo[3.3.1]-2,6-nonadiene:



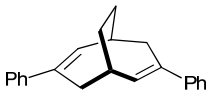
	Rh-Ph 230+1	**EB-*si*-*anti* 231a**	**CR-TS-*si* 232a**	**EB-*re*-anti 233a**	**CR-TS-*re* 234a**
ΔG	0.0	7.5	20.2	6.8	16.0
ΔH	0.0	–7.6	4.4	–7.8	0.2
–TΔS	0.0	15.2	15.8	14.6	15.8

Ligand **XIX**: (*S*,*S*)-Bicyclo[3.3.2]-2,6-decadiene:



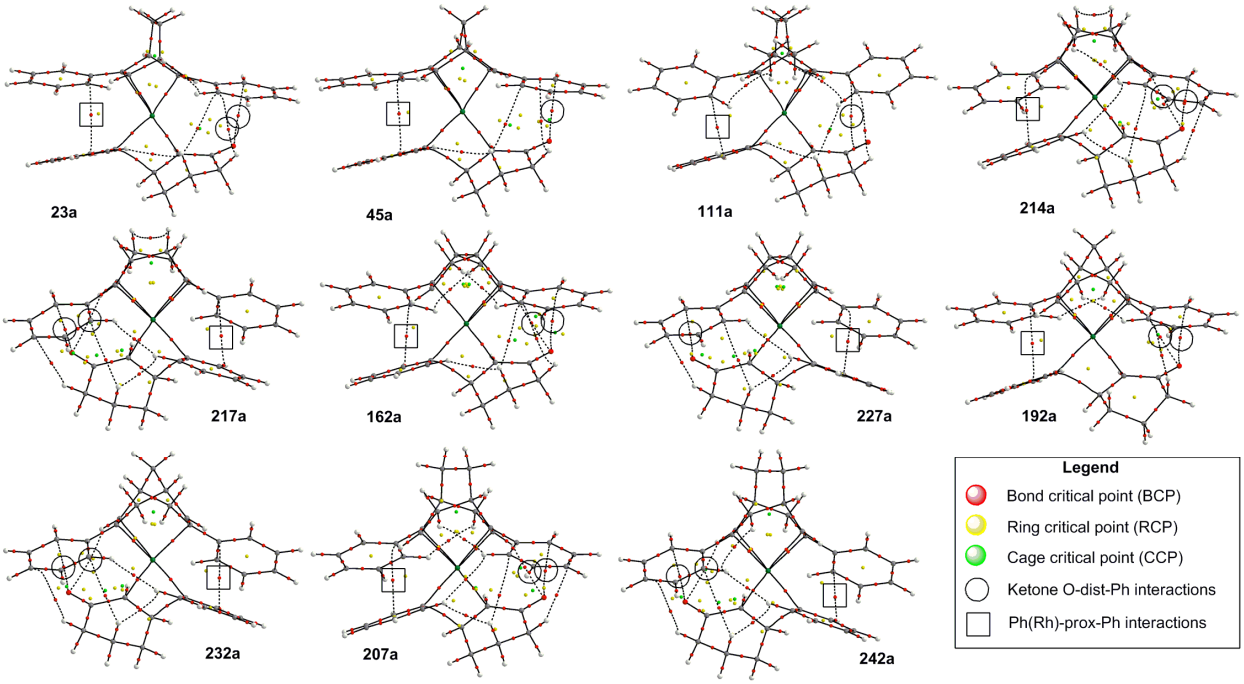
	Rh-Ph 235+1	**EB-*si*-*anti* 236a**	**CR-TS-*si* 237a**	**EB-*re*-anti 238a**	**CR-TS-*re* 239a**
ΔG	0.0	0.8	9.5	–0.2	8.7
ΔH	0.0	–13.7	–6.2	–14.5	–7.2
–TΔS	0.0	14.5	15.7	14.3	15.9

Ligand **XX**: (*S*,*S*)-3,7-diphenylbicyclo[3.3.2]-2,6-decadiene:



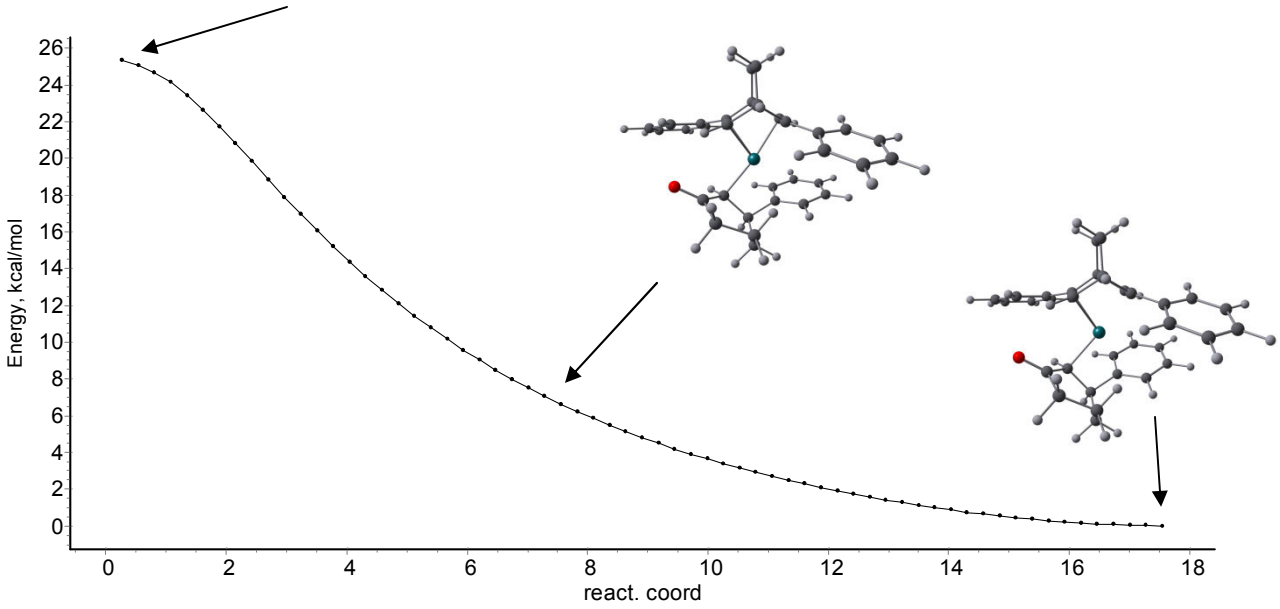
	Rh-Ph 240+1	**EB-*si*-*anti* 241a**	**CR-TS-*si* 242a**	**EB-*re*-anti 243a**	**CR-TS-*re* 244a**
ΔG	0.0	8.8	20.5	7.9	17.4
ΔH	0.0	–6.4	4.9	–6.2	1.8
–TΔS	0.0	15.2	15.6	14.1	15.7

2.3. AIM plots for the minor CR-TSs for phenyl-substituted, C2-symmetric 1,4- and 1,5-diene ligands (Table 5).

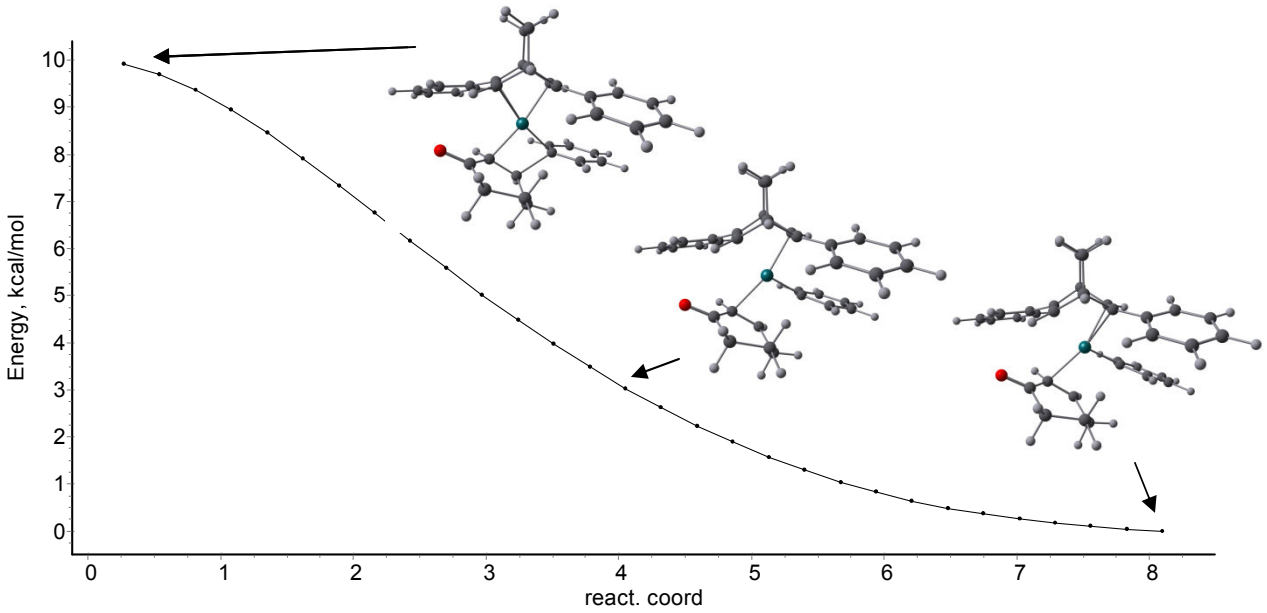


2.4 IRC for the major CR-TS (U/*si*-pathway) for Ligand I (PhBOD) (gas phase)

Forward direction



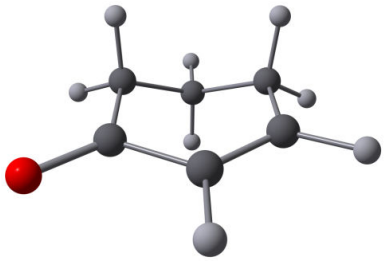
Reverse direction:



2.5. Structure plots, Cartesian coordinates, SCF energies and convergences and frequencies (for the first 3 normal modes only) for selected structures (Table 2).

Cyclohexenone (1)

Conformation M (303.15K, 1,4-dioxane)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.962786	1.316500	0.026452
2	1	0	-1.472304	2.279416	0.022905
3	6	0	0.378388	1.285575	-0.058478
4	1	0	0.965700	2.195826	-0.153244
5	6	0	1.134987	0.021818	0.015786
6	8	0	2.356376	0.001849	-0.074855
7	6	0	-1.810895	0.087597	0.133428
8	1	0	-2.735892	0.230605	-0.435904
9	1	0	-2.124409	-0.027400	1.181831
10	6	0	0.327111	-1.233624	0.267527
11	1	0	0.254269	-1.345523	1.358615
12	1	0	0.896279	-2.090369	-0.102278
13	6	0	-1.068843	-1.157153	-0.341705
14	1	0	-1.639526	-2.058480	-0.096772
15	1	0	-0.982898	-1.123150	-1.434372

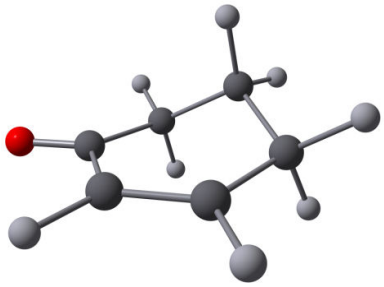
```
SCF Done:  E(RPBE1PBE) =  -308.332694733     A.U. after    1 cycles
             Convg  =    0.2930D-08             -V/T =  2.0137
Zero-point correction=                           0.128507 (Hartree/Particle)
 Thermal correction to Energy=                    0.134787
 Thermal correction to Enthalpy=                  0.135747
 Thermal correction to Gibbs Free Energy=         0.097953
 Sum of electronic and zero-point Energies=           -308.204188
 Sum of electronic and thermal Energies=              -308.197907
 Sum of electronic and thermal Enthalpies=            -308.196947
 Sum of electronic and thermal Free Energies=         -308.234742
                    1                    2                    3
Frequencies --   103.2147              246.0748              307.9643
```

(298.15K, methanol)

```
SCF Done:  E(RPBE1PBE) =  -308.337156064     A.U. after    1 cycles
             Convg  =    0.3535D-08             -V/T =  2.0137
Zero-point correction=                           0.128412 (Hartree/Particle)
 Thermal correction to Energy=                    0.134498
 Thermal correction to Enthalpy=                  0.135442
 Thermal correction to Gibbs Free Energy=         0.098502
 Sum of electronic and zero-point Energies=           -308.208744
 Sum of electronic and thermal Energies=              -308.202658
```

```
 Sum of electronic and thermal Enthalpies=           -308.201714
 Sum of electronic and thermal Free Energies=        -308.238654
```

Conformation P (303.15K, 1,4-dioxane)



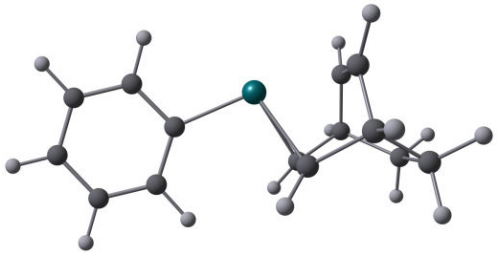
```
---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1          6           0        0.961610    1.316738    0.026174
      2          1           0        1.470109    2.280220    0.022793
      3          6           0       -0.379822    1.285364   -0.060053
      4          1           0       -0.966240    2.195990   -0.155174
      5          6           0       -1.134183    0.021733    0.015765
      6          8           0       -2.356602    0.000547   -0.073159
      7          6           0        1.810634    0.088667    0.134539
      8          6           0       -0.326721   -1.233556    0.265436
      9          6           0        1.070625   -1.157069   -0.341130
     10          1           0        2.736723    0.232616   -0.432741
     11          1           0        2.122137   -0.025576    1.183718
     12          1           0        0.986874   -1.123727   -1.433907
     13          1           0        1.641107   -2.057961   -0.094196
     14          1           0       -0.255290   -1.347474    1.356520
     15          1           0       -0.895465   -2.089725   -0.106131
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -308.332697511     A.U. after    1 cycles
             Convg  =    0.9829D-09             -V/T =  2.0137
Zero-point correction=                           0.128513 (Hartree/Particle)
 Thermal correction to Energy=                    0.134789
 Thermal correction to Enthalpy=                  0.135749
 Thermal correction to Gibbs Free Energy=         0.097969
 Sum of electronic and zero-point Energies=           -308.204184
 Sum of electronic and thermal Energies=              -308.197908
 Sum of electronic and thermal Enthalpies=            -308.196948
 Sum of electronic and thermal Free Energies=         -308.234729
1                    2                     3
Frequencies --   104.4117               245.7871               308.7082
```

(303.15K, 1,4-dioxane)

```
SCF Done:  E(RPBE1PBE) =  -308.337155523     A.U. after    1 cycles
             Convg  =    0.1404D-08             -V/T =  2.0137
Zero-point correction=                           0.128413 (Hartree/Particle)
 Thermal correction to Energy=                    0.134496
 Thermal correction to Enthalpy=                  0.135441
 Thermal correction to Gibbs Free Energy=         0.098508
 Sum of electronic and zero-point Energies=           -308.208743
 Sum of electronic and thermal Energies=              -308.202659
 Sum of electronic and thermal Enthalpies=            -308.201715
 Sum of electronic and thermal Free Energies=         -308.238648
```

BOD-Rh pathway

BOD-Rh(I)-Ph (4)

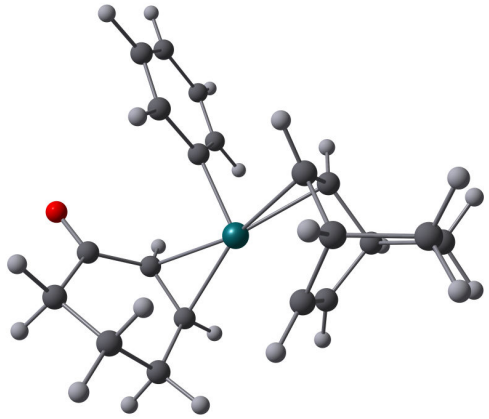


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.019857	-0.721191	-0.000302
2	6	0	-2.195349	-1.105605	-0.686140
3	6	0	-2.264319	0.283450	1.293351
4	6	0	-2.195215	-1.105972	0.685661
5	6	0	-2.264563	0.284151	-1.293053
6	6	0	-3.535212	1.001634	0.772132
7	6	0	-1.034075	0.959883	-0.709185
8	6	0	-1.033945	0.959510	0.709619
9	6	0	-3.535352	1.002061	-0.771199
10	1	0	-2.237808	0.256247	2.384390
11	1	0	-2.238262	0.257549	-2.384111
12	1	0	-4.420918	0.491819	1.165021
13	1	0	-3.551587	2.022988	1.166384
14	1	0	-3.551788	2.023635	-1.164879
15	1	0	-4.421136	0.492475	-1.164207
16	1	0	-0.465054	1.678279	-1.295500
17	1	0	-2.312872	-2.005581	1.285211
18	6	0	1.846904	0.006522	-0.000077
19	6	0	2.289945	1.338669	-0.000294
20	6	0	2.832284	-0.996040	0.000339
21	6	0	3.649900	1.653800	-0.000149
22	1	0	1.568054	2.154991	-0.000588
23	6	0	4.195942	-0.692977	0.000492
24	1	0	2.539357	-2.049797	0.000572
25	6	0	4.609056	0.639304	0.000240
26	1	0	3.965460	2.695467	-0.000341
27	1	0	4.933877	-1.492787	0.000812
28	1	0	5.668143	0.885296	0.000352
29	1	0	-0.464801	1.677588	1.296203
30	1	0	-2.313122	-2.004888	-1.286156

SCF Done: E(RPBE1PBE) = -5229.13925857 A.U. after 1 cycles
Convg = 0.4123D-08 -V/T = 2.0032
Zero-point correction= 0.251314 (Hartree/Particle)
Thermal correction to Energy= 0.264337
Thermal correction to Enthalpy= 0.265297
Thermal correction to Gibbs Free Energy= 0.210539
Sum of electronic and zero-point Energies= -5228.887944
Sum of electronic and thermal Energies= -5228.874921
Sum of electronic and thermal Enthalpies= -5228.873961
Sum of electronic and thermal Free Energies= -5228.928720

	1	2	3
Frequencies --	47.8055	62.1886	68.7912

BOD-Rh(I)-Ph-CH-si-confU-syn (5a)

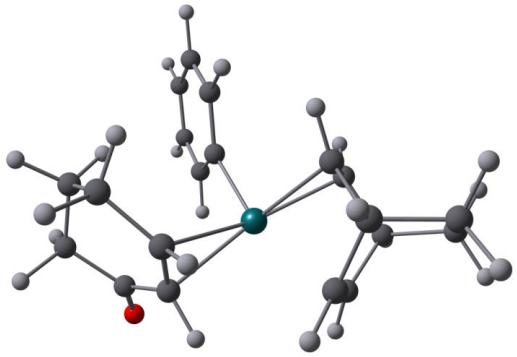


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.284381	0.096657	-0.305569
2	6	0	-2.356668	0.869993	0.336849
3	6	0	-2.719322	-1.113450	-0.998082
4	6	0	-2.459213	0.380692	-0.945085
5	6	0	-2.516821	-0.190653	1.407400
6	6	0	-4.022268	-1.415800	-0.211923
7	6	0	-1.431810	-1.188374	1.058760
8	6	0	-1.543765	-1.689940	-0.232657
9	6	0	-3.899043	-0.871441	1.225624
10	1	0	-2.768865	-1.488558	-2.021568
11	1	0	-2.397126	0.217358	2.412548
12	1	0	-4.867466	-0.958184	-0.736064
13	1	0	-4.191031	-2.497267	-0.210625
14	1	0	-3.995453	-1.676240	1.961219
15	1	0	-4.687197	-0.142603	1.440355
16	1	0	-0.817838	-1.660159	1.820158
17	1	0	-2.577622	1.015870	-1.818921
18	6	0	1.338909	-1.148814	-0.059800
19	6	0	1.778829	-1.946414	-1.126528
20	6	0	1.950843	-1.341041	1.186220
21	6	0	2.784328	-2.900941	-0.956536
22	1	0	1.337152	-1.825331	-2.115496
23	6	0	2.961067	-2.289848	1.360857
24	1	0	1.652808	-0.734179	2.040112
25	6	0	3.381650	-3.078295	0.291059
26	1	0	3.104705	-3.503182	-1.804675
27	1	0	3.424110	-2.408192	2.338639
28	1	0	4.169033	-3.815855	0.425705
29	6	0	0.220351	2.043449	-1.269126
30	6	0	1.427387	1.393981	-1.025691
31	1	0	-0.225219	1.936969	-2.258625
32	1	0	1.892053	0.774708	-1.787565
33	6	0	2.343274	1.858792	0.038775
34	8	0	3.489333	1.436636	0.125994
35	6	0	1.863273	2.972881	0.950405
36	1	0	2.379772	3.876226	0.597612
37	6	0	-0.180007	3.261119	-0.477119
38	1	0	0.231871	4.141882	-0.993729
39	1	0	-2.386167	1.927486	0.578670
40	1	0	-1.026954	-2.585921	-0.563253

41	6	0	0.357107	3.205921	0.947553
42	1	0	-1.266528	3.393592	-0.489572
43	1	0	0.121336	4.132563	1.482350
44	1	0	2.248797	2.777543	1.955285
45	1	0	-0.140297	2.387919	1.484366

```
SCF Done:  E(RPBE1PBE) =  -5537.49662416     A.U. after    1 cycles
             Convg  =    0.2024D-08             -V/T =  2.0039
Zero-point correction=                           0.382271 (Hartree/Particle)
 Thermal correction to Energy=                    0.402655
 Thermal correction to Enthalpy=                  0.403615
 Thermal correction to Gibbs Free Energy=         0.332519
 Sum of electronic and zero-point Energies=          -5537.114353
 Sum of electronic and thermal Energies=             -5537.093969
 Sum of electronic and thermal Enthalpies=           -5537.093009
 Sum of electronic and thermal Free Energies=        -5537.164106
                     1                      2                      3
Frequencies --    36.7075                41.3819                54.3205
```

BOD-Rh(I)-Ph-CH-si-confU-close (6a)

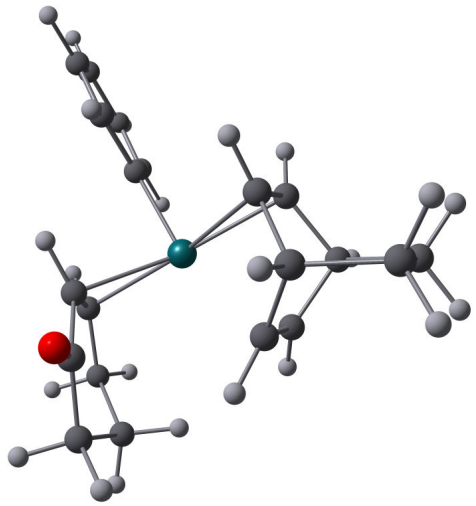


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.395633	-0.184259	-0.203611
2	6	0	2.499637	-1.316855	0.115623
3	6	0	2.893888	0.658564	-1.207738
4	6	0	2.490738	-0.803747	-1.146460
5	6	0	2.893289	-0.314302	1.181403
6	6	0	4.313811	0.789727	-0.595751
7	6	0	1.901417	0.821174	1.007077
8	6	0	1.906468	1.357867	-0.282541
9	6	0	4.309347	0.226318	0.839641
10	1	0	2.856804	1.054376	-2.223995
11	1	0	2.859807	-0.742661	2.184979
12	1	0	5.027591	0.251524	-1.227616
13	1	0	4.604794	1.844842	-0.604564
14	1	0	4.577028	0.998390	1.567919
15	1	0	5.036635	-0.584555	0.947748
16	1	0	1.519176	1.361172	1.868913
17	1	0	2.351199	-1.407754	-2.039353
18	6	0	-1.072017	1.170095	-0.041780
19	6	0	-1.880373	1.292806	-1.185006
20	6	0	-1.276622	2.087630	0.998892
21	6	0	-2.851222	2.291493	-1.285760
22	1	0	-1.771051	0.589438	-2.011308
23	6	0	-2.257740	3.078422	0.908786

24	1	0	-0.680522	2.027340	1.907721
25	6	0	-3.048768	3.188026	-0.234932
26	1	0	-3.463414	2.359147	-2.182889
27	1	0	-2.403427	3.769068	1.737297
28	1	0	-3.811358	3.959623	-0.305358
29	6	0	-0.544237	-1.727093	1.132026
30	6	0	-0.744414	-2.104699	-0.200887
31	1	0	0.345596	-2.091052	1.645483
32	1	0	-0.017118	-2.721431	-0.727355
33	6	0	-2.090665	-2.122779	-0.803607
34	8	0	-2.255897	-2.386338	-1.991869
35	6	0	-3.264817	-1.941527	0.132960
36	1	0	-3.507104	-2.959354	0.473997
37	6	0	-1.688778	-1.382854	2.045797
38	1	0	-1.837393	-2.266441	2.687152
39	1	0	2.371250	-2.374510	0.331237
40	1	0	1.520277	2.347817	-0.509848
41	6	0	-2.992852	-1.039694	1.332576
42	1	0	-1.401668	-0.571258	2.723670
43	1	0	-3.824614	-1.116169	2.041695
44	1	0	-4.123337	-1.595096	-0.448550
45	1	0	-2.962027	-0.001544	0.998582

```
SCF Done:  E(RPBE1PBE) =  -5537.49735556     A.U. after    1 cycles
             Convg  =    0.4338D-08             -V/T =  2.0039
Zero-point correction=                           0.381726 (Hartree/Particle)
 Thermal correction to Energy=                    0.402264
 Thermal correction to Enthalpy=                  0.403224
 Thermal correction to Gibbs Free Energy=         0.331813
 Sum of electronic and zero-point Energies=          -5537.115630
 Sum of electronic and thermal Energies=             -5537.095092
 Sum of electronic and thermal Enthalpies=           -5537.094132
 Sum of electronic and thermal Free Energies=        -5537.165542
                     1                      2                      3
Frequencies --    33.0220                47.7435                54.9662
```

BOD-Rh(I)-Ph-CH-si-confU-far (7a)

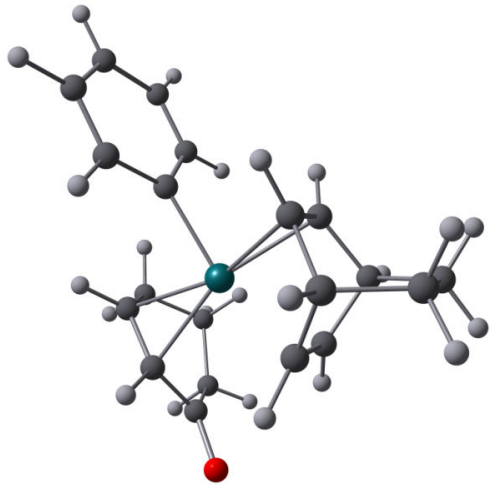


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.107762	-0.046820	-0.325537

2	6	0	-1.926461	-1.009505	-1.206710
3	6	0	-1.898187	-1.494053	1.157550
4	6	0	-2.254786	-0.548357	0.031682
5	6	0	-1.286613	-2.385235	-1.185022
6	6	0	-2.641275	-2.835940	0.899984
7	6	0	-0.080855	-2.224032	-0.273147
8	6	0	-0.414470	-1.743204	0.988690
9	6	0	-2.283468	-3.363257	-0.504103
10	1	0	-2.140413	-1.075440	2.135100
11	1	0	-1.007336	-2.727838	-2.183051
12	1	0	-3.718819	-2.669820	0.996667
13	1	0	-2.354661	-3.551991	1.676507
14	1	0	-1.820592	-4.353586	-0.448129
15	1	0	-3.177506	-3.458780	-1.128840
16	1	0	0.859837	-2.728462	-0.478085
17	1	0	-2.871534	0.326160	0.209284
18	6	0	2.081448	-0.118989	0.036089
19	6	0	2.689200	-0.208558	1.296258
20	6	0	2.917181	-0.152885	-1.092630
21	6	0	4.075797	-0.331962	1.423983
22	1	0	2.082126	-0.183139	2.199801
23	6	0	4.302360	-0.283402	-0.970236
24	1	0	2.487646	-0.077317	-2.092978
25	6	0	4.889278	-0.372507	0.292528
26	1	0	4.520870	-0.397623	2.414936
27	1	0	4.924036	-0.310008	-1.863085
28	1	0	5.967528	-0.468786	0.392559
29	6	0	0.374852	2.157964	-0.608000
30	1	0	1.433566	2.216297	-0.861424
31	6	0	0.044155	1.910607	0.724926
32	1	0	0.813876	1.772751	1.479751
33	6	0	-1.291370	2.261210	1.254738
34	8	0	-1.605496	2.034055	2.418488
35	6	0	-0.560510	2.851564	-1.563452
36	1	0	-0.258869	3.910372	-1.600289
37	6	0	-2.219305	3.027941	0.332005
38	1	0	-2.235940	-0.529508	-2.131917
39	1	0	0.242155	-1.832831	1.848998
40	6	0	-2.025423	2.752552	-1.156855
41	1	0	-0.418538	2.471033	-2.581680
42	1	0	-2.404144	1.756420	-1.403407
43	1	0	-2.623831	3.460084	-1.740954
44	1	0	-3.250649	2.859575	0.655861
45	1	0	-2.003424	4.087171	0.535940

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5537.49700131     A.U. after    1 cycles
           Convg  =    0.2771D-08             -V/T =  2.0039
Zero-point correction=                           0.381585 (Hartree/Particle)
 Thermal correction to Energy=                    0.402263
 Thermal correction to Enthalpy=                  0.403223
 Thermal correction to Gibbs Free Energy=         0.331284
 Sum of electronic and zero-point Energies=          -5537.115416
 Sum of electronic and thermal Energies=             -5537.094738
 Sum of electronic and thermal Enthalpies=           -5537.093778
 Sum of electronic and thermal Free Energies=        -5537.165717
                    1                      2                      3
Frequencies --    39.3569                40.8268                55.4066
```

BOD-Rh(I)-Ph-CH-si-confU-anti (8a)

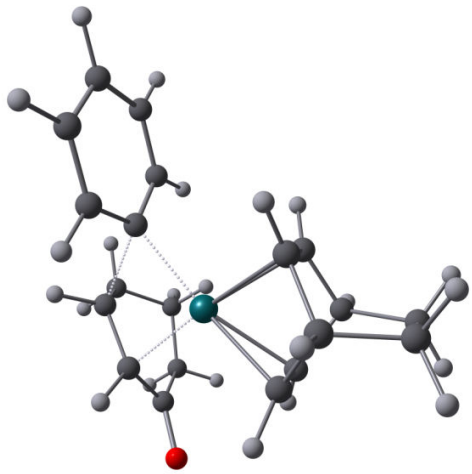


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.108191	-0.024039	-0.259794
2	6	0	2.190181	-0.674004	-0.880583
3	6	0	1.955214	-1.319324	1.440870
4	6	0	2.288506	-0.246751	0.423561
5	6	0	1.774335	-2.128733	-1.007591
6	6	0	2.904796	-2.526169	1.218950
7	6	0	0.451191	-2.173003	-0.264103
8	6	0	0.548603	-1.727623	1.050570
9	6	0	2.800681	-3.005708	-0.243032
10	1	0	2.008386	-0.947344	2.465573
11	1	0	1.672734	-2.440149	-2.048491
12	1	0	3.928105	-2.222915	1.462061
13	1	0	2.630999	-3.324585	1.916042
14	1	0	2.479608	-4.051019	-0.293296
15	1	0	3.769145	-2.940646	-0.749092
16	1	0	-0.395244	-2.746077	-0.631165
17	1	0	2.766600	0.687428	0.702322
18	6	0	-1.914964	-0.415353	-0.105751
19	6	0	-2.586778	-0.411756	1.126911
20	6	0	-2.643425	-0.846331	-1.227541
21	6	0	-3.920485	-0.816463	1.236911
22	1	0	-2.067901	-0.085184	2.027830
23	6	0	-3.974666	-1.256094	-1.124585
24	1	0	-2.169176	-0.861550	-2.208605
25	6	0	-4.622831	-1.242932	0.110894
26	1	0	-4.410300	-0.797965	2.208797
27	1	0	-4.507999	-1.584063	-2.014937
28	1	0	-5.659965	-1.558442	0.193423
29	6	0	-0.926615	1.970979	-0.741694
30	6	0	0.390087	1.960176	-1.191779
31	1	0	-1.717966	1.743206	-1.449837
32	1	0	0.621614	1.679652	-2.219163
33	6	0	1.456630	2.695742	-0.486060
34	8	0	2.593416	2.772142	-0.945008
35	6	0	1.071883	3.423989	0.785090
36	1	0	0.888009	4.464477	0.480611
37	6	0	-1.325531	2.726850	0.494588
38	1	0	-1.668211	3.723948	0.176794

39	1	0	2.576181	-0.098693	-1.717516
40	1	0	-0.222645	-1.918408	1.791262
41	6	0	-0.167600	2.864229	1.474763
42	1	0	-2.185864	2.241529	0.964621
43	1	0	-0.451570	3.508537	2.313748
44	1	0	0.060656	1.874215	1.892074
45	1	0	1.943597	3.448331	1.445423

```
SCF Done:  E(RPBE1PBE) =  -5537.50421460     A.U. after    1 cycles
             Convg  =    0.2243D-08             -V/T =  2.0039
Zero-point correction=                           0.382318 (Hartree/Particle)
 Thermal correction to Energy=                    0.402700
 Thermal correction to Enthalpy=                  0.403660
 Thermal correction to Gibbs Free Energy=         0.332263
 Sum of electronic and zero-point Energies=          -5537.121896
 Sum of electronic and thermal Energies=             -5537.101515
 Sum of electronic and thermal Enthalpies=           -5537.100555
 Sum of electronic and thermal Free Energies=        -5537.171952
                     1                      2                      3
Frequencies --    27.0925               49.4442                54.6532
```

BOD-Rh(I)-Ph-CH-si-confU-CR-TS (9a)

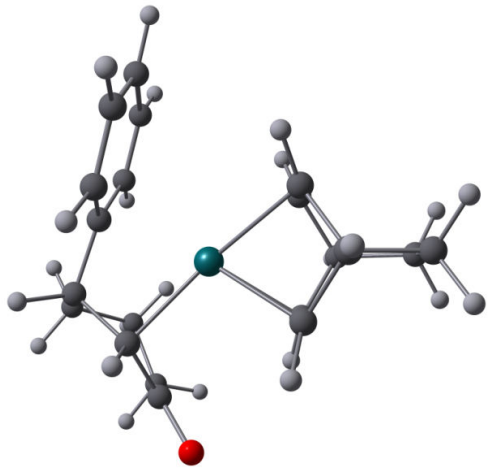


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.200864	0.039539	-0.297534
2	6	0	2.239174	-0.287691	-1.001516
3	6	0	2.305979	-0.700724	1.391181
4	6	0	2.310660	0.304290	0.252971
5	6	0	2.168668	-1.804369	-0.941890
6	6	0	3.500071	-1.672787	1.203215
7	6	0	0.938412	-2.050616	-0.084957
8	6	0	1.011649	-1.459134	1.161173
9	6	0	3.416523	-2.333800	-0.187917
10	1	0	2.332923	-0.215762	2.368798
11	1	0	2.076377	-2.252544	-1.932820
12	1	0	4.433626	-1.112391	1.317214
13	1	0	3.476266	-2.424420	1.998904
14	1	0	3.344619	-3.422889	-0.102715
15	1	0	4.309926	-2.115059	-0.781567
16	1	0	0.192206	-2.796593	-0.345376
17	1	0	2.616520	1.337822	0.394080

18	6	0	-1.874995	-0.442449	-0.142754
19	6	0	-2.431289	-0.763631	1.105417
20	6	0	-2.326123	-1.161766	-1.264830
21	6	0	-3.372783	-1.784689	1.232260
22	1	0	-2.112854	-0.228406	1.997606
23	6	0	-3.254275	-2.192817	-1.138458
24	1	0	-1.949117	-0.905932	-2.254460
25	6	0	-3.785148	-2.509124	0.113441
26	1	0	-3.781945	-2.019409	2.212545
27	1	0	-3.575784	-2.740855	-2.021366
28	1	0	-4.520452	-3.303193	0.213681
29	6	0	-1.642836	1.515819	-0.593001
30	6	0	-0.364599	1.889451	-1.156705
31	1	0	-2.427279	1.364307	-1.329533
32	1	0	-0.216796	1.780703	-2.232543
33	6	0	0.501181	2.887278	-0.527872
34	8	0	1.499836	3.336061	-1.097107
35	6	0	0.116122	3.412710	0.844181
36	1	0	1.029690	3.518299	1.437096
37	6	0	-2.103724	2.282654	0.626814
38	1	0	-2.911196	1.753889	1.139268
39	1	0	2.481647	0.246400	-1.916762
40	1	0	0.331201	-1.700882	1.973280
41	6	0	-0.947167	2.592914	1.564746
42	1	0	-2.534681	3.225007	0.257835
43	1	0	-0.253981	4.432910	0.672886
44	1	0	-1.304450	3.132312	2.448892
45	1	0	-0.507045	1.649859	1.917947

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5537.48689464     A.U. after    1 cycles
             Convg  =    0.4605D-08             -V/T =  2.0039
Zero-point correction=                           0.381908 (Hartree/Particle)
 Thermal correction to Energy=                   0.401369
 Thermal correction to Enthalpy=                 0.402329
 Thermal correction to Gibbs Free Energy=        0.333716
 Sum of electronic and zero-point Energies=          -5537.104987
 Sum of electronic and thermal Energies=             -5537.085526
 Sum of electronic and thermal Enthalpies=           -5537.084566
 Sum of electronic and thermal Free Energies=        -5537.153178
                    1                    2                    3
Frequencies --  -301.5608               34.8408              58.7332
```

BOD-Rh(I)-Ph-CH-si-confU-α-Rhketone (10a)

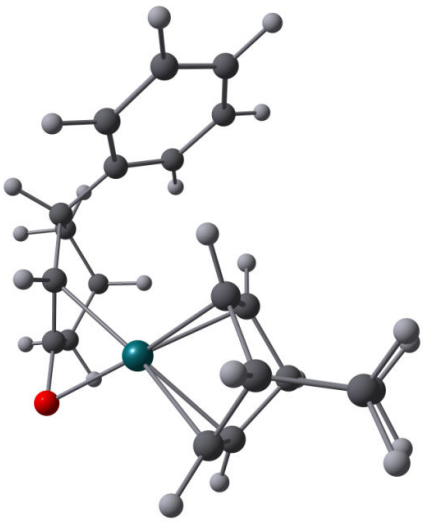


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.141465	0.053823	-0.228618
2	6	0	-1.794462	-1.108147	-0.924234
3	6	0	-2.253290	-0.681266	1.433364
4	6	0	-1.495511	-1.486492	0.392657
5	6	0	-2.800505	0.026683	-0.994696
6	6	0	-3.775653	-0.821994	1.179439
7	6	0	-2.116921	1.115945	-0.182967
8	6	0	-1.827236	0.741012	1.111671
9	6	0	-4.101868	-0.400024	-0.268096
10	1	0	-1.986809	-0.970932	2.451696
11	1	0	-2.996960	0.341888	-2.021214
12	1	0	-4.070479	-1.860481	1.361734
13	1	0	-4.317601	-0.202079	1.901284
14	1	0	-4.809460	0.435477	-0.284407
15	1	0	-4.563131	-1.223018	-0.823423
16	1	0	-2.053448	2.143583	-0.530908
17	1	0	-1.038345	-2.445210	0.623632
18	6	0	1.818413	1.241515	-0.265766
19	6	0	1.709385	1.786848	1.030976
20	6	0	1.177630	1.943145	-1.316187
21	6	0	1.077330	3.011561	1.251773
22	1	0	2.172207	1.278169	1.870804
23	6	0	0.553433	3.175127	-1.091706
24	1	0	1.263631	1.569128	-2.333773
25	6	0	0.510027	3.717223	0.190242
26	1	0	1.037376	3.417148	2.259436
27	1	0	0.111409	3.709544	-1.928639
28	1	0	0.034904	4.679104	0.363034
29	6	0	2.587970	-0.042298	-0.607837
30	6	0	1.498314	-1.017578	-1.070533
31	1	0	3.260590	0.201673	-1.441263
32	1	0	1.293278	-0.991270	-2.145220
33	6	0	1.415420	-2.374758	-0.555330
34	8	0	0.784156	-3.272281	-1.133471
35	6	0	2.102994	-2.693516	0.762508
36	1	0	1.404471	-3.269324	1.378848
37	6	0	3.442747	-0.601829	0.532062
38	1	0	3.958887	0.209979	1.057735
39	1	0	-1.571810	-1.748709	-1.773865
40	1	0	-1.512652	1.443118	1.879472
41	6	0	2.644485	-1.474674	1.496653
42	1	0	2.924826	-3.379742	0.517762
43	1	0	4.230941	-1.222552	0.087411
44	1	0	3.276964	-1.788254	2.335370
45	1	0	1.807671	-0.909919	1.926097

SCF Done: E(RPBE1PBE) = -5537.52891837 A.U. after 1 cycles
Convg = 0.2172D-08 -V/T = 2.0039
Zero-point correction= 0.383971 (Hartree/Particle)
Thermal correction to Energy= 0.403518
Thermal correction to Enthalpy= 0.404478
Thermal correction to Gibbs Free Energy= 0.335938
Sum of electronic and zero-point Energies= -5537.144947
Sum of electronic and thermal Energies= -5537.125400
Sum of electronic and thermal Enthalpies= -5537.124440
Sum of electronic and thermal Free Energies= -5537.192980

	1	2	3
Frequencies --	38.6164	52.0743	67.3153

BOD-Rh(I)-Ph-CH-si-confU-Rh-oxa-π-allyl (11a)

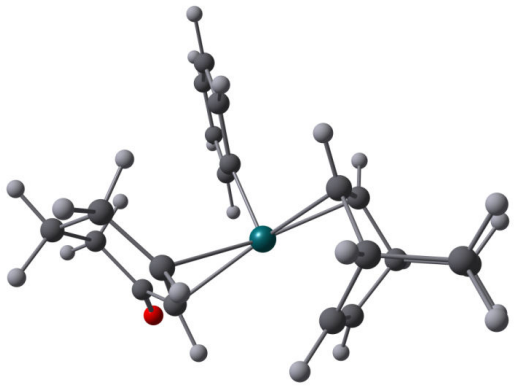


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.807604	-0.856082	-0.415385
2	6	0	-2.941188	-0.453553	-0.659613
3	6	0	-2.319677	0.395140	1.530798
4	6	0	-2.708140	-0.791645	0.667953
5	6	0	-2.750542	1.027562	-0.941779
6	6	0	-3.425132	1.476849	1.452859
7	6	0	-1.304382	1.230414	-0.519107
8	6	0	-1.073865	0.885152	0.815190
9	6	0	-3.681036	1.854695	-0.021397
10	1	0	-2.113716	0.102121	2.562170
11	1	0	-2.908394	1.267110	-1.995102
12	1	0	-4.335389	1.091449	1.923993
13	1	0	-3.108781	2.349756	2.033276
14	1	0	-3.494222	2.919977	-0.192129
15	1	0	-4.722162	1.662478	-0.301249
16	1	0	-0.617352	1.850028	-1.088962
17	1	0	-3.003962	-1.745827	1.096882
18	6	0	2.648724	-0.576665	-0.535442
19	6	0	1.334849	-1.219229	-0.960867
20	1	0	3.312936	-0.646451	-1.407744
21	1	0	1.031573	-1.040428	-1.997072
22	6	0	0.828296	-2.401054	-0.381464
23	8	0	-0.294332	-2.875269	-0.829513
24	6	0	1.457970	-3.011052	0.842613
25	1	0	2.051245	-3.875940	0.514750
26	6	0	3.329290	-1.372591	0.591138
27	1	0	3.912309	-2.179512	0.129606
28	6	0	2.498649	0.915940	-0.277125
29	6	0	2.526800	1.483981	1.000178
30	6	0	2.335613	1.775934	-1.371156
31	6	0	2.385877	2.861340	1.179938
32	1	0	2.662625	0.854063	1.875057
33	6	0	2.193341	3.150479	-1.199234
34	1	0	2.325498	1.360435	-2.377430
35	6	0	2.215469	3.701874	0.082403
36	1	0	2.412876	3.276992	2.184413

37	1	0	2.073142	3.793830	-2.067527
38	1	0	2.109768	4.774506	0.221982
39	1	0	-0.191046	1.211218	1.357436
40	1	0	-3.442280	-1.116628	-1.360386
41	6	0	2.350463	-2.013015	1.570646
42	1	0	0.661823	-3.399650	1.484450
43	1	0	1.719315	-1.250956	2.044248
44	1	0	2.900131	-2.516450	2.373624
45	1	0	4.052639	-0.739608	1.114949

```
SCF Done:  E(RPBE1PBE) =  -5537.53302854     A.U. after    1 cycles
            Convg  =    0.2156D-08             -V/T =  2.0038
Zero-point correction=                           0.384927 (Hartree/Particle)
 Thermal correction to Energy=                    0.404244
 Thermal correction to Enthalpy=                  0.405204
 Thermal correction to Gibbs Free Energy=         0.336143
 Sum of electronic and zero-point Energies=          -5537.148102
 Sum of electronic and thermal Energies=             -5537.128785
 Sum of electronic and thermal Enthalpies=           -5537.127825
 Sum of electronic and thermal Free Energies=        -5537.196886
                     1                      2                      3
Frequencies --    25.7927                39.1178                52.5098
```

BOD-Rh(I)-Ph-CH-si-confD-close (6b)

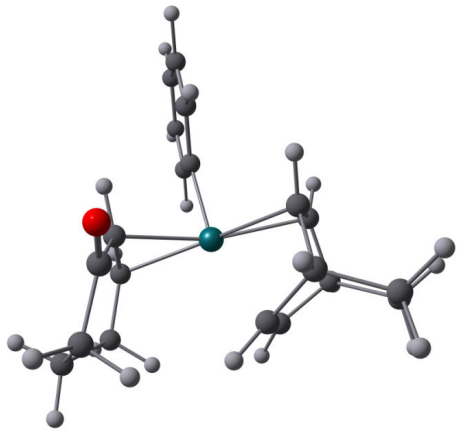


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.394878	-0.177047	-0.203563
2	6	0	2.478688	-1.335021	0.120012
3	6	0	2.909487	0.651221	-1.175218
4	6	0	2.489820	-0.807375	-1.136111
5	6	0	2.871383	-0.349909	1.202698
6	6	0	4.323896	0.759146	-0.545361
7	6	0	1.895199	0.799304	1.031288
8	6	0	1.919545	1.349879	-0.252754
9	6	0	4.297286	0.178268	0.882884
10	1	0	2.888818	1.059568	-2.186984
11	1	0	2.821283	-0.790178	2.200344
12	1	0	5.038730	0.220760	-1.175862
13	1	0	4.626610	1.810949	-0.537900
14	1	0	4.565666	0.938149	1.623595
15	1	0	5.014063	-0.642170	0.988915
16	1	0	1.508133	1.335595	1.893384
17	1	0	2.355020	-1.399506	-2.037607
18	6	0	-1.053372	1.198237	-0.000526

19	6	0	-1.746437	1.498640	-1.186051
20	6	0	-1.345558	1.973446	1.130581
21	6	0	-2.698397	2.518779	-1.236921
22	1	0	-1.559347	0.918381	-2.090944
23	6	0	-2.303521	2.990753	1.087624
24	1	0	-0.827298	1.788144	2.070378
25	6	0	-2.985107	3.269849	-0.096153
26	1	0	-3.222474	2.720313	-2.169031
27	1	0	-2.514095	3.569714	1.984880
28	1	0	-3.729584	4.061288	-0.130389
29	6	0	-0.603206	-1.762085	1.071926
30	6	0	-0.769735	-2.081389	-0.280013
31	1	0	0.273101	-2.156099	1.584200
32	1	0	-0.053047	-2.711874	-0.804228
33	6	0	-2.080902	-1.960512	-0.945033
34	8	0	-2.222608	-2.243538	-2.132328
35	6	0	-3.245375	-1.505382	-0.092518
36	1	0	-3.300904	-0.412058	-0.167329
37	1	0	-4.158669	-1.906056	-0.541662
38	6	0	-3.091430	-1.923077	1.366784
39	1	0	-3.936344	-1.549472	1.954938
40	1	0	-3.116611	-3.018089	1.435374
41	6	0	-1.777537	-1.411711	1.956557
42	1	0	-1.841960	-0.330319	2.106286
43	1	0	2.337075	-2.393800	0.321342
44	1	0	1.547576	2.347237	-0.471730
45	1	0	-1.612745	-1.851428	2.946798

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5537.49764500     A.U. after    1 cycles
             Convg  =    0.2565D-08             -V/T =  2.0039
Zero-point correction=                           0.381958 (Hartree/Particle)
 Thermal correction to Energy=                    0.402477
 Thermal correction to Enthalpy=                  0.403437
 Thermal correction to Gibbs Free Energy=         0.332053
 Sum of electronic and zero-point Energies=          -5537.115687
 Sum of electronic and thermal Energies=             -5537.095168
 Sum of electronic and thermal Enthalpies=           -5537.094208
 Sum of electronic and thermal Free Energies=        -5537.165592
                     A                      A                      A
 Frequencies --    33.4030                49.6329                54.4221
```

BOD-Rh(I)-Ph-CH-si-confD-far (7b)



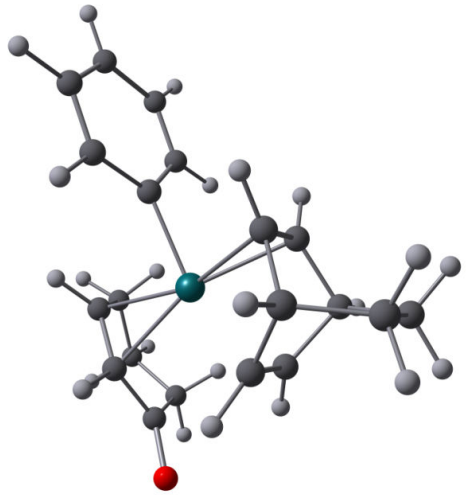
```
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
```

1	45	0	0.081947	-0.121174	-0.354784
2	6	0	-1.811370	-1.242367	-1.231071
3	6	0	-1.923072	-1.484470	1.169172
4	6	0	-2.237173	-0.670346	-0.068595
5	6	0	-1.127048	-2.582635	-1.026689
6	6	0	-2.598809	-2.874989	1.008064
7	6	0	0.010640	-2.281748	-0.063442
8	6	0	-0.422010	-1.683844	1.116139
9	6	0	-2.134941	-3.524360	-0.311441
10	1	0	-2.240097	-0.982412	2.084237
11	1	0	-0.771713	-3.013343	-1.964449
12	1	0	-3.685678	-2.746096	1.023442
13	1	0	-2.336268	-3.497484	1.869106
14	1	0	-1.646765	-4.486618	-0.127664
15	1	0	-2.983282	-3.713151	-0.977216
16	1	0	0.980232	-2.762533	-0.159560
17	1	0	-2.899192	0.187837	-0.036378
18	6	0	2.060843	-0.076250	0.003570
19	6	0	2.684615	-0.083549	1.259331
20	6	0	2.883675	-0.119463	-1.133616
21	6	0	4.075581	-0.143554	1.374708
22	1	0	2.083445	-0.033502	2.165473
23	6	0	4.275054	-0.183915	-1.022330
24	1	0	2.441690	-0.110622	-2.131241
25	6	0	4.878222	-0.197095	0.235206
26	1	0	4.533716	-0.146482	2.361825
27	1	0	4.887648	-0.220177	-1.921127
28	1	0	5.960593	-0.243650	0.325637
29	6	0	0.001766	1.995388	-1.005070
30	1	0	0.932489	2.030263	-1.574198
31	6	0	0.098309	1.996552	0.386914
32	1	0	1.060793	2.030697	0.888405
33	6	0	-1.052299	2.368946	1.240397
34	8	0	-1.008252	2.271387	2.461829
35	6	0	-1.251703	2.478259	-1.705365
36	1	0	-0.977232	2.924969	-2.666787
37	1	0	-1.925317	1.645061	-1.942679
38	6	0	-2.276236	2.949934	0.550865
39	1	0	-3.040081	2.164499	0.500434
40	1	0	-2.682205	3.716529	1.217691
41	6	0	-1.987955	3.501766	-0.841692
42	1	0	-2.921912	3.809913	-1.324161
43	1	0	-1.365494	4.400162	-0.751179
44	1	0	-2.085240	-0.877074	-2.217895
45	1	0	0.181739	-1.648595	2.018614

SCF Done: E(RPBE1PBE) = -5537.49498936 A.U. after 1 cycles
Convg = 0.4202D-08 -V/T = 2.0039
Zero-point correction= 0.381489 (Hartree/Particle)
Thermal correction to Energy= 0.402214
Thermal correction to Enthalpy= 0.403174
Thermal correction to Gibbs Free Energy= 0.330594
Sum of electronic and zero-point Energies= -5537.113500
Sum of electronic and thermal Energies= -5537.092775
Sum of electronic and thermal Enthalpies= -5537.091815
Sum of electronic and thermal Free Energies= -5537.164396

	1	2	3
Frequencies --	27.2806	40.9996	49.6059

BOD-Rh(I)-Ph-CH-si-confD-anti (8b)

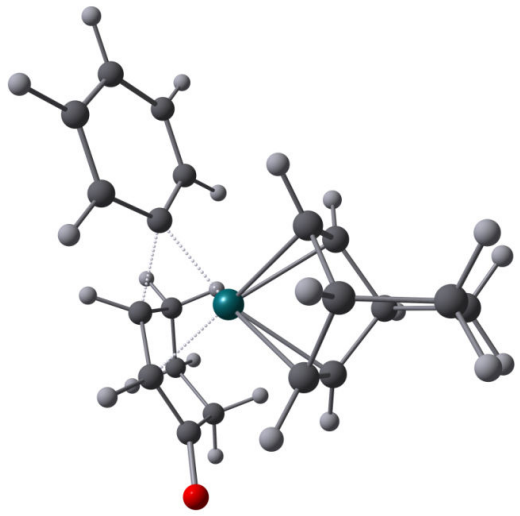


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.114713	-0.049260	-0.230155
2	6	0	2.217508	-0.612215	-0.874584
3	6	0	2.026160	-1.287109	1.442271
4	6	0	2.311943	-0.193572	0.432524
5	6	0	1.854391	-2.080048	-1.012632
6	6	0	3.017446	-2.455929	1.201000
7	6	0	0.540295	-2.178989	-0.259671
8	6	0	0.631889	-1.742035	1.059048
9	6	0	2.919153	-2.925031	-0.264711
10	1	0	2.074855	-0.923049	2.470085
11	1	0	1.756077	-2.385305	-2.055693
12	1	0	4.030834	-2.117231	1.438953
13	1	0	2.779445	-3.270514	1.892567
14	1	0	2.637464	-3.981238	-0.323062
15	1	0	3.880221	-2.818700	-0.777885
16	1	0	-0.285973	-2.782214	-0.624448
17	1	0	2.761412	0.753609	0.715283
18	6	0	-1.891714	-0.529288	-0.083427
19	6	0	-2.563013	-0.573652	1.147772
20	6	0	-2.601692	-0.973409	-1.211980
21	6	0	-3.879473	-1.032953	1.250707
22	1	0	-2.058843	-0.243092	2.055660
23	6	0	-3.914861	-1.439168	-1.116800
24	1	0	-2.126677	-0.954934	-2.192721
25	6	0	-4.563673	-1.470702	0.117995
26	1	0	-4.369674	-1.049443	2.222422
27	1	0	-4.433565	-1.775778	-2.012559
28	1	0	-5.586985	-1.829706	0.194970
29	6	0	-0.992496	1.908740	-0.695222
30	6	0	0.319765	1.961811	-1.151998
31	1	0	-1.764648	1.623312	-1.402140
32	1	0	0.559226	1.700333	-2.182227
33	6	0	1.367185	2.702468	-0.422988
34	8	0	2.497380	2.837164	-0.883077
35	6	0	0.967896	3.306572	0.906980
36	1	0	1.085335	2.530214	1.675934
37	1	0	1.675031	4.106931	1.140772

38	6	0	-0.478030	3.795643	0.886491
39	1	0	-0.742982	4.230865	1.855739
40	1	0	-0.574256	4.595808	0.142220
41	6	0	-1.440018	2.662229	0.539083
42	1	0	-1.536317	1.981300	1.391294
43	1	0	-2.445449	3.057963	0.361764
44	1	0	2.575379	-0.016037	-1.709526
45	1	0	-0.122990	-1.973899	1.805037

```
SCF Done:  E(RPBE1PBE) =  -5537.50010489     A.U. after    1 cycles
             Convg  =    0.4077D-08             -V/T =  2.0039
Zero-point correction=                           0.382445 (Hartree/Particle)
 Thermal correction to Energy=                    0.402905
 Thermal correction to Enthalpy=                  0.403865
 Thermal correction to Gibbs Free Energy=         0.332484
 Sum of electronic and zero-point Energies=          -5537.117659
 Sum of electronic and thermal Energies=             -5537.097200
 Sum of electronic and thermal Enthalpies=           -5537.096240
 Sum of electronic and thermal Free Energies=        -5537.167621
                     1                      2                      3
Frequencies --    31.9062                53.0136                57.5389
```

BOD-Rh(I)-Ph-CH-si-confD-CR-TS (9b)

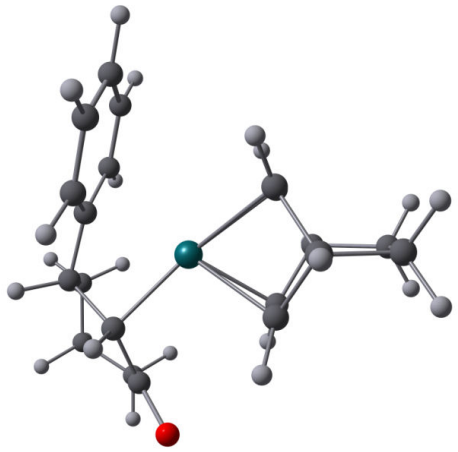


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.196790	-0.007578	-0.263715
2	6	0	2.235744	-0.281846	-0.993561
3	6	0	2.341526	-0.668736	1.402412
4	6	0	2.306871	0.324014	0.254028
5	6	0	2.207309	-1.799619	-0.917748
6	6	0	3.557692	-1.612358	1.211158
7	6	0	0.993436	-2.069693	-0.044974
8	6	0	1.063881	-1.461018	1.194256
9	6	0	3.477117	-2.288023	-0.173277
10	1	0	2.366291	-0.172831	2.374657
11	1	0	2.115692	-2.259871	-1.903149
12	1	0	4.478458	-1.028631	1.311196
13	1	0	3.559717	-2.357070	2.013695
14	1	0	3.435892	-3.377841	-0.077697
15	1	0	4.357761	-2.050398	-0.778608

16	1	0	0.265971	-2.839329	-0.288997
17	1	0	2.589344	1.365924	0.382095
18	6	0	-1.860503	-0.552997	-0.082715
19	6	0	-2.437221	-0.962176	1.128262
20	6	0	-2.300369	-1.178202	-1.265199
21	6	0	-3.385532	-1.985062	1.162285
22	1	0	-2.137441	-0.493027	2.062498
23	6	0	-3.230850	-2.213885	-1.229910
24	1	0	-1.911331	-0.846803	-2.227112
25	6	0	-3.781666	-2.622437	-0.013302
26	1	0	-3.814182	-2.287939	2.115187
27	1	0	-3.539420	-2.693350	-2.156280
28	1	0	-4.520843	-3.418655	0.015578
29	6	0	-1.624706	1.442521	-0.313898
30	6	0	-0.458379	1.839863	-1.072101
31	1	0	-2.530372	1.361467	-0.907845
32	1	0	-0.489613	1.716205	-2.156534
33	6	0	0.446454	2.900984	-0.625597
34	8	0	1.377778	3.304450	-1.324336
35	6	0	0.167897	3.531107	0.728110
36	1	0	0.732699	2.973052	1.487479
37	1	0	0.575847	4.545545	0.708090
38	6	0	-1.318029	3.510961	1.073351
39	1	0	-1.485494	3.951986	2.062219
40	1	0	-1.871747	4.125811	0.352772
41	6	0	-1.846288	2.079133	1.051599
42	1	0	-1.322232	1.514117	1.829259
43	1	0	-2.910797	2.045311	1.303583
44	1	0	2.450754	0.250251	-1.916721
45	1	0	0.400957	-1.713720	2.017432

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5537.48273485     A.U. after    1 cycles
             Convg  =    0.8501D-08             -V/T =  2.0038
Zero-point correction=                           0.382074 (Hartree/Particle)
 Thermal correction to Energy=                    0.401554
 Thermal correction to Enthalpy=                  0.402514
 Thermal correction to Gibbs Free Energy=         0.334005
 Sum of electronic and zero-point Energies=          -5537.100661
 Sum of electronic and thermal Energies=             -5537.081181
 Sum of electronic and thermal Enthalpies=           -5537.080221
 Sum of electronic and thermal Free Energies=        -5537.148730
                    1                    2                    3
Frequencies --  -299.5886               45.8692              57.6815
```

BOD-Rh(I)-Ph-CH-si-confD-α-Rhketone (10b)

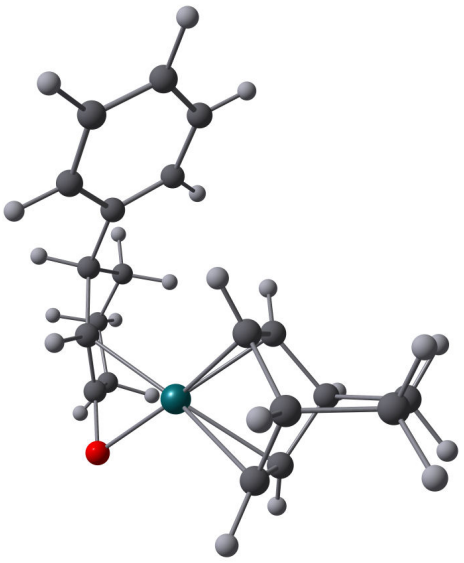


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.203248	0.055419	-0.181042
2	6	0	-1.633844	-1.375364	-0.861526
3	6	0	-2.201968	-0.940832	1.470474
4	6	0	-1.305299	-1.654220	0.473448
5	6	0	-2.804544	-0.416635	-0.990736
6	6	0	-3.677885	-1.328278	1.200423
7	6	0	-2.314744	0.796304	-0.214617
8	6	0	-1.994733	0.518718	1.098524
9	6	0	-4.037779	-1.012663	-0.265630
10	1	0	-1.913739	-1.146673	2.503195
11	1	0	-3.027350	-0.175582	-2.031915
12	1	0	-3.808777	-2.393611	1.416478
13	1	0	-4.324681	-0.777907	1.891664
14	1	0	-4.863781	-0.296106	-0.322268
15	1	0	-4.358149	-1.915521	-0.795404
16	1	0	-2.412282	1.807290	-0.601895
17	1	0	-0.709309	-2.520902	0.749484
18	6	0	1.584545	1.535355	-0.169834
19	6	0	1.333546	2.176843	1.061192
20	6	0	0.927466	2.054349	-1.312180
21	6	0	0.528364	3.313512	1.136856
22	1	0	1.807874	1.812187	1.966392
23	6	0	0.123077	3.195974	-1.231772
24	1	0	1.123418	1.615248	-2.286956
25	6	0	-0.073718	3.832691	-0.009386
26	1	0	0.376553	3.796552	2.098720
27	1	0	-0.340067	3.586018	-2.134382
28	1	0	-0.691351	4.724729	0.051430
29	6	0	2.515359	0.325618	-0.332328
30	6	0	1.609505	-0.762444	-0.918886
31	1	0	3.314528	0.599790	-1.039115
32	1	0	1.442450	-0.662715	-1.997609
33	6	0	1.800926	-2.171119	-0.588221
34	8	0	1.256466	-3.079590	-1.228913
35	6	0	2.684320	-2.523833	0.598007
36	1	0	2.042641	-2.580160	1.488143
37	1	0	3.076986	-3.530585	0.428491
38	6	0	3.790419	-1.500384	0.830712
39	1	0	4.361410	-1.757887	1.729774
40	1	0	4.498502	-1.519164	-0.008219
41	6	0	3.184140	-0.110657	0.970000
42	1	0	2.442983	-0.153465	1.778452
43	1	0	3.942120	0.624053	1.265914
44	1	0	-1.292492	-1.999961	-1.683112
45	1	0	-1.815948	1.289621	1.843838

SCF Done: E(RPBE1PBE) = -5537.52786184 A.U. after 1 cycles
Convg = 0.6417D-08 -V/T = 2.0039
Zero-point correction= 0.384187 (Hartree/Particle)
Thermal correction to Energy= 0.403754
Thermal correction to Enthalpy= 0.404714
Thermal correction to Gibbs Free Energy= 0.335839
Sum of electronic and zero-point Energies= -5537.143675
Sum of electronic and thermal Energies= -5537.124108
Sum of electronic and thermal Enthalpies= -5537.123148
Sum of electronic and thermal Free Energies= -5537.192023

	1	2	3
Frequencies --	40.0380	43.5289	63.5205

BOD-Rh(I)-Ph-CH-si-confD-Rh-oxa-π-allyl (11b)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.861711	-0.756927	-0.453772
2	6	0	-2.908530	-0.091018	-0.861987
3	6	0	-2.490713	0.345549	1.489832
4	6	0	-2.877862	-0.648016	0.409328
5	6	0	-2.544607	1.384625	-0.879702
6	6	0	-3.470244	1.544339	1.467406
7	6	0	-1.150098	1.360369	-0.274455
8	6	0	-1.123795	0.794975	1.004023
9	6	0	-3.502480	2.163925	0.054556
10	1	0	-2.444731	-0.118702	2.476932
11	1	0	-2.546124	1.794483	-1.891459
12	1	0	-4.464660	1.198660	1.768506
13	1	0	-3.147616	2.279505	2.212064
14	1	0	-3.197681	3.215292	0.079357
15	1	0	-4.513402	2.132612	-0.365093
16	1	0	-0.342276	1.978025	-0.659574
17	1	0	-3.313665	-1.616172	0.643121
18	6	0	2.507574	-0.712571	-0.072569
19	6	0	1.275708	-1.195244	-0.814841
20	1	0	3.385351	-1.054399	-0.645764
21	1	0	1.147609	-0.838695	-1.841307
22	6	0	0.657664	-2.431391	-0.519522
23	8	0	-0.437366	-2.731444	-1.143184
24	6	0	1.129047	-3.313287	0.610336
25	1	0	0.368523	-3.285783	1.399332
26	1	0	1.143061	-4.343838	0.238311
27	6	0	2.495345	-2.898039	1.151138
28	1	0	2.676855	-3.387619	2.113730
29	1	0	3.283163	-3.245191	0.470652
30	6	0	2.596644	-1.382142	1.297344
31	1	0	1.779802	-1.032572	1.942419
32	1	0	3.538174	-1.107612	1.786339
33	6	0	2.586506	0.804113	-0.060908
34	6	0	2.480333	1.567744	1.104715
35	6	0	2.775053	1.481812	-1.273256

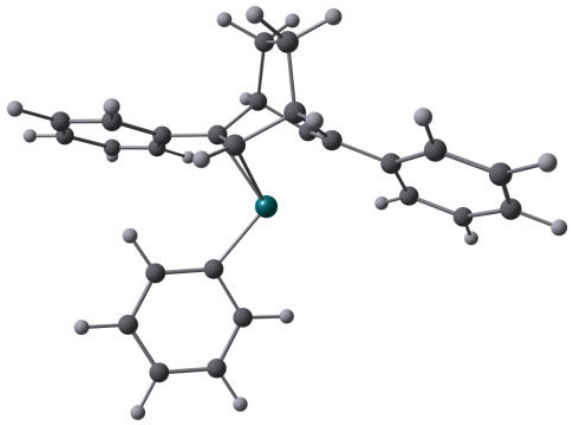
36	6	0	2.540936	2.962198	1.059958
37	1	0	2.353949	1.079572	2.066948
38	6	0	2.835899	2.871316	-1.324929
39	1	0	2.878948	0.909704	-2.193572
40	6	0	2.714081	3.621475	-0.154049
41	1	0	2.454900	3.533162	1.981340
42	1	0	2.983426	3.370499	-2.279487
43	1	0	2.761961	4.706714	-0.188906
44	1	0	-0.294594	0.943306	1.689811
45	1	0	-3.373830	-0.582077	-1.713011

SCF Done: E(RPBE1PBE) = -5537.53736410 A.U. after 1 cycles
Convg = 0.3645D-08 -V/T = 2.0038
Zero-point correction= 0.384547 (Hartree/Particle)
Thermal correction to Energy= 0.403942
Thermal correction to Enthalpy= 0.404902
Thermal correction to Gibbs Free Energy= 0.335808
Sum of electronic and zero-point Energies= -5537.152817
Sum of electronic and thermal Energies= -5537.133422
Sum of electronic and thermal Enthalpies= -5537.132462
Sum of electronic and thermal Free Energies= -5537.201556

	1	2	3
Frequencies --	32.2971	42.2653	47.2655

(S)-PhBOD-Rh pathway

(*S*)-PhBOD-Rh(I)-Ph (12)

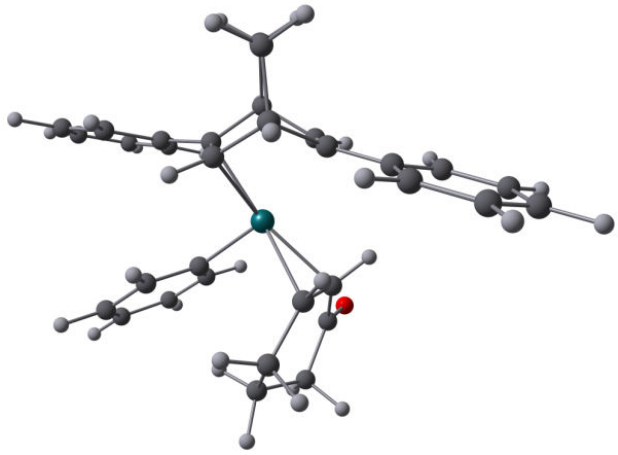


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.192605	0.527314	0.336416
2	6	0	1.907399	-0.962327	0.017016
3	6	0	-0.007811	-2.178658	0.896160
4	6	0	-2.993649	-1.223348	1.338901
5	6	0	3.243361	-0.334783	0.020546
6	6	0	3.673979	0.434043	1.116823
7	6	0	1.223888	-1.340199	1.156557
8	6	0	1.230877	-1.480749	-1.248360
9	6	0	5.399737	0.078523	-1.030292
10	6	0	-5.147149	-1.597844	0.309202
11	6	0	0.386132	-3.442852	0.093200
12	6	0	-0.162877	-0.881580	-1.154807
13	6	0	4.937884	1.011143	1.138945

14	6	0	-0.874358	-1.285660	0.007588
15	6	0	-3.132145	-1.658806	-1.023702
16	6	0	4.130658	-0.497074	-1.053130
17	6	0	1.136747	-3.024122	-1.186970
18	6	0	5.810665	0.836748	0.063383
19	6	0	-2.347394	-1.380042	0.103534
20	6	0	-4.519092	-1.763973	-0.923057
21	6	0	-4.376043	-1.327523	1.441785
22	1	0	-2.404219	-0.982517	2.220465
23	1	0	-6.228086	-1.677141	0.388797
24	1	0	-2.652394	-1.803067	-1.988259
25	1	0	-5.108524	-1.980216	-1.810518
26	1	0	-4.857342	-1.187228	2.406276
27	1	0	3.002960	0.592225	1.957979
28	1	0	6.069843	-0.068197	-1.873428
29	1	0	5.242312	1.606561	1.995928
30	1	0	3.839514	-1.092481	-1.913617
31	1	0	6.797752	1.290700	0.077903
32	1	0	-0.519891	-2.445354	1.822613
33	1	0	1.735647	-1.143759	-2.154805
34	1	0	1.010482	-4.083257	0.724356
35	1	0	-0.520562	-4.009130	-0.144284
36	1	0	0.619148	-3.382857	-2.082809
37	1	0	2.146069	-3.448524	-1.208125
38	1	0	-0.671586	-0.536707	-2.052863
39	1	0	1.641939	-1.251779	2.156515
40	6	0	-1.102854	1.988521	-0.129711
41	6	0	-2.433296	2.000391	-0.572325
42	6	0	-0.485442	3.232043	0.094912
43	6	0	-3.116876	3.201667	-0.771868
44	1	0	-2.956162	1.063921	-0.755214
45	6	0	-1.160868	4.439011	-0.101502
46	1	0	0.557489	3.279412	0.426774
47	6	0	-2.485456	4.424647	-0.537774
48	1	0	-4.151702	3.184028	-1.108652
49	1	0	-0.654962	5.385152	0.080218
50	1	0	-3.021069	5.357894	-0.694305

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5690.72610703     A.U. after    1 cycles
             Convg  =    0.2906D-08             -V/T =  2.0042
Zero-point correction=                           0.414010 (Hartree/Particle)
 Thermal correction to Energy=                    0.437129
 Thermal correction to Enthalpy=                  0.438089
 Thermal correction to Gibbs Free Energy=         0.359176
 Sum of electronic and zero-point Energies=          -5690.312097
 Sum of electronic and thermal Energies=             -5690.288978
 Sum of electronic and thermal Enthalpies=           -5690.288018
 Sum of electronic and thermal Free Energies=        -5690.366931
                    1                      2                      3
Frequencies --    27.8539               33.9789                38.7313
```

(*S*)-PhBOD-Rh(I)-Ph-CH-si-confU-close (13a)

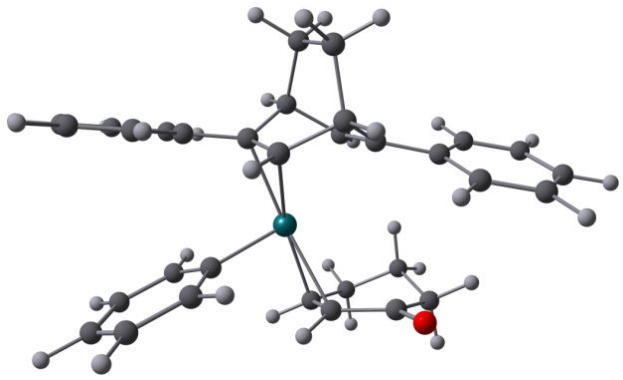


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.087353	0.174976	0.195132
2	6	0	1.854461	-1.590831	0.070490
3	6	0	-0.164602	-2.471880	1.101200
4	6	0	-3.145002	-1.473856	1.344118
5	6	0	3.267943	-1.170835	-0.012699
6	6	0	3.988496	-0.805755	1.139736
7	6	0	1.128876	-1.699795	1.228914
8	6	0	1.095081	-2.184371	-1.107701
9	6	0	5.288785	-0.746493	-1.312132
10	6	0	-5.284405	-1.974846	0.340757
11	6	0	0.165197	-3.872887	0.520280
12	6	0	-0.268288	-1.517833	-1.109873
13	6	0	5.319513	-0.414653	1.067491
14	6	0	-1.005264	-1.727814	0.063434
15	6	0	-3.251928	-2.201974	-0.945030
16	6	0	3.951985	-1.132572	-1.238350
17	6	0	0.889688	-3.698451	-0.827259
18	6	0	5.981068	-0.382083	-0.160914
19	6	0	-2.481411	-1.784717	0.148442
20	6	0	-4.638987	-2.293278	-0.852277
21	6	0	-4.529106	-1.564973	1.440061
22	1	0	-2.571839	-1.130036	2.201837
23	1	0	-6.366332	-2.045888	0.415063
24	1	0	-2.758388	-2.474579	-1.874354
25	1	0	-5.216113	-2.621836	-1.713043
26	1	0	-5.022753	-1.305844	2.373196
27	1	0	3.509043	-0.833356	2.113651
28	1	0	5.787886	-0.729761	-2.277439
29	1	0	5.845023	-0.135976	1.977030
30	1	0	3.446158	-1.408566	-2.157850
31	1	0	7.022703	-0.078177	-0.216751
32	1	0	-0.679541	-2.555233	2.059683
33	1	0	1.599575	-2.034134	-2.061332
34	1	0	0.788502	-4.416983	1.237033
35	1	0	-0.765837	-4.436606	0.403742
36	1	0	0.307146	-4.128938	-1.648100
37	1	0	1.862712	-4.200194	-0.824195
38	1	0	-0.746227	-1.282534	-2.057683
39	1	0	1.522474	-1.453809	2.211099

40	6	0	-1.539589	1.259121	-0.230673
41	6	0	-2.088025	1.973140	0.845839
42	6	0	-2.219117	1.298098	-1.454971
43	6	0	-3.268898	2.704526	0.703247
44	1	0	-1.583522	1.982071	1.812338
45	6	0	-3.394113	2.037518	-1.604784
46	1	0	-1.829583	0.757167	-2.315439
47	6	0	-3.926002	2.745183	-0.526675
48	1	0	-3.668858	3.252871	1.553902
49	1	0	-3.897931	2.058299	-2.569356
50	1	0	-4.840766	3.320943	-0.643343
51	6	0	1.470244	1.621324	-0.864289
52	6	0	1.573503	1.803099	0.516896
53	1	0	2.135379	0.900060	-1.336504
54	1	0	2.293728	1.231293	1.100759
55	6	0	1.126862	3.051565	1.166421
56	8	0	1.129490	3.174145	2.388475
57	6	0	0.808897	4.217731	0.257300
58	1	0	0.168608	4.918366	0.799632
59	6	0	0.970469	2.703026	-1.781581
60	6	0	0.209802	3.833545	-1.092712
61	1	0	1.775177	4.723106	0.109388
62	1	0	-0.831349	3.540229	-0.950768
63	1	0	1.869455	3.106618	-2.274470
64	1	0	0.362036	2.274187	-2.585398
65	1	0	0.199814	4.712301	-1.747279

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5999.08060756     A.U. after    1 cycles
             Convg  =    0.6934D-08             -V/T =  2.0047
Zero-point correction=                           0.544529 (Hartree/Particle)
 Thermal correction to Energy=                    0.575121
 Thermal correction to Enthalpy=                  0.576081
 Thermal correction to Gibbs Free Energy=         0.481129
 Sum of electronic and zero-point Energies=          -5998.536079
 Sum of electronic and thermal Energies=             -5998.505486
 Sum of electronic and thermal Enthalpies=           -5998.504526
 Sum of electronic and thermal Free Energies=        -5998.599479
                     1                    2                    3
Frequencies --    17.4036              27.8160              38.5945
```

(*S*)-PhBOD-Rh(I)-Ph-CH-si-confU-far (14a)

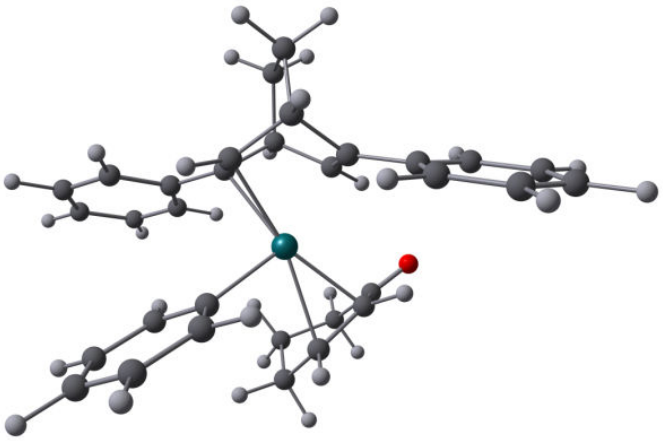


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.272361	-0.501945	0.329192
2	6	0	-1.089136	1.670699	1.062021

3	6	0	-0.921039	1.769438	-1.308423
4	6	0	-1.760253	1.429150	-0.094537
5	6	0	0.238757	2.366349	0.885885
6	6	0	-0.690598	3.311270	-1.255237
7	6	0	1.124699	1.500013	-0.003137
8	6	0	0.437455	1.117541	-1.160847
9	6	0	-0.032729	3.675612	0.086901
10	1	0	-1.401057	1.487271	-2.245199
11	1	0	0.701649	2.591133	1.847070
12	1	0	-1.650084	3.822484	-1.383249
13	1	0	-0.055632	3.596794	-2.099733
14	1	0	0.915534	4.201559	-0.062992
15	1	0	-0.679360	4.328495	0.681642
16	6	0	1.933204	-1.423121	-0.272915
17	6	0	2.183729	-1.798879	-1.600124
18	6	0	2.917161	-1.704932	0.685695
19	6	0	3.383964	-2.418101	-1.958711
20	1	0	1.439621	-1.609008	-2.371358
21	6	0	4.117055	-2.323384	0.329553
22	1	0	2.761210	-1.426165	1.727423
23	6	0	4.358013	-2.681127	-0.996941
24	1	0	3.554014	-2.697233	-2.996783
25	1	0	4.867212	-2.521082	1.092610
26	1	0	5.292210	-3.162032	-1.276046
27	6	0	-0.392700	-2.475098	1.123185
28	1	0	0.575763	-2.922186	1.350437
29	6	0	-0.787495	-2.421944	-0.211492
30	1	0	-0.137947	-2.793275	-0.999140
31	6	0	-2.215932	-2.343265	-0.584148
32	8	0	-2.570158	-2.387610	-1.758068
33	6	0	-1.377442	-2.415514	2.260176
34	1	0	-1.546874	-3.448387	2.603896
35	6	0	-3.223475	-2.356431	0.545353
36	6	0	-2.699890	-1.779405	1.855342
37	1	0	-0.938906	-1.888424	3.116130
38	1	0	-2.561994	-0.700425	1.741628
39	1	0	-3.445191	-1.916547	2.646128
40	1	0	-4.134766	-1.856269	0.208786
41	1	0	-3.480318	-3.417225	0.685976
42	1	0	-1.535767	1.571690	2.048652
43	1	0	0.950058	0.782475	-2.058755
44	6	0	-3.201195	1.137128	-0.211092
45	6	0	-4.084470	1.484040	0.826870
46	6	0	-3.744682	0.568721	-1.372480
47	6	0	-5.450790	1.253930	0.715713
48	1	0	-3.699898	1.965700	1.721666
49	6	0	-5.114264	0.344335	-1.488126
50	1	0	-3.094891	0.258797	-2.183943
51	6	0	-5.974248	0.683777	-0.446103
52	1	0	-6.112450	1.536308	1.530582
53	1	0	-5.505742	-0.111348	-2.393375
54	1	0	-7.043183	0.510463	-0.537877
55	6	0	2.596252	1.583335	0.143815
56	6	0	3.447972	1.563336	-0.970866
57	6	0	3.185439	1.698042	1.412820
58	6	0	4.829192	1.635163	-0.822835
59	1	0	3.025771	1.493373	-1.968731
60	6	0	4.566873	1.778231	1.563618
61	1	0	2.560793	1.702580	2.302479
62	6	0	5.398452	1.743686	0.445597
63	1	0	5.464914	1.610630	-1.704232
64	1	0	4.995526	1.859998	2.559429
65	1	0	6.477508	1.802675	0.560599

```
 ----------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5999.07462228     A.U. after    1 cycles
             Convg  =    0.2587D-08             -V/T =  2.0047
Zero-point correction=                           0.544601 (Hartree/Particle)
 Thermal correction to Energy=                    0.575160
 Thermal correction to Enthalpy=                  0.576120
 Thermal correction to Gibbs Free Energy=         0.482196
 Sum of electronic and zero-point Energies=          -5998.530021
 Sum of electronic and thermal Energies=             -5998.499462
 Sum of electronic and thermal Enthalpies=           -5998.498502
 Sum of electronic and thermal Free Energies=        -5998.592426
                    1                    2                    3
Frequencies --    23.6611              35.7842              37.8011
```

(*S*)-PhBOD-Rh(I)-Ph-CH-si-confU-anti (15a)

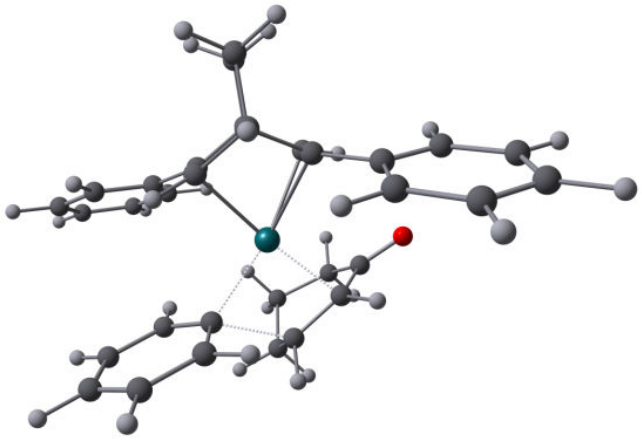


```
---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1         45           0       -0.166185   -0.324353   -0.061371
      2          6           0       -1.813642    1.263833   -0.322855
      3          6           0       -0.012791    2.313211    0.929366
      4          6           0        2.876011    1.428011    1.590555
      5          6           0       -3.160894    0.721249   -0.589750
      6          6           0       -4.175010    0.788906    0.376239
      7          6           0       -1.246781    1.439337    0.925873
      8          6           0       -1.011364    1.970497   -1.408210
      9          6           0       -4.721235   -0.400191   -2.081100
     10          6           0        5.166844    1.627061    0.851072
     11          6           0       -0.362314    3.692260    0.314237
     12          6           0        0.382774    1.394598   -1.266745
     13          6           0       -5.440533    0.269995    0.118265
     14          6           0        0.960661    1.610306   -0.010390
     15          6           0        3.353758    1.809343   -0.735952
     16          6           0       -3.456594    0.119659   -1.823061
     17          6           0       -0.976979    3.485164   -1.081916
     18          6           0       -5.720886   -0.325369   -1.111004
     19          6           0        2.408183    1.608724    0.279607
     20          6           0        4.716931    1.817574   -0.454434
     21          6           0        4.238114    1.431762    1.873753
     22          1           0        2.167936    1.258496    2.397494
     23          1           0        6.231090    1.633291    1.071074
     24          1           0        3.020335    1.965240   -1.757588
     25          1           0        5.430603    1.975230   -1.258848
```

26	1	0	4.576462	1.279760	2.895505
27	1	0	-3.972124	1.250119	1.337654
28	1	0	-4.926190	-0.868757	-3.040203
29	1	0	-6.211648	0.333098	0.881442
30	1	0	-2.681202	0.033302	-2.580017
31	1	0	-6.709898	-0.728639	-1.311573
32	1	0	0.393573	2.429300	1.934538
33	1	0	-1.419491	1.796412	-2.404192
34	1	0	-1.061104	4.205649	0.982216
35	1	0	0.545496	4.302274	0.264558
36	1	0	-0.390522	3.994967	-1.852980
37	1	0	-1.994891	3.884926	-1.132854
38	1	0	0.968175	1.138202	-2.144803
39	1	0	-1.749028	1.163108	1.848257
40	6	0	1.288429	-1.371925	-1.098718
41	6	0	2.633694	-1.493701	-0.724361
42	6	0	0.927503	-1.888470	-2.356504
43	6	0	3.576299	-2.093930	-1.564791
44	1	0	2.969873	-1.112652	0.238021
45	6	0	1.864659	-2.481713	-3.204765
46	1	0	-0.108928	-1.831057	-2.689612
47	6	0	3.199594	-2.588726	-2.811908
48	1	0	4.612240	-2.168838	-1.239376
49	1	0	1.548763	-2.865192	-4.173300
50	1	0	3.932339	-3.053820	-3.466987
51	6	0	-0.428724	-2.522912	0.564149
52	6	0	-1.449985	-1.735206	1.087536
53	1	0	-0.609838	-3.042900	-0.373879
54	1	0	-2.400976	-1.635254	0.567352
55	6	0	-1.470716	-1.369629	2.518458
56	8	0	-2.427218	-0.779115	3.016742
57	6	0	-0.320181	-1.837390	3.385335
58	1	0	-0.157040	-1.090569	4.167903
59	6	0	0.656953	-3.083428	1.439691
60	6	0	0.955213	-2.173870	2.622267
61	1	0	-0.694209	-2.736670	3.895898
62	1	0	1.415517	-1.251030	2.247546
63	1	0	1.679922	-2.645540	3.294969
64	1	0	0.311454	-4.064855	1.800954
65	1	0	1.557439	-3.268978	0.848948

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5999.08904453     A.U. after    1 cycles
             Convg  =    0.6309D-08             -V/T =  2.0047
Zero-point correction=                           0.545455 (Hartree/Particle)
 Thermal correction to Energy=                    0.575734
 Thermal correction to Enthalpy=                  0.576694
 Thermal correction to Gibbs Free Energy=         0.483204
 Sum of electronic and zero-point Energies=          -5998.543590
 Sum of electronic and thermal Energies=             -5998.513311
 Sum of electronic and thermal Enthalpies=           -5998.512351
 Sum of electronic and thermal Free Energies=        -5998.605840
                     1                      2                      3
Frequencies --    24.7900                38.5193                39.9303
```

(*S*)-PhBOD-Rh(I)-Ph-CH-si-confU-CR-TS (16a)

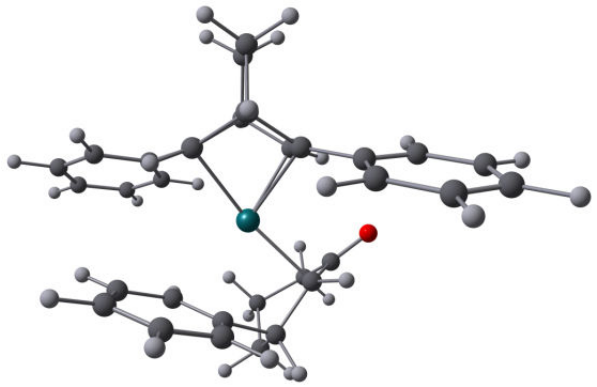


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.087353	0.174976	0.195132
2	6	0	1.854461	-1.590831	0.070490
3	6	0	-0.164602	-2.471880	1.101200
4	6	0	-3.145002	-1.473856	1.344118
5	6	0	3.267943	-1.170835	-0.012699
6	6	0	3.988496	-0.805755	1.139736
7	6	0	1.128876	-1.699795	1.228914
8	6	0	1.095081	-2.184371	-1.107701
9	6	0	5.288785	-0.746493	-1.312132
10	6	0	-5.284405	-1.974846	0.340757
11	6	0	0.165197	-3.872887	0.520280
12	6	0	-0.268288	-1.517833	-1.109873
13	6	0	5.319513	-0.414653	1.067491
14	6	0	-1.005264	-1.727814	0.063434
15	6	0	-3.251928	-2.201974	-0.945030
16	6	0	3.951985	-1.132572	-1.238350
17	6	0	0.889688	-3.698451	-0.827259
18	6	0	5.981068	-0.382083	-0.160914
19	6	0	-2.481411	-1.784717	0.148442
20	6	0	-4.638987	-2.293278	-0.852277
21	6	0	-4.529106	-1.564973	1.440061
22	1	0	-2.571839	-1.130036	2.201837
23	1	0	-6.366332	-2.045888	0.415063
24	1	0	-2.758388	-2.474579	-1.874354
25	1	0	-5.216113	-2.621836	-1.713043
26	1	0	-5.022753	-1.305844	2.373196
27	1	0	3.509043	-0.833356	2.113651
28	1	0	5.787886	-0.729761	-2.277439
29	1	0	5.845023	-0.135976	1.977030
30	1	0	3.446158	-1.408566	-2.157850
31	1	0	7.022703	-0.078177	-0.216751
32	1	0	-0.679541	-2.555233	2.059683
33	1	0	1.599575	-2.034134	-2.061332
34	1	0	0.788502	-4.416983	1.237033
35	1	0	-0.765837	-4.436606	0.403742
36	1	0	0.307146	-4.128938	-1.648100
37	1	0	1.862712	-4.200194	-0.824195
38	1	0	-0.746227	-1.282534	-2.057683
39	1	0	1.522474	-1.453809	2.211099

40	6	0	-1.539589	1.259121	-0.230673
41	6	0	-2.088025	1.973140	0.845839
42	6	0	-2.219117	1.298098	-1.454971
43	6	0	-3.268898	2.704526	0.703247
44	1	0	-1.583522	1.982071	1.812338
45	6	0	-3.394113	2.037518	-1.604784
46	1	0	-1.829583	0.757167	-2.315439
47	6	0	-3.926002	2.745183	-0.526675
48	1	0	-3.668858	3.252871	1.553902
49	1	0	-3.897931	2.058299	-2.569356
50	1	0	-4.840766	3.320943	-0.643343
51	6	0	1.470244	1.621324	-0.864289
52	6	0	1.573503	1.803099	0.516896
53	1	0	2.135379	0.900060	-1.336504
54	1	0	2.293728	1.231293	1.100759
55	6	0	1.126862	3.051565	1.166421
56	8	0	1.129490	3.174145	2.388475
57	6	0	0.808897	4.217731	0.257300
58	1	0	0.168608	4.918366	0.799632
59	6	0	0.970469	2.703026	-1.781581
60	6	0	0.209802	3.833545	-1.092712
61	1	0	1.775177	4.723106	0.109388
62	1	0	-0.831349	3.540229	-0.950768
63	1	0	1.869455	3.106618	-2.274470
64	1	0	0.362036	2.274187	-2.585398
65	1	0	0.199814	4.712301	-1.747279

```
SCF Done:  E(RPBE1PBE) =  -5999.08060756     A.U. after    1 cycles
             Convg  =    0.6934D-08             -V/T =  2.0047
Zero-point correction=                           0.544867 (Hartree/Particle)
 Thermal correction to Energy=                    0.574309
 Thermal correction to Enthalpy=                  0.575269
 Thermal correction to Gibbs Free Energy=         0.483991
 Sum of electronic and zero-point Energies=          -5998.528151
 Sum of electronic and thermal Energies=             -5998.498709
 Sum of electronic and thermal Enthalpies=           -5998.497749
 Sum of electronic and thermal Free Energies=        -5998.589027
                     1                      2                      3
Frequencies --  -296.0813               24.3296                37.5715
```

(*S*)-PhBOD-Rh(I)-Ph-CH-si-confU-α-Rhketone (17a)

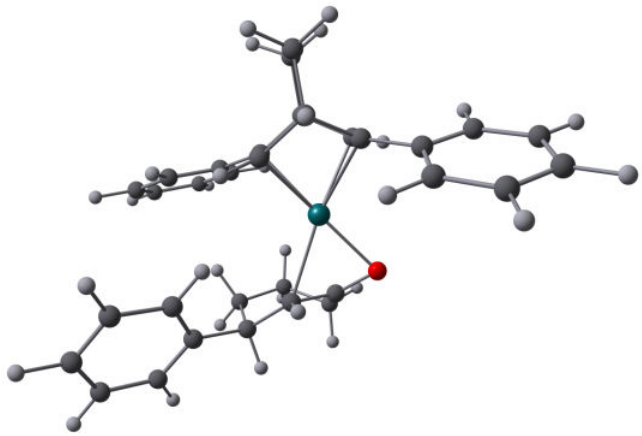


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.023842	0.193355	0.036312

2	6	0	-1.469675	-1.412003	-0.153517
3	6	0	0.491757	-2.054848	-1.472686
4	6	0	3.259443	-0.588929	-1.511900
5	6	0	-2.899852	-1.108608	0.069405
6	6	0	-3.788594	-0.954244	-1.003818
7	6	0	-0.770217	-1.217911	-1.362557
8	6	0	-0.727564	-2.379053	0.766465
9	6	0	-4.752740	-0.698527	1.594240
10	6	0	5.513636	-0.732163	-0.652361
11	6	0	0.147214	-3.552004	-1.287688
12	6	0	0.638730	-1.743244	0.917313
13	6	0	-5.134919	-0.678427	-0.782666
14	6	0	1.323211	-1.589794	-0.279536
15	6	0	3.680005	-1.732806	0.563942
16	6	0	-3.407594	-0.974682	1.372063
17	6	0	-0.593486	-3.744295	0.049060
18	6	0	-5.625800	-0.551888	0.515706
19	6	0	2.765322	-1.298679	-0.406427
20	6	0	5.038674	-1.451032	0.444102
21	6	0	4.616346	-0.303962	-1.631509
22	1	0	2.569117	-0.237586	-2.275250
23	1	0	6.573917	-0.513836	-0.747542
24	1	0	3.323607	-2.310523	1.412678
25	1	0	5.730855	-1.802935	1.204962
26	1	0	4.975496	0.255870	-2.491299
27	1	0	-3.422163	-1.037031	-2.021108
28	1	0	-5.120875	-0.593623	2.611837
29	1	0	-5.803183	-0.559809	-1.631549
30	1	0	-2.738311	-1.060560	2.224248
31	1	0	-6.677577	-0.337771	0.686833
32	1	0	1.006661	-1.885614	-2.419889
33	1	0	-1.224776	-2.494982	1.729862
34	1	0	-0.470118	-3.875804	-2.131819
35	1	0	1.070587	-4.139783	-1.318998
36	1	0	-0.051828	-4.433390	0.705177
37	1	0	-1.592235	-4.165009	-0.106222
38	1	0	1.108080	-1.632535	1.891747
39	1	0	-1.234717	-0.774750	-2.240582
40	6	0	0.284885	2.149062	1.393143
41	6	0	1.617665	1.715894	1.255782
42	6	0	-0.374052	1.842908	2.607834
43	6	0	2.287463	1.086625	2.323022
44	1	0	2.194135	1.978318	0.373785
45	6	0	0.286055	1.216501	3.652676
46	1	0	-1.410233	2.151332	2.730906
47	6	0	1.633253	0.845719	3.518322
48	1	0	3.327566	0.799704	2.195090
49	1	0	-0.239458	1.029550	4.585841
50	1	0	2.156619	0.376198	4.347138
51	6	0	-0.462404	2.947361	0.322721
52	6	0	-1.232291	1.892490	-0.477715
53	1	0	-1.168256	3.598511	0.854596
54	1	0	-2.214808	1.654876	-0.062857
55	6	0	-1.267389	1.935722	-1.933119
56	8	0	-2.148606	1.376265	-2.605199
57	6	0	-0.180033	2.699911	-2.671055
58	1	0	0.161838	2.078599	-3.505255
59	6	0	0.433581	3.849311	-0.539344
60	6	0	0.971814	3.169739	-1.796126
61	1	0	-0.680523	3.565384	-3.125710
62	1	0	1.610027	2.314600	-1.545454
63	1	0	1.605964	3.870464	-2.352117
64	1	0	1.249612	4.257681	0.067899

```
     65          1           0       -0.167959    4.708491   -0.862036
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5999.11212653     A.U. after    1 cycles
             Convg  =    0.3928D-08             -V/T =  2.0047
Zero-point correction=                           0.546798 (Hartree/Particle)
 Thermal correction to Energy=                    0.576582
 Thermal correction to Enthalpy=                  0.577542
 Thermal correction to Gibbs Free Energy=         0.484157
 Sum of electronic and zero-point Energies=          -5998.565328
 Sum of electronic and thermal Energies=             -5998.535545
 Sum of electronic and thermal Enthalpies=           -5998.534585
 Sum of electronic and thermal Free Energies=        -5998.627969
                     1                      2                      3
Frequencies --    14.6293                26.3670                38.7693
```

(*S*)-PhBOD-Rh(I)-Ph-CH-si-confU-Rh-oxa-π-allyl (18a)

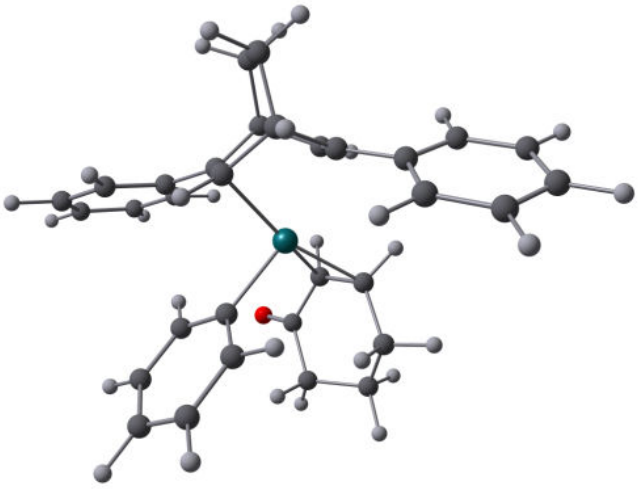


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.757023	-0.180178	0.405016
2	6	0	-2.618300	0.600718	-0.459647
3	6	0	-1.286538	2.527199	0.226112
4	6	0	1.629236	2.799175	1.182085
5	6	0	-3.765667	-0.330925	-0.444751
6	6	0	-4.864900	-0.110342	0.396777
7	6	0	-2.232493	1.410051	0.609212
8	6	0	-1.933727	1.024861	-1.757107
9	6	0	-4.858970	-2.343198	-1.260397
10	6	0	3.919010	3.117124	0.478579
11	6	0	-1.904961	3.392140	-0.897482
12	6	0	-0.462681	0.932313	-1.397413
13	6	0	-5.941203	-0.993380	0.414874
14	6	0	-0.084658	1.765278	-0.330145
15	6	0	2.306903	2.121858	-1.021652
16	6	0	-3.784510	-1.460056	-1.277119
17	6	0	-2.312904	2.489542	-2.077069
18	6	0	-5.943610	-2.114384	-0.413466
19	6	0	1.295319	2.223417	-0.054178
20	6	0	3.602293	2.557081	-0.758073
21	6	0	2.922642	3.238420	1.447046
22	1	0	0.875157	2.886019	1.959485
23	1	0	4.930162	3.457606	0.684786
24	1	0	2.080264	1.706130	-1.998694

25	1	0	4.366600	2.459575	-1.524570
26	1	0	3.154861	3.671072	2.416875
27	1	0	-4.884061	0.768570	1.035427
28	1	0	-4.847079	-3.218181	-1.905164
29	1	0	-6.783999	-0.801624	1.074008
30	1	0	-2.935550	-1.665420	-1.924427
31	1	0	-6.783377	-2.804031	-0.400282
32	1	0	-1.024830	3.141966	1.087490
33	1	0	-2.188648	0.363244	-2.586433
34	1	0	-2.769447	3.929382	-0.494266
35	1	0	-1.173607	4.145711	-1.207528
36	1	0	-1.807353	2.791922	-2.999840
37	1	0	-3.389844	2.545399	-2.266789
38	1	0	0.249536	0.537246	-2.116815
39	1	0	-2.742247	1.404440	1.569624
40	6	0	2.306537	-1.881119	0.883656
41	6	0	0.806858	-1.808580	0.720508
42	1	0	2.514206	-2.821845	1.420170
43	1	0	0.351277	-2.376329	-0.094532
44	6	0	0.051465	-1.699054	1.904179
45	8	0	-1.240083	-1.658791	1.835294
46	6	0	0.786300	-1.471574	3.195899
47	1	0	1.197670	-2.438072	3.520025
48	6	0	2.823494	-0.738789	1.785244
49	6	0	3.100323	-1.957894	-0.402205
50	6	0	4.396289	-2.488623	-0.379675
51	6	0	2.599515	-1.500965	-1.623176
52	6	0	5.170739	-2.552075	-1.535191
53	1	0	4.802662	-2.864373	0.557961
54	6	0	3.367740	-1.565589	-2.786000
55	1	0	1.591787	-1.097938	-1.659074
56	6	0	4.658512	-2.088290	-2.747599
57	1	0	6.173202	-2.970811	-1.492148
58	1	0	2.953930	-1.210645	-3.727246
59	1	0	5.257474	-2.141904	-3.653068
60	6	0	1.919428	-0.456184	3.004287
61	1	0	0.083740	-1.141018	3.965235
62	1	0	1.460382	0.530300	2.887156
63	1	0	2.518619	-0.411990	3.920059
64	1	0	3.838456	-0.990315	2.111229
65	1	0	2.911832	0.165334	1.176623

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5999.11584272     A.U. after    1 cycles
             Convg  =    0.3529D-08             -V/T =  2.0047
Zero-point correction=                           0.547160 (Hartree/Particle)
 Thermal correction to Energy=                    0.576849
 Thermal correction to Enthalpy=                  0.577809
 Thermal correction to Gibbs Free Energy=         0.484531
 Sum of electronic and zero-point Energies=          -5998.568683
 Sum of electronic and thermal Energies=             -5998.538994
 Sum of electronic and thermal Enthalpies=           -5998.538034
 Sum of electronic and thermal Free Energies=        -5998.631312
                     1                      2                      3
Frequencies --    19.0497               24.9027               35.3594
```

(*S*)-PhBOD-Rh(I)-Ph-CH-si-confD-close (13b)

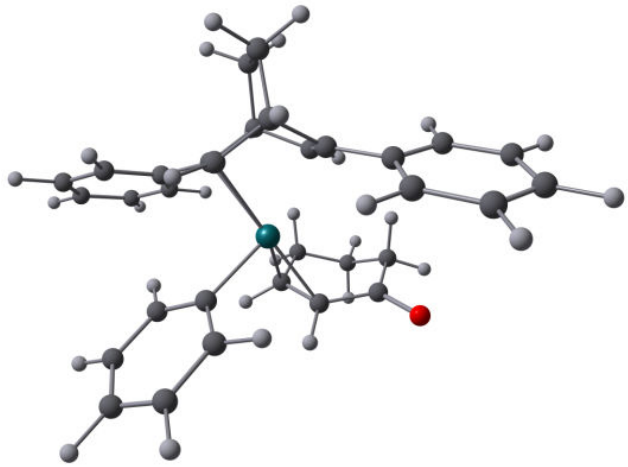


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.239730	0.113142	-0.028414
2	6	0	-1.942298	-1.476604	0.043492
3	6	0	-0.041147	-2.530637	-1.041859
4	6	0	2.899540	-1.574794	-1.434503
5	6	0	-3.286453	-0.883629	0.184889
6	6	0	-4.232292	-0.976355	-0.846958
7	6	0	-1.271565	-1.658833	-1.142999
8	6	0	-1.235012	-2.180709	1.200589
9	6	0	-4.903940	0.384830	1.484769
10	6	0	5.115687	-1.883446	-0.524931
11	6	0	-0.452012	-3.908699	-0.459110
12	6	0	0.181302	-1.628473	1.189801
13	6	0	-5.489550	-0.391392	-0.719053
14	6	0	0.856391	-1.845526	-0.016836
15	6	0	3.173345	-2.158297	0.885465
16	6	0	-3.647920	-0.199984	1.356015
17	6	0	-1.189188	-3.696377	0.876234
18	6	0	-5.831029	0.293480	0.446544
19	6	0	2.322094	-1.857010	-0.186790
20	6	0	4.555631	-2.170658	0.718788
21	6	0	4.280136	-1.583866	-1.601608
22	1	0	2.264393	-1.302238	-2.273132
23	1	0	6.194700	-1.888981	-0.654521
24	1	0	2.749529	-2.392102	1.858029
25	1	0	5.197307	-2.406787	1.563722
26	1	0	4.705593	-1.341697	-2.571828
27	1	0	-3.988056	-1.529471	-1.749972
28	1	0	-5.159268	0.917071	2.397352
29	1	0	-6.209228	-0.480265	-1.528709
30	1	0	-2.930314	-0.105838	2.167499
31	1	0	-6.813498	0.746452	0.547940
32	1	0	0.454736	-2.646624	-2.006442
33	1	0	-1.732505	-2.002555	2.155033
34	1	0	-1.088441	-4.423438	-1.185782
35	1	0	0.446538	-4.519674	-0.326550
36	1	0	-0.681035	-4.214042	1.695915
37	1	0	-2.212067	-4.084477	0.831673

38	1	0	0.699513	-1.405967	2.118735
39	1	0	-1.672955	-1.362734	-2.109294
40	6	0	1.133897	1.220383	0.969202
41	6	0	2.499706	1.361560	0.694830
42	6	0	0.637918	1.839571	2.130681
43	6	0	3.332797	2.105870	1.533913
44	1	0	2.927948	0.905456	-0.194469
45	6	0	1.467843	2.581515	2.974868
46	1	0	-0.415973	1.745781	2.397539
47	6	0	2.823624	2.721270	2.677240
48	1	0	4.387933	2.205556	1.286916
49	1	0	1.052421	3.050010	3.865282
50	1	0	3.473264	3.301306	3.328245
51	6	0	-1.313118	1.631075	-1.274414
52	6	0	-0.095339	1.365385	-1.897000
53	1	0	-2.191367	1.067501	-1.585492
54	1	0	-0.009700	0.582889	-2.649089
55	6	0	0.988334	2.370201	-1.944908
56	8	0	2.021283	2.152200	-2.569752
57	6	0	0.742360	3.694863	-1.254514
58	1	0	1.147301	3.607665	-0.238839
59	1	0	1.338019	4.451569	-1.773167
60	6	0	-0.736592	4.068660	-1.199293
61	1	0	-0.866059	4.995318	-0.629715
62	1	0	-1.103332	4.265069	-2.214814
63	6	0	-1.571493	2.948970	-0.578122
64	1	0	-1.338723	2.878452	0.491211
65	1	0	-2.639031	3.183766	-0.643179

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5999.08528477     A.U. after    1 cycles
             Convg  =    0.2653D-08             -V/T =  2.0047
Zero-point correction=                           0.544464 (Hartree/Particle)
 Thermal correction to Energy=                   0.575017
 Thermal correction to Enthalpy=                 0.575977
 Thermal correction to Gibbs Free Energy=        0.481764
 Sum of electronic and zero-point Energies=          -5998.540821
 Sum of electronic and thermal Energies=             -5998.510267
 Sum of electronic and thermal Enthalpies=           -5998.509307
 Sum of electronic and thermal Free Energies=        -5998.603521
                    1                    2                    3
Frequencies --    27.6050              33.6996              38.6892
```

(*S*)-PhBOD-Rh(I)-Ph-CH-si-confD-far (14b)

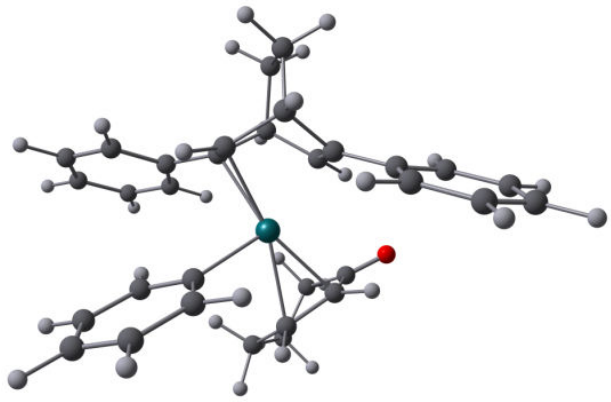


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.000392	0.358818	-0.052221
2	6	0	1.523330	-1.390417	-0.658907
3	6	0	-0.356474	-2.452112	0.445555
4	6	0	-3.117007	-1.399241	1.426831
5	6	0	2.906090	-0.921354	-0.871188
6	6	0	3.952927	-1.362219	-0.048699
7	6	0	0.987121	-1.770041	0.541494
8	6	0	0.594810	-1.731442	-1.821948
9	6	0	4.502997	0.442376	-2.093461
10	6	0	-5.441403	-1.296083	0.776116
11	6	0	-0.204354	-3.700826	-0.467540
12	6	0	-0.732799	-1.071222	-1.495888
13	6	0	5.251230	-0.898594	-0.237331
14	6	0	-1.280413	-1.474672	-0.273949
15	6	0	-3.706455	-1.368412	-0.905051
16	6	0	3.205317	-0.021147	-1.904337
17	6	0	0.394538	-3.270731	-1.818827
18	6	0	5.531511	0.007431	-1.259247
19	6	0	-2.711871	-1.407665	0.082613
20	6	0	-5.055198	-1.310631	-0.562993
21	6	0	-4.463622	-1.341021	1.770771
22	1	0	-2.368311	-1.410022	2.214739
23	1	0	-6.493772	-1.251791	1.043527
24	1	0	-3.422794	-1.390172	-1.953253
25	1	0	-5.807366	-1.280924	-1.347008
26	1	0	-4.751993	-1.325065	2.818764
27	1	0	3.750782	-2.091006	0.732155
28	1	0	4.710368	1.153391	-2.888608
29	1	0	6.048859	-1.251670	0.410977
30	1	0	2.410725	0.343479	-2.551043
31	1	0	6.544853	0.371399	-1.404770
32	1	0	-0.740047	-2.735775	1.426894
33	1	0	0.993407	-1.392109	-2.778865
34	1	0	0.437838	-4.429995	0.036201
35	1	0	-1.186171	-4.167715	-0.595780
36	1	0	-0.267392	-3.537437	-2.648632
37	1	0	1.357581	-3.758335	-2.001634
38	1	0	-1.325828	-0.611274	-2.281856
39	1	0	1.544900	-1.757768	1.472573
40	6	0	-1.284963	1.771051	-0.696325
41	6	0	-2.626860	1.945939	-0.336338
42	6	0	-0.748987	2.644963	-1.657981
43	6	0	-3.407931	2.945931	-0.923129
44	1	0	-3.084361	1.296382	0.407560
45	6	0	-1.528135	3.639490	-2.252847
46	1	0	0.297739	2.558346	-1.953102
47	6	0	-2.865566	3.794799	-1.886678
48	1	0	-4.448333	3.057897	-0.623951
49	1	0	-1.085479	4.298721	-2.996991
50	1	0	-3.474322	4.571752	-2.342598
51	6	0	-0.197936	1.270437	1.969067
52	6	0	0.873966	1.882851	1.306002
53	1	0	-1.174346	1.743710	1.902011
54	1	0	0.705755	2.781914	0.714056
55	6	0	2.273632	1.669350	1.714091
56	8	0	3.201270	2.263046	1.173744
57	6	0	2.520187	0.730155	2.880607
58	1	0	2.710197	-0.269674	2.471723
59	1	0	3.449964	1.045468	3.362382

60	6	0	1.351941	0.697718	3.862060
61	1	0	1.547632	-0.025790	4.661313
62	1	0	1.262362	1.680329	4.341173
63	6	0	0.033059	0.368087	3.162450
64	1	0	0.030735	-0.685148	2.859294
65	1	0	-0.801794	0.481247	3.862791

```
SCF Done:  E(RPBE1PBE) =  -5999.08468186     A.U. after    1 cycles
             Convg  =    0.3321D-08             -V/T =  2.0047
Zero-point correction=                           0.544635 (Hartree/Particle)
 Thermal correction to Energy=                    0.575161
 Thermal correction to Enthalpy=                  0.576121
 Thermal correction to Gibbs Free Energy=         0.481888
 Sum of electronic and zero-point Energies=          -5998.540046
 Sum of electronic and thermal Energies=             -5998.509521
 Sum of electronic and thermal Enthalpies=           -5998.508561
 Sum of electronic and thermal Free Energies=        -5998.602794
                     1                      2                      3
Frequencies --    26.6968                33.6857                38.1004
```

(*S*)-PhBOD-Rh(I)-Ph-CH-si-confD-anti (15b)

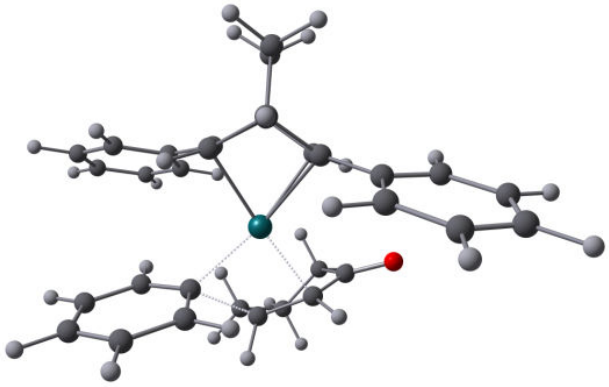


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.144259	-0.300130	-0.091837
2	6	0	-1.771296	1.316716	-0.258833
3	6	0	0.034717	2.264237	1.067485
4	6	0	2.895262	1.206962	1.678680
5	6	0	-3.116423	0.791508	-0.569191
6	6	0	-4.132093	0.775678	0.397582
7	6	0	-1.214409	1.415265	1.003171
8	6	0	-0.953000	2.080386	-1.293670
9	6	0	-4.670092	-0.215840	-2.147332
10	6	0	5.195589	1.478196	0.994040
11	6	0	-0.284392	3.684085	0.533293
12	6	0	0.431964	1.476236	-1.181518
13	6	0	-5.394285	0.272340	0.097414
14	6	0	1.000411	1.598129	0.093027
15	6	0	3.402199	1.867176	-0.578575
16	6	0	-3.408545	0.288695	-1.847086
17	6	0	-0.901099	3.570361	-0.872788
18	6	0	-5.670906	-0.224129	-1.175774
19	6	0	2.444777	1.550811	0.394730
20	6	0	4.762504	1.830597	-0.283046
21	6	0	4.253648	1.165590	1.975373

22	1	0	2.173629	0.943504	2.448102
23	1	0	6.257185	1.448817	1.224525
24	1	0	3.080255	2.149616	-1.576601
25	1	0	5.486702	2.080101	-1.054129
26	1	0	4.579538	0.885663	2.973869
27	1	0	-3.933933	1.157502	1.393826
28	1	0	-4.871465	-0.606976	-3.141246
29	1	0	-6.165667	0.269614	0.862893
30	1	0	-2.634477	0.268119	-2.609910
31	1	0	-6.657665	-0.615204	-1.408991
32	1	0	0.438611	2.310725	2.079702
33	1	0	-1.357407	1.975931	-2.300747
34	1	0	-0.973018	4.173279	1.229337
35	1	0	0.636543	4.276085	0.519448
36	1	0	-0.308927	4.120810	-1.610882
37	1	0	-1.914332	3.984289	-0.897878
38	1	0	1.023568	1.275147	-2.069780
39	1	0	-1.733906	1.105563	1.904410
40	6	0	1.258463	-1.297387	-1.248094
41	6	0	2.622321	-1.444037	-0.967262
42	6	0	0.810362	-1.759779	-2.499080
43	6	0	3.501327	-2.020757	-1.889830
44	1	0	3.026735	-1.100220	-0.016968
45	6	0	1.683087	-2.327247	-3.429208
46	1	0	-0.245404	-1.681714	-2.759460
47	6	0	3.039242	-2.462601	-3.127754
48	1	0	4.555269	-2.118320	-1.636000
49	1	0	1.300718	-2.669344	-4.389225
50	1	0	3.722744	-2.908675	-3.846182
51	6	0	-0.297082	-2.504195	0.537808
52	6	0	-1.404796	-1.802706	1.003851
53	1	0	-0.394013	-3.019918	-0.413021
54	1	0	-2.332131	-1.778505	0.433465
55	6	0	-1.515368	-1.412526	2.423425
56	8	0	-2.548264	-0.936201	2.887816
57	6	0	-0.305125	-1.674457	3.294949
58	1	0	0.405702	-0.849686	3.149488
59	1	0	-0.629865	-1.651090	4.338567
60	6	0	0.355944	-2.998075	2.920996
61	1	0	1.213024	-3.192506	3.574304
62	1	0	-0.360324	-3.812433	3.087115
63	6	0	0.798092	-2.995146	1.461030
64	1	0	1.698258	-2.384139	1.345644
65	1	0	1.085816	-4.005087	1.149617

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5999.08488956     A.U. after    1 cycles
           Convg  =    0.2723D-08             -V/T =  2.0047
Zero-point correction=                           0.544995 (Hartree/Particle)
 Thermal correction to Energy=                    0.575548
 Thermal correction to Enthalpy=                  0.576508
 Thermal correction to Gibbs Free Energy=         0.481764
 Sum of electronic and zero-point Energies=          -5998.539895
 Sum of electronic and thermal Energies=             -5998.509341
 Sum of electronic and thermal Enthalpies=           -5998.508381
 Sum of electronic and thermal Free Energies=        -5998.603126
                    1                    2                    3
Frequencies --    23.9514              27.8111              38.3765
```

(*S*)-PhBOD-Rh(I)-Ph-CH-si-confD-CR-TS (16b)

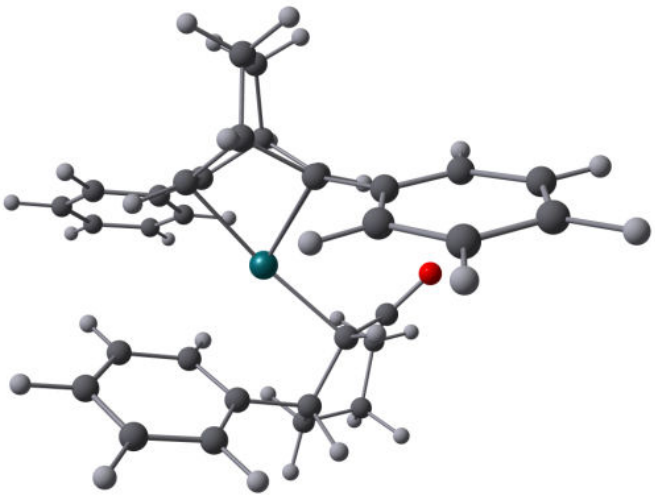


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.177345	-0.256580	0.070336
2	6	0	1.746977	1.292634	0.067510
3	6	0	-0.065832	2.153765	-1.320493
4	6	0	-2.931944	1.029261	-1.741784
5	6	0	3.113988	0.826903	0.383640
6	6	0	4.090724	0.704045	-0.614196
7	6	0	1.144450	1.252130	-1.190532
8	6	0	0.983835	2.212195	1.019353
9	6	0	4.757586	0.073246	2.012514
10	6	0	-5.226809	1.242470	-1.016610
11	6	0	0.331382	3.610159	-0.973370
12	6	0	-0.425816	1.654557	1.010885
13	6	0	5.377405	0.272837	-0.305468
14	6	0	-1.021080	1.644076	-0.244571
15	6	0	-3.417541	1.863708	0.461155
16	6	0	3.472380	0.505959	1.703013
17	6	0	0.979760	3.641865	0.423247
18	6	0	5.718871	-0.043749	1.008005
19	6	0	-2.467132	1.509090	-0.506949
20	6	0	-4.780781	1.730438	0.210830
21	6	0	-4.293564	0.892723	-1.993398
22	1	0	-2.218022	0.738272	-2.508420
23	1	0	-6.290735	1.140300	-1.213115
24	1	0	-3.086090	2.256018	1.418278
25	1	0	-5.497954	2.014756	0.976618
26	1	0	-4.628337	0.510262	-2.954333
27	1	0	3.843712	0.949303	-1.641926
28	1	0	5.009785	-0.176071	3.040176
29	1	0	6.116389	0.182826	-1.097278
30	1	0	2.732195	0.573952	2.496289
31	1	0	6.724434	-0.379186	1.247927
32	1	0	-0.503356	2.099246	-2.318249
33	1	0	1.410368	2.210992	2.022750
34	1	0	1.021995	3.978106	-1.738905
35	1	0	-0.561379	4.242960	-1.012672
36	1	0	0.430250	4.304407	1.099683
37	1	0	2.009538	4.010701	0.375331
38	1	0	-0.982301	1.513329	1.933820
39	1	0	1.639973	0.844627	-2.068218
40	6	0	-1.150414	-1.457215	1.239989
41	6	0	-2.548409	-1.412197	1.173711

42	6	0	-0.555521	-1.682090	2.497416
43	6	0	-3.324097	-1.543233	2.326902
44	1	0	-3.049275	-1.251782	0.222323
45	6	0	-1.328005	-1.785991	3.651284
46	1	0	0.526225	-1.785514	2.572066
47	6	0	-2.721316	-1.720398	3.571127
48	1	0	-4.408024	-1.495889	2.248470
49	1	0	-0.843113	-1.938981	4.613029
50	1	0	-3.328369	-1.821447	4.467137
51	6	0	-0.235759	-2.530919	-0.223144
52	6	0	1.083911	-2.072532	-0.594725
53	1	0	-0.229807	-3.307053	0.536005
54	1	0	1.915907	-2.305573	0.071156
55	6	0	1.473049	-1.891909	-1.996087
56	8	0	2.631779	-1.641213	-2.331854
57	6	0	0.395007	-2.088511	-3.049038
58	1	0	-0.123265	-1.131393	-3.198714
59	1	0	0.895886	-2.336394	-3.988929
60	6	0	-0.609187	-3.156390	-2.627964
61	1	0	-1.371453	-3.293397	-3.403147
62	1	0	-0.094819	-4.118829	-2.513563
63	6	0	-1.274804	-2.757904	-1.314976
64	1	0	-1.854996	-1.847230	-1.493275
65	1	0	-1.987992	-3.519636	-0.984271

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5999.06907812     A.U. after    1 cycles
             Convg  =    0.2166D-08             -V/T =  2.0047
Zero-point correction=                           0.544486 (Hartree/Particle)
 Thermal correction to Energy=                    0.574164
 Thermal correction to Enthalpy=                  0.575124
 Thermal correction to Gibbs Free Energy=         0.482731
 Sum of electronic and zero-point Energies=          -5998.524592
 Sum of electronic and thermal Energies=             -5998.494914
 Sum of electronic and thermal Enthalpies=           -5998.493954
 Sum of electronic and thermal Free Energies=        -5998.586347
                    1                    2                    3
Frequencies --  -296.3662               24.0519              30.0269
```

(*S*)-PhBOD-Rh(I)-Ph-CH-si-confD-α-Rhketone (17b)



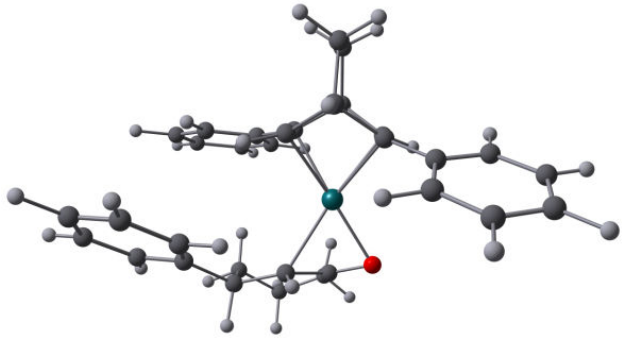
```
---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
```

1	45	0	0.050995	0.110490	0.009677
2	6	0	-1.307538	-1.572856	-0.025770
3	6	0	0.650479	-2.204647	-1.355090
4	6	0	3.320844	-0.572855	-1.563722
5	6	0	-2.750815	-1.357163	0.214982
6	6	0	-3.685951	-1.449799	-0.823760
7	6	0	-0.649697	-1.425297	-1.265900
8	6	0	-0.494578	-2.437216	0.935790
9	6	0	-4.575790	-0.876615	1.750719
10	6	0	5.599894	-0.521425	-0.761043
11	6	0	0.390751	-3.700548	-1.059300
12	6	0	0.838411	-1.722681	1.004508
13	6	0	-5.043978	-1.262047	-0.580153
14	6	0	1.482082	-1.611983	-0.219585
15	6	0	3.863921	-1.555530	0.565847
16	6	0	-3.219937	-1.068382	1.506314
17	6	0	-0.307257	-3.839274	0.306962
18	6	0	-5.496648	-0.976066	0.706693
19	6	0	2.899949	-1.242370	-0.403831
20	6	0	5.198565	-1.197114	0.390849
21	6	0	4.653584	-0.212615	-1.738840
22	1	0	2.590823	-0.313083	-2.326810
23	1	0	6.641371	-0.243749	-0.899044
24	1	0	3.566533	-2.101025	1.457717
25	1	0	5.929760	-1.455758	1.152589
26	1	0	4.955485	0.313401	-2.640925
27	1	0	-3.347222	-1.663136	-1.832081
28	1	0	-4.915599	-0.644103	2.756932
29	1	0	-5.751394	-1.336994	-1.401965
30	1	0	-2.510423	-0.961100	2.323370
31	1	0	-6.556902	-0.828607	0.895195
32	1	0	1.134283	-2.075169	-2.324773
33	1	0	-0.964729	-2.510102	1.917387
34	1	0	-0.228162	-4.113280	-1.862522
35	1	0	1.342787	-4.241375	-1.076166
36	1	0	0.283262	-4.456525	0.991861
37	1	0	-1.287243	-4.316992	0.206248
38	1	0	1.325399	-1.523625	1.955671
39	1	0	-1.165780	-1.071820	-2.156086
40	6	0	0.140337	2.392690	1.286777
41	6	0	1.400425	1.801199	1.063428
42	6	0	-0.327340	2.463428	2.611516
43	6	0	2.174577	1.334109	2.140683
44	1	0	1.857023	1.829065	0.070822
45	6	0	0.440749	1.999792	3.670357
46	1	0	-1.301350	2.908766	2.802430
47	6	0	1.701700	1.433196	3.439433
48	1	0	3.151108	0.900961	1.939979
49	1	0	0.063706	2.085360	4.686604
50	1	0	2.304416	1.081251	4.272397
51	6	0	-0.695128	2.921016	0.131313
52	6	0	-1.291963	1.686559	-0.555518
53	1	0	-1.511383	3.521715	0.556601
54	1	0	-2.205306	1.347587	-0.057256
55	6	0	-1.487064	1.691758	-2.007455
56	8	0	-2.278883	0.932681	-2.582672
57	6	0	-0.692776	2.688615	-2.837310
58	1	0	0.311166	2.279116	-3.014962
59	1	0	-1.184410	2.770130	-3.810716
60	6	0	-0.573022	4.036326	-2.133092
61	1	0	-0.007470	4.741989	-2.752135
62	1	0	-1.571993	4.469948	-1.993071

63	6	0	0.111881	3.846681	-0.788320
64	1	0	1.109918	3.434523	-0.975665
65	1	0	0.266606	4.805819	-0.280627

```
SCF Done:  E(RPBE1PBE) =  -5999.11252020     A.U. after    1 cycles
             Convg  =    0.2116D-08             -V/T =  2.0047
Zero-point correction=                           0.546476 (Hartree/Particle)
 Thermal correction to Energy=                    0.576259
 Thermal correction to Enthalpy=                  0.577219
 Thermal correction to Gibbs Free Energy=         0.483773
 Sum of electronic and zero-point Energies=          -5998.566044
 Sum of electronic and thermal Energies=             -5998.536262
 Sum of electronic and thermal Enthalpies=           -5998.535302
 Sum of electronic and thermal Free Energies=        -5998.628747
                     1                      2                      3
Frequencies --    18.8633                23.0575                36.8197
```

(*S*)-PhBOD-Rh(I)-Ph-CH-si-confD-Rh-oxa-π-allyl (18b)

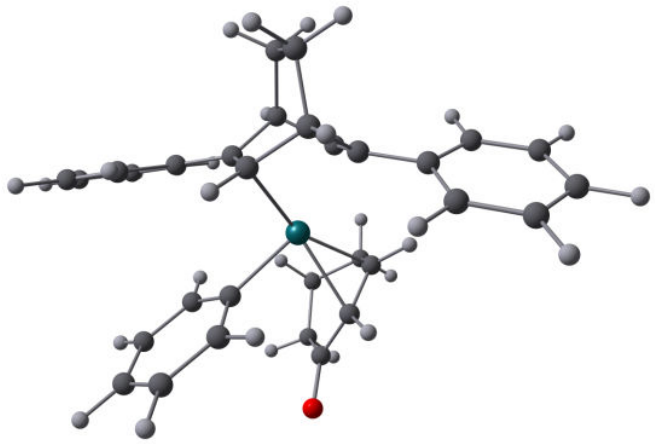


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.735081	-0.282715	-0.447270
2	6	0	2.506024	0.814420	0.271184
3	6	0	0.990412	2.452696	-0.709472
4	6	0	-1.905462	2.166598	-1.721965
5	6	0	3.743196	0.016896	0.406473
6	6	0	4.835842	0.226389	-0.446434
7	6	0	2.053583	1.395259	-0.912614
8	6	0	1.768413	1.370156	1.488188
9	6	0	5.022515	-1.714231	1.537045
10	6	0	-4.221454	2.437443	-1.091122
11	6	0	1.499011	3.549150	0.255021
12	6	0	0.318978	1.063103	1.160671
13	6	0	6.001526	-0.523660	-0.313579
14	6	0	-0.127585	1.663110	-0.030092
15	6	0	-2.553024	1.921284	0.581143
16	6	0	3.859284	-0.963321	1.403713
17	6	0	1.990385	2.898305	1.561895
18	6	0	6.100621	-1.497903	0.678363
19	6	0	-1.541630	1.909538	-0.389770
20	6	0	-3.876583	2.179980	0.234394
21	6	0	-3.227034	2.426894	-2.069896
22	1	0	-1.149278	2.141012	-2.502316
23	1	0	-5.254009	2.644233	-1.360161
24	1	0	-2.305832	1.729095	1.621149
25	1	0	-4.640628	2.181870	1.007250
26	1	0	-3.482514	2.618328	-3.109104

27	1	0	4.777809	0.994663	-1.212720
28	1	0	5.086703	-2.475808	2.309971
29	1	0	6.837951	-0.341933	-0.983555
30	1	0	3.019521	-1.158233	2.066164
31	1	0	7.010215	-2.083285	0.782967
32	1	0	0.670436	2.887160	-1.656927
33	1	0	2.086957	0.883360	2.411521
34	1	0	2.304012	4.105911	-0.235598
35	1	0	0.686918	4.258602	0.444994
36	1	0	1.448537	3.292232	2.427836
37	1	0	3.054027	3.097410	1.729899
38	1	0	-0.362238	0.706625	1.927847
39	1	0	2.570360	1.283133	-1.862667
40	6	0	-2.176824	-2.201708	-0.315716
41	6	0	-0.679052	-2.048705	-0.467982
42	1	0	-2.372067	-3.288765	-0.312103
43	1	0	-0.053992	-2.508547	0.301311
44	6	0	-0.054464	-1.977345	-1.731180
45	8	0	1.236714	-1.872050	-1.768115
46	6	0	-0.842415	-1.858020	-3.011538
47	1	0	-0.745039	-0.827474	-3.373113
48	1	0	-0.353288	-2.490814	-3.760116
49	6	0	-2.308246	-2.236350	-2.829238
50	1	0	-2.887443	-1.905423	-3.697920
51	1	0	-2.400989	-3.329518	-2.791124
52	6	0	-2.896906	-1.647202	-1.550464
53	1	0	-2.822138	-0.553577	-1.562361
54	1	0	-3.961638	-1.894754	-1.511692
55	6	0	-2.735591	-1.705892	1.013349
56	6	0	-4.110218	-1.487997	1.177899
57	6	0	-1.919712	-1.532964	2.137724
58	6	0	-4.644744	-1.097722	2.403887
59	1	0	-4.787218	-1.617013	0.338798
60	6	0	-2.447944	-1.143745	3.368771
61	1	0	-0.849813	-1.696318	2.058409
62	6	0	-3.815464	-0.918967	3.510062
63	1	0	-5.715861	-0.932689	2.493392
64	1	0	-1.784740	-1.019034	4.221812
65	1	0	-4.229714	-0.614821	4.467891

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5999.12036933     A.U. after    1 cycles
             Convg  =    0.2988D-08             -V/T =  2.0047
Zero-point correction=                           0.547282 (Hartree/Particle)
 Thermal correction to Energy=                    0.576793
 Thermal correction to Enthalpy=                  0.577753
 Thermal correction to Gibbs Free Energy=         0.485311
 Sum of electronic and zero-point Energies=          -5998.573087
 Sum of electronic and thermal Energies=             -5998.543576
 Sum of electronic and thermal Enthalpies=           -5998.542616
 Sum of electronic and thermal Free Energies=        -5998.635058
                     1                      2                      3
Frequencies --    21.0929               24.2204                36.7395
```

(*S*)-PhBOD-Rh(I)-Ph-CH-re-confU-syn (19a)

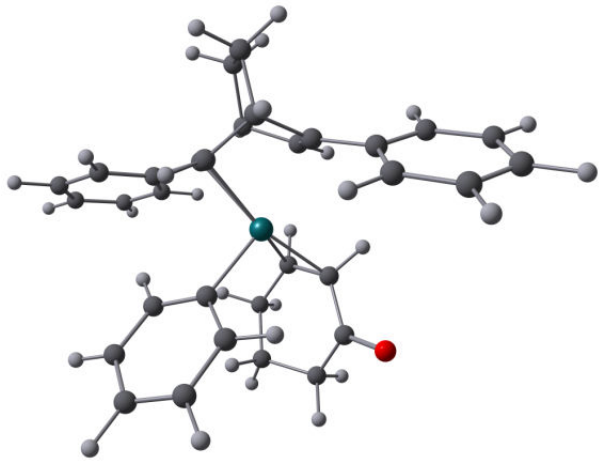


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.229960	0.199856	0.039982
2	6	0	1.977899	-1.287023	-0.145484
3	6	0	0.182750	-2.447099	1.016894
4	6	0	-2.780427	-1.759968	1.539287
5	6	0	3.324883	-0.710809	-0.334156
6	6	0	4.323947	-0.874291	0.636318
7	6	0	1.356161	-1.492658	1.072531
8	6	0	1.274770	-2.038574	-1.268085
9	6	0	4.901761	0.564230	-1.674087
10	6	0	-5.022743	-2.050733	0.690269
11	6	0	0.658369	-3.798920	0.426046
12	6	0	-0.159858	-1.559850	-1.194813
13	6	0	5.590580	-0.321758	0.458062
14	6	0	-0.787943	-1.814644	0.024497
15	6	0	-3.132871	-2.107984	-0.814246
16	6	0	3.638129	0.010713	-1.496178
17	6	0	1.322609	-3.553456	-0.941365
18	6	0	5.884395	0.401354	-0.696604
19	6	0	-2.245086	-1.888703	0.248384
20	6	0	-4.505079	-2.185985	-0.597045
21	6	0	-4.152280	-1.836837	1.758864
22	1	0	-2.120360	-1.569414	2.381767
23	1	0	-6.094395	-2.112328	0.859927
24	1	0	-2.746690	-2.224091	-1.822646
25	1	0	-5.173232	-2.354567	-1.437447
26	1	0	-4.543647	-1.724448	2.766777
27	1	0	4.111854	-1.454263	1.530774
28	1	0	5.119717	1.130522	-2.575753
29	1	0	6.352387	-0.464043	1.220154
30	1	0	2.873471	0.163129	-2.253974
31	1	0	6.872032	0.832259	-0.836599
32	1	0	-0.266247	-2.590390	2.000050
33	1	0	1.721010	-1.831121	-2.241718
34	1	0	1.359064	-4.261805	1.128408
35	1	0	-0.201615	-4.470380	0.336427
36	1	0	0.805981	-4.099514	-1.736873
37	1	0	2.364979	-3.887984	-0.944392
38	1	0	-0.712223	-1.319214	-2.098759
39	1	0	1.806246	-1.215609	2.021732

40	6	0	-1.349052	1.158693	-0.883749
41	6	0	-2.610987	1.315071	-0.295331
42	6	0	-1.206406	1.581462	-2.215484
43	6	0	-3.684353	1.863920	-1.002119
44	1	0	-2.781866	0.998130	0.731990
45	6	0	-2.276835	2.119847	-2.931179
46	1	0	-0.239515	1.502670	-2.710976
47	6	0	-3.525562	2.265777	-2.326419
48	1	0	-4.650332	1.970735	-0.511981
49	1	0	-2.130409	2.437192	-3.962027
50	1	0	-4.359337	2.693504	-2.878019
51	6	0	1.465447	1.583295	1.299881
52	1	0	2.479847	1.219719	1.145434
53	6	0	0.883255	2.357429	0.304159
54	1	0	1.403096	2.527316	-0.637486
55	6	0	-0.157640	3.356455	0.626230
56	8	0	-0.420567	4.269619	-0.145479
57	6	0	0.968219	1.645324	2.720572
58	1	0	1.570405	2.398007	3.253295
59	6	0	-0.783122	3.299582	2.006299
60	6	0	-0.507940	2.018452	2.783646
61	1	0	1.152048	0.695135	3.233160
62	1	0	-1.095232	1.194776	2.360705
63	1	0	-0.826751	2.136450	3.825145
64	1	0	-1.853622	3.493749	1.895506
65	1	0	-0.370264	4.161513	2.548490

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5999.08315533     A.U. after    1 cycles
             Convg  =    0.6187D-08             -V/T =  2.0047
Zero-point correction=                           0.544623 (Hartree/Particle)
 Thermal correction to Energy=                    0.575147
 Thermal correction to Enthalpy=                  0.576107
 Thermal correction to Gibbs Free Energy=         0.481888
 Sum of electronic and zero-point Energies=          -5998.538533
 Sum of electronic and thermal Energies=             -5998.508008
 Sum of electronic and thermal Enthalpies=           -5998.507048
 Sum of electronic and thermal Free Energies=        -5998.601268
                     1                      2                      3
Frequencies --    20.5852                36.1503                38.6848
```

(*S*)-PhBOD-Rh(I)-Ph-CH-re-confU-close (20a)



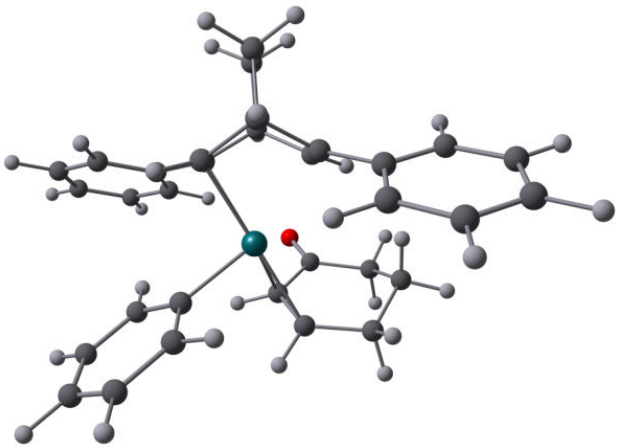
```
---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
```

Number	Number	Type	X	Y	Z
1	45	0	-0.168274	0.105580	-0.048989
2	6	0	-1.742163	-1.675619	0.106962
3	6	0	0.241009	-2.576120	-0.958981
4	6	0	3.108907	-1.457800	-1.432652
5	6	0	-3.130893	-1.197506	0.245267
6	6	0	-4.087022	-1.461501	-0.746256
7	6	0	-1.077720	-1.850327	-1.077350
8	6	0	-0.947643	-2.231069	1.286180
9	6	0	-4.826107	0.016424	1.492672
10	6	0	5.342253	-1.589771	-0.520748
11	6	0	-0.012768	-3.957025	-0.296469
12	6	0	0.407188	-1.544215	1.219948
13	6	0	-5.391027	-0.990177	-0.622192
14	6	0	1.084535	-1.755198	0.012514
15	6	0	3.420629	-1.886236	0.914331
16	6	0	-3.524459	-0.458341	1.370500
17	6	0	-0.744716	-3.749634	1.042556
18	6	0	-5.765673	-0.247919	0.497056
19	6	0	2.548863	-1.691097	-0.166604
20	6	0	4.801587	-1.833646	0.740312
21	6	0	4.487573	-1.402936	-1.608363
22	1	0	2.456108	-1.290243	-2.285748
23	1	0	6.419562	-1.548098	-0.657084
24	1	0	3.013602	-2.086488	1.901241
25	1	0	5.457031	-1.987097	1.593671
26	1	0	4.898145	-1.208731	-2.595964
27	1	0	-3.811529	-2.058870	-1.611474
28	1	0	-5.105581	0.603547	2.363223
29	1	0	-6.119292	-1.209847	-1.398541
30	1	0	-2.797228	-0.225735	2.144669
31	1	0	-6.782837	0.122012	0.592663
32	1	0	0.728255	-2.693783	-1.928065
33	1	0	-1.448658	-2.052187	2.238550
34	1	0	-0.605355	-4.572882	-0.980204
35	1	0	0.946792	-4.463873	-0.152490
36	1	0	-0.168564	-4.161843	1.876960
37	1	0	-1.719779	-4.247536	1.044789
38	1	0	0.916438	-1.240167	2.130985
39	1	0	-1.519606	-1.629369	-2.045978
40	6	0	1.005843	1.422067	0.914068
41	6	0	2.405120	1.489401	0.943830
42	6	0	0.293926	2.296503	1.754765
43	6	0	3.068557	2.393382	1.777824
44	1	0	2.997586	0.846144	0.297670
45	6	0	0.953940	3.192095	2.599148
46	1	0	-0.796506	2.303127	1.742140
47	6	0	2.348200	3.246926	2.613193
48	1	0	4.156410	2.430071	1.771017
49	1	0	0.374787	3.857893	3.236127
50	1	0	2.865005	3.951026	3.260769
51	6	0	0.011462	1.055154	-2.077584
52	1	0	0.011787	0.154760	-2.692232
53	6	0	-1.193325	1.458476	-1.492113
54	1	0	-2.106182	0.877174	-1.617070
55	6	0	-1.432753	2.867721	-1.114043
56	8	0	-2.452298	3.209413	-0.523621
57	6	0	1.114670	2.028371	-2.396250
58	1	0	1.075195	2.181615	-3.486805
59	6	0	-0.431840	3.884920	-1.614132
60	6	0	1.002831	3.373730	-1.684230
61	1	0	2.091665	1.574643	-2.196031

62	1	0	1.399263	3.283678	-0.671665
63	1	0	1.627980	4.110031	-2.201634
64	1	0	-0.512999	4.784365	-0.998383
65	1	0	-0.784691	4.156062	-2.620581

```
SCF Done:  E(RPBE1PBE) =  -5999.08426443     A.U. after    1 cycles
             Convg  =    0.3451D-08             -V/T =  2.0047
Zero-point correction=                           0.544472 (Hartree/Particle)
 Thermal correction to Energy=                    0.575065
 Thermal correction to Enthalpy=                  0.576025
 Thermal correction to Gibbs Free Energy=         0.481347
 Sum of electronic and zero-point Energies=          -5998.539792
 Sum of electronic and thermal Energies=             -5998.509199
 Sum of electronic and thermal Enthalpies=           -5998.508239
 Sum of electronic and thermal Free Energies=        -5998.602918
                     1                      2                      3
Frequencies --    25.2405                29.9962                39.7848
```

(*S*)-PhBOD-Rh(I)-Ph-CH-re-confU-far (21a)

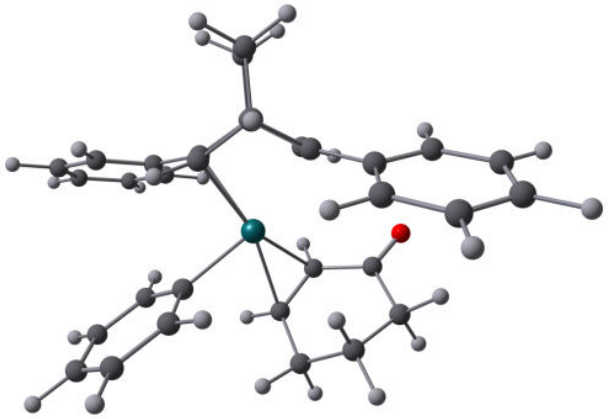


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.038230	0.476733	-0.019847
2	6	0	1.726996	-1.125310	-0.798642
3	6	0	-0.126803	-2.398322	0.099892
4	6	0	-2.970026	-1.621014	1.072429
5	6	0	3.088969	-0.568489	-0.916031
6	6	0	4.167073	-1.141902	-0.227015
7	6	0	1.175553	-1.669669	0.326033
8	6	0	0.860474	-1.368447	-2.029581
9	6	0	4.617442	1.075532	-1.848217
10	6	0	-5.272251	-1.632794	0.331042
11	6	0	0.132388	-3.522851	-0.941895
12	6	0	-0.509007	-0.815612	-1.683922
13	6	0	5.449638	-0.610625	-0.340381
14	6	0	-1.079267	-1.400861	-0.548707
15	6	0	-3.479878	-1.408980	-1.273704
16	6	0	3.337639	0.540978	-1.738363
17	6	0	0.745146	-2.906059	-2.212913
18	6	0	5.679632	0.501932	-1.148358
19	6	0	-2.523578	-1.470563	-0.250644
20	6	0	-4.840462	-1.487050	-0.986347
21	6	0	-4.329635	-1.697855	1.358482

22	1	0	-2.249120	-1.632532	1.887003
23	1	0	-6.333860	-1.694594	0.555934
24	1	0	-3.156229	-1.307838	-2.305863
25	1	0	-5.564916	-1.438165	-1.795316
26	1	0	-4.654853	-1.800959	2.390669
27	1	0	3.999712	-2.022545	0.388020
28	1	0	4.787328	1.942905	-2.480755
29	1	0	6.273214	-1.072505	0.197867
30	1	0	2.515267	1.001391	-2.281619
31	1	0	6.680512	0.915403	-1.238346
32	1	0	-0.527647	-2.802571	1.029442
33	1	0	1.278244	-0.898308	-2.921572
34	1	0	0.802630	-4.266362	-0.499213
35	1	0	-0.813719	-4.028653	-1.159148
36	1	0	0.122005	-3.105460	-3.090418
37	1	0	1.737349	-3.321075	-2.418956
38	1	0	-1.102701	-0.302224	-2.436295
39	1	0	1.695872	-1.743468	1.276159
40	6	0	-1.373119	1.829604	-0.481918
41	6	0	-2.711464	1.862672	-0.074983
42	6	0	-0.931799	2.836391	-1.357902
43	6	0	-3.580016	2.858296	-0.532688
44	1	0	-3.098625	1.099548	0.597207
45	6	0	-1.797822	3.827105	-1.824551
46	1	0	0.108194	2.857879	-1.688712
47	6	0	-3.130695	3.842702	-1.411041
48	1	0	-4.616483	2.857876	-0.200995
49	1	0	-1.428680	4.590609	-2.506679
50	1	0	-3.808182	4.614831	-1.767271
51	6	0	0.654022	1.924737	1.588017
52	1	0	0.232663	2.852149	1.200273
53	6	0	-0.235916	0.985183	2.113432
54	1	0	-1.306401	1.173976	2.133405
55	6	0	0.227185	-0.057003	3.056809
56	8	0	-0.523721	-0.932325	3.478386
57	6	0	2.100224	1.996903	2.001104
58	1	0	2.178773	2.806126	2.744432
59	6	0	1.641468	0.076088	3.581171
60	6	0	2.627927	0.699735	2.598785
61	1	0	2.726939	2.307226	1.157423
62	1	0	2.841487	-0.003039	1.790278
63	1	0	3.583654	0.881815	3.102058
64	1	0	1.974336	-0.901827	3.941214
65	1	0	1.552449	0.719285	4.469457

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5999.08562930     A.U. after    1 cycles
           Convg  =    0.2833D-08             -V/T =  2.0047
Zero-point correction=                           0.544349 (Hartree/Particle)
 Thermal correction to Energy=                    0.575065
 Thermal correction to Enthalpy=                  0.576025
 Thermal correction to Gibbs Free Energy=         0.481034
 Sum of electronic and zero-point Energies=          -5998.541281
 Sum of electronic and thermal Energies=             -5998.510564
 Sum of electronic and thermal Enthalpies=           -5998.509604
 Sum of electronic and thermal Free Energies=        -5998.604595
                    1                      2                      3
Frequencies --    24.2624                33.0168                37.0454
```

(*S*)-PhBOD-Rh(I)-Ph-CH-re-confU-anti (22a)

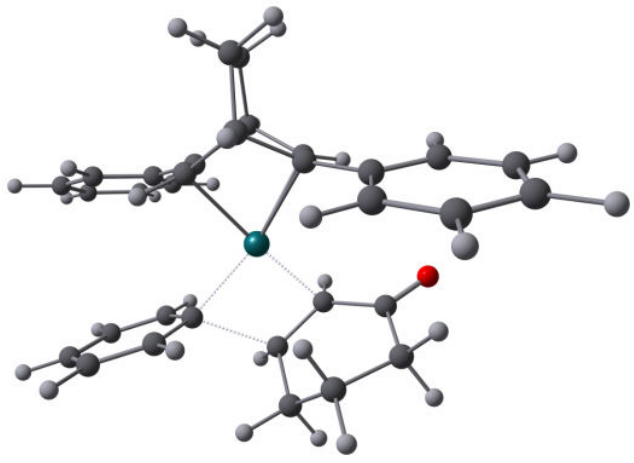


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.044680	0.241158	0.195210
2	6	0	1.442713	-1.456925	-0.455627
3	6	0	-0.460409	-2.494781	0.640830
4	6	0	-3.210378	-1.399035	1.561990
5	6	0	2.844106	-1.048153	-0.679252
6	6	0	3.871462	-1.477229	0.173542
7	6	0	0.879151	-1.799573	0.755392
8	6	0	0.540271	-1.831251	-1.624704
9	6	0	4.507275	0.122288	-2.015186
10	6	0	-5.521467	-1.255782	0.874320
11	6	0	-0.301964	-3.760248	-0.240862
12	6	0	-0.761415	-1.117217	-1.323797
13	6	0	5.193584	-1.110365	-0.061836
14	6	0	-1.349476	-1.505666	-0.107047
15	6	0	-3.761545	-1.345873	-0.779351
16	6	0	3.186875	-0.247806	-1.781232
17	6	0	0.314255	-3.362896	-1.594775
18	6	0	5.518356	-0.309677	-1.156105
19	6	0	-2.785291	-1.407367	0.224274
20	6	0	-5.114398	-1.268977	-0.458600
21	6	0	-4.561077	-1.321019	1.884766
22	1	0	-2.473800	-1.425463	2.361278
23	1	0	-6.577321	-1.196750	1.124859
24	1	0	-3.460147	-1.363978	-1.822700
25	1	0	-5.853510	-1.221772	-1.254101
26	1	0	-4.866145	-1.306395	2.928047
27	1	0	3.634151	-2.106189	1.025598
28	1	0	4.748097	0.750273	-2.869069
29	1	0	5.972849	-1.453968	0.613062
30	1	0	2.409238	0.106145	-2.453671
31	1	0	6.551264	-0.025991	-1.339934
32	1	0	-0.865312	-2.751700	1.620439
33	1	0	0.958433	-1.520099	-2.582514
34	1	0	0.332536	-4.478481	0.288039
35	1	0	-1.282865	-4.229027	-0.370105
36	1	0	-0.345642	-3.634082	-2.425167
37	1	0	1.269600	-3.871244	-1.761907
38	1	0	-1.327670	-0.640653	-2.119192
39	1	0	1.423076	-1.760774	1.695690
40	6	0	-1.408074	1.619121	-0.507675

41	6	0	-2.678661	1.872550	0.027708
42	6	0	-1.062729	2.306102	-1.685013
43	6	0	-3.565240	2.764432	-0.580808
44	1	0	-2.996686	1.365758	0.937607
45	6	0	-1.945600	3.196873	-2.301500
46	1	0	-0.084676	2.147979	-2.140208
47	6	0	-3.205476	3.431935	-1.751128
48	1	0	-4.544004	2.934571	-0.136188
49	1	0	-1.644985	3.708454	-3.214167
50	1	0	-3.894933	4.125490	-2.226454
51	6	0	0.203076	2.085659	1.582754
52	1	0	-0.806712	2.300872	1.919708
53	6	0	0.864287	0.992730	2.123754
54	1	0	0.360618	0.340885	2.835342
55	6	0	2.334982	0.908782	2.138970
56	8	0	2.909686	0.037994	2.788388
57	6	0	0.957072	3.214261	0.936616
58	1	0	1.116301	3.985811	1.705825
59	6	0	3.106751	1.992205	1.418566
60	6	0	2.295611	2.753639	0.375494
61	1	0	0.340798	3.675390	0.159380
62	1	0	2.117421	2.105754	-0.492045
63	1	0	2.871116	3.611224	0.010738
64	1	0	4.011343	1.545020	0.996627
65	1	0	3.440941	2.682462	2.206769

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5999.08617280     A.U. after    1 cycles
             Convg  =    0.1882D-08             -V/T =  2.0047
Zero-point correction=                           0.544923 (Hartree/Particle)
 Thermal correction to Energy=                    0.575344
 Thermal correction to Enthalpy=                  0.576304
 Thermal correction to Gibbs Free Energy=         0.482513
 Sum of electronic and zero-point Energies=          -5998.541250
 Sum of electronic and thermal Energies=             -5998.510829
 Sum of electronic and thermal Enthalpies=           -5998.509869
 Sum of electronic and thermal Free Energies=        -5998.603659
                     1                    2                    3
Frequencies --    16.7183              41.2851              42.7949
```

(*S*)-PhBOD-Rh(I)-Ph-CH-re-confU-CR-TS (23a)



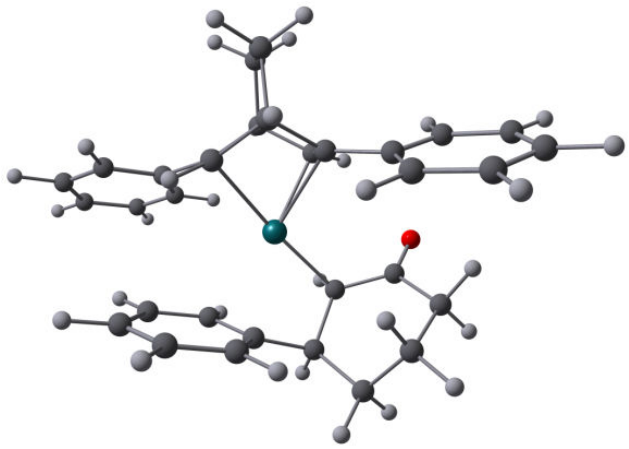
```
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
```

1	45	0	-0.017678	0.187400	-0.310970
2	6	0	-1.434808	-1.450293	0.258298
3	6	0	0.515019	-2.486858	-0.781911
4	6	0	3.286429	-1.310516	-1.522156
5	6	0	-2.871798	-1.150341	0.434985
6	6	0	-3.813723	-1.472490	-0.553095
7	6	0	-0.794008	-1.739473	-0.949012
8	6	0	-0.601143	-1.908125	1.450778
9	6	0	-4.698149	-0.332585	1.825265
10	6	0	5.563063	-1.107645	-0.740413
11	6	0	0.267599	-3.790855	0.018100
12	6	0	0.732381	-1.221056	1.258898
13	6	0	-5.170058	-1.227355	-0.358936
14	6	0	1.371206	-1.556944	0.074030
15	6	0	3.747171	-1.327997	0.838733
16	6	0	-3.342713	-0.574531	1.627503
17	6	0	-0.414689	-3.443751	1.353570
18	6	0	-5.621325	-0.660797	0.831859
19	6	0	2.811683	-1.385276	-0.203644
20	6	0	5.106584	-1.187051	0.574477
21	6	0	4.644819	-1.171083	-1.788890
22	1	0	2.582998	-1.339185	-2.350607
23	1	0	6.624948	-1.003083	-0.947041
24	1	0	3.408019	-1.405049	1.867911
25	1	0	5.813413	-1.146805	1.399298
26	1	0	4.988285	-1.109092	-2.818464
27	1	0	-3.484914	-1.921825	-1.484368
28	1	0	-5.034601	0.117645	2.755783
29	1	0	-5.877032	-1.481108	-1.144102
30	1	0	-2.640278	-0.294033	2.407678
31	1	0	-6.681054	-0.473937	0.984114
32	1	0	0.980429	-2.703662	-1.744088
33	1	0	-1.057035	-1.637195	2.402855
34	1	0	-0.356595	-4.458919	-0.583966
35	1	0	1.224001	-4.298996	0.178932
36	1	0	0.186513	-3.779105	2.204826
37	1	0	-1.393396	-3.927282	1.438598
38	1	0	1.237621	-0.725730	2.083967
39	1	0	-1.303154	-1.711123	-1.909062
40	6	0	1.300141	1.809208	0.220200
41	6	0	2.548941	1.927367	-0.412988
42	6	0	1.223726	2.184096	1.573328
43	6	0	3.677756	2.359301	0.278114
44	1	0	2.642807	1.683986	-1.470106
45	6	0	2.352366	2.613607	2.270759
46	1	0	0.272500	2.131803	2.098678
47	6	0	3.586942	2.703275	1.627554
48	1	0	4.631221	2.427993	-0.240166
49	1	0	2.263374	2.885379	3.320568
50	1	0	4.464964	3.047773	2.167933
51	6	0	-0.163740	2.474982	-0.996284
52	1	0	0.623256	2.928419	-1.592209
53	6	0	-0.948129	1.491510	-1.707146
54	1	0	-0.544802	1.106663	-2.647000
55	6	0	-2.409476	1.483782	-1.673168
56	8	0	-3.064607	0.872894	-2.520279
57	6	0	-0.940154	3.474216	-0.162792
58	6	0	-3.107443	2.303951	-0.608021
59	6	0	-2.175426	2.847215	0.467828
60	1	0	-0.296810	3.945782	0.583495
61	1	0	-1.255731	4.270597	-0.853168
62	1	0	-1.873124	2.030549	1.136222
63	1	0	-2.702004	3.583469	1.085032

64	1	0	-3.588298	3.135392	-1.141373
65	1	0	-3.917415	1.699580	-0.189222

```
SCF Done:  E(RPBE1PBE) =  -5999.06822577     A.U. after    1 cycles
             Convg  =    0.4214D-08             -V/T =  2.0047
Zero-point correction=                          0.544661 (Hartree/Particle)
 Thermal correction to Energy=                   0.574116
 Thermal correction to Enthalpy=                 0.575076
 Thermal correction to Gibbs Free Energy=        0.484199
 Sum of electronic and zero-point Energies=          -5998.523564
 Sum of electronic and thermal Energies=             -5998.494109
 Sum of electronic and thermal Enthalpies=           -5998.493149
 Sum of electronic and thermal Free Energies=        -5998.584026
                     1                      2                      3
Frequencies --  -304.6525               23.2506                40.1843
```

(*S*)-PhBOD-Rh(I)-Ph-CH-re-confU-α-Rhketone (24a)



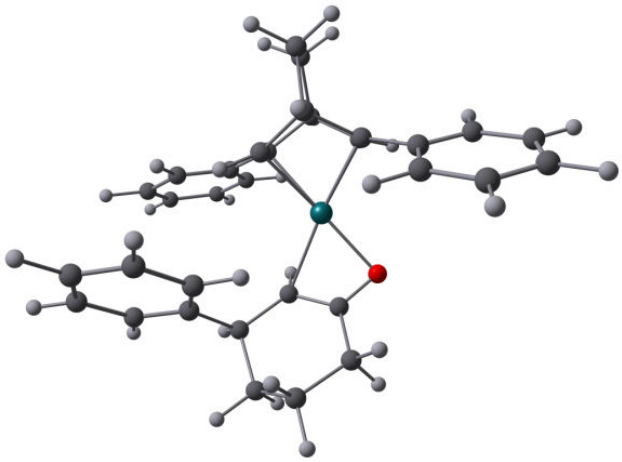
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.181814	0.247773	-0.255627
2	6	0	-1.051157	-1.506618	0.231555
3	6	0	0.978979	-2.310229	-0.864933
4	6	0	3.554821	-0.636239	-1.525460
5	6	0	-2.517406	-1.441733	0.409612
6	6	0	-3.387306	-1.973024	-0.553737
7	6	0	-0.385165	-1.659265	-0.999618
8	6	0	-0.179841	-1.958482	1.400929
9	6	0	-4.453336	-0.911202	1.787147
10	6	0	5.830220	-0.333575	-0.769626
11	6	0	0.840189	-3.672295	-0.142887
12	6	0	1.086043	-1.144101	1.250637
13	6	0	-4.765370	-1.973328	-0.351675
14	6	0	1.740565	-1.350594	0.046010
15	6	0	4.116098	-1.042251	0.779962
16	6	0	-3.077445	-0.913485	1.584363
17	6	0	0.141727	-3.462585	1.213906
18	6	0	-5.305946	-1.445447	0.819428
19	6	0	3.148556	-0.999237	-0.233002
20	6	0	5.443208	-0.710795	0.515687
21	6	0	4.878852	-0.300400	-1.790618
22	1	0	2.817518	-0.589231	-2.323568
23	1	0	6.865257	-0.075133	-0.976868

24	1	0	3.826164	-1.347391	1.781890
25	1	0	6.178984	-0.754095	1.314823
26	1	0	5.170462	-0.009192	-2.796527
27	1	0	-2.982209	-2.391252	-1.469065
28	1	0	-4.863074	-0.488274	2.700980
29	1	0	-5.418239	-2.388346	-1.114976
30	1	0	-2.428912	-0.480361	2.341890
31	1	0	-6.381312	-1.447154	0.976989
32	1	0	1.470327	-2.425702	-1.832506
33	1	0	-0.662678	-1.781972	2.362706
34	1	0	0.266792	-4.350875	-0.782677
35	1	0	1.834406	-4.112815	-0.014813
36	1	0	0.778644	-3.791843	2.041444
37	1	0	-0.788954	-4.036136	1.275051
38	1	0	1.544185	-0.636243	2.096299
39	1	0	-0.910530	-1.624017	-1.951855
40	6	0	0.350936	2.570461	0.247716
41	6	0	1.666323	2.281159	-0.176424
42	6	0	0.116823	2.616541	1.639560
43	6	0	2.719302	2.155983	0.744814
44	1	0	1.896767	2.293802	-1.240720
45	6	0	1.159104	2.477760	2.548494
46	1	0	-0.884638	2.811947	2.010472
47	6	0	2.470340	2.264966	2.104063
48	1	0	3.726796	1.975492	0.380564
49	1	0	0.952140	2.550473	3.613444
50	1	0	3.284094	2.180471	2.819434
51	6	0	-0.707437	2.871957	-0.816613
52	1	0	-0.242787	3.580578	-1.515502
53	6	0	-0.948839	1.534255	-1.530350
54	1	0	-0.307506	1.389918	-2.409847
55	6	0	-2.297643	1.074209	-1.828901
56	8	0	-2.530093	0.237298	-2.713170
57	6	0	-1.989879	3.522562	-0.293000
58	1	0	-1.756110	4.239388	0.502793
59	6	0	-3.453221	1.644619	-1.027425
60	6	0	-3.028107	2.500389	0.157262
61	1	0	-2.427447	4.110250	-1.110053
62	1	0	-2.622776	1.854385	0.944143
63	1	0	-3.900224	3.008200	0.585505
64	1	0	-4.037835	2.250666	-1.733537
65	1	0	-4.102115	0.816435	-0.728579

SCF Done: E(RPBE1PBE) = -5999.11049477 A.U. after 1 cycles
Convg = 0.2705D-08 -V/T = 2.0047
Zero-point correction= 0.546915 (Hartree/Particle)
Thermal correction to Energy= 0.576381
Thermal correction to Enthalpy= 0.577341
Thermal correction to Gibbs Free Energy= 0.486727
Sum of electronic and zero-point Energies= -5998.563580
Sum of electronic and thermal Energies= -5998.534113
Sum of electronic and thermal Enthalpies= -5998.533153
Sum of electronic and thermal Free Energies= -5998.623768

	1	2	3
Frequencies --	23.1707	39.4424	49.2722

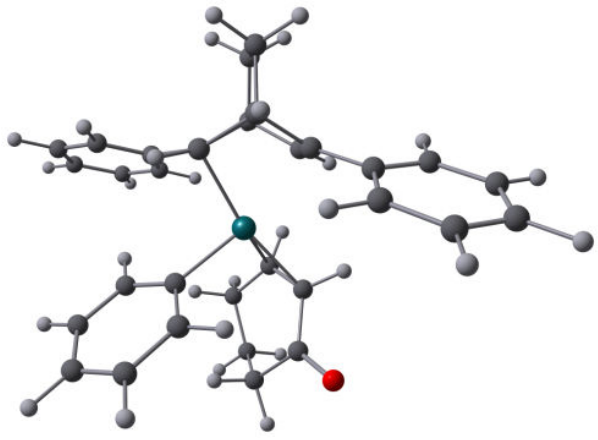
(*S*)-PhBOD-Rh(I)-Ph-CH-re-confU-Rh-oxa-π-allyl (25a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.572931	-0.120880	-0.671653
2	6	0	-2.286234	-0.994730	0.373718
3	6	0	-0.847404	-2.831026	-0.365258
4	6	0	1.995491	-2.689725	-1.617306
5	6	0	-3.513941	-0.173413	0.431776
6	6	0	-4.644394	-0.500076	-0.330039
7	6	0	-1.911615	-1.804953	-0.705011
8	6	0	-1.484599	-1.334737	1.628576
9	6	0	-4.733672	1.731492	1.326210
10	6	0	4.361399	-2.733992	-1.129043
11	6	0	-1.309233	-3.713768	0.816093
12	6	0	-0.059921	-1.121451	1.158053
13	6	0	-5.798356	0.277016	-0.269959
14	6	0	0.314115	-1.944735	0.085540
15	6	0	2.781549	-2.018911	0.555227
16	6	0	-3.581809	0.954367	1.264005
17	6	0	-1.714438	-2.816815	2.001271
18	6	0	-5.849391	1.396902	0.558164
19	6	0	1.708941	-2.220040	-0.325508
20	6	0	4.091886	-2.270436	0.157596
21	6	0	3.304312	-2.942276	-2.015707
22	1	0	1.187317	-2.836027	-2.329370
23	1	0	5.384147	-2.932860	-1.438424
24	1	0	2.592391	-1.665537	1.564835
25	1	0	4.905100	-2.105593	0.859717
26	1	0	3.500832	-3.298626	-3.023770
27	1	0	-4.626051	-1.380557	-0.966430
28	1	0	-4.760105	2.605504	1.972081
29	1	0	-6.663603	0.002052	-0.867715
30	1	0	-2.713077	1.241563	1.851427
31	1	0	-6.750255	2.002754	0.606855
32	1	0	-0.587990	-3.441749	-1.230954
33	1	0	-1.736826	-0.679285	2.463886
34	1	0	-2.148419	-4.334720	0.486104
35	1	0	-0.496246	-4.393507	1.091834
36	1	0	-1.124643	-3.051542	2.893421
37	1	0	-2.767429	-2.959460	2.265880
38	1	0	0.664171	-0.607900	1.783616

```
     39          1           0       -2.497642   -1.882679   -1.617758
     40          8           0       -1.228954    1.270169   -2.108351
     41          6           0       -0.209898    1.963996   -1.705910
     42          6           0        1.007927    1.299121   -1.489781
     43          6           0        2.247550    2.023896   -0.997587
     44          1           0        3.085700    1.667021   -1.607244
     45          6           0        2.107695    3.536587   -1.276595
     46          1           0        2.954960    4.071542   -0.833700
     47          6           0        2.652272    1.784526    0.447331
     48          6           0        1.733707    1.789998    1.502542
     49          6           0        4.007315    1.626655    0.760808
     50          6           0        2.155237    1.653413    2.824726
     51          1           0        0.672133    1.880952    1.285676
     52          6           0        4.435880    1.482040    2.079083
     53          1           0        4.739779    1.610215   -0.044360
     54          6           0        3.509108    1.497953    3.120785
     55          1           0        1.421846    1.665604    3.628031
     56          1           0        5.494470    1.354808    2.292529
     57          1           0        3.837445    1.388129    4.151192
     58          6           0       -0.407205    3.428755   -1.414916
     59          1           0       -1.326338    3.556097   -0.834477
     60          1           0        1.181795    0.422659   -2.122906
     61          6           0        0.793256    4.104473   -0.754006
     62          1           0        2.161441    3.689239   -2.362483
     63          1           0        0.748115    3.978370    0.332943
     64          1           0        0.754192    5.184145   -0.935476
     65          1           0       -0.606846    3.887020   -2.393008
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5999.11893951     A.U. after    1 cycles
             Convg  =    0.2615D-08             -V/T =  2.0047
Zero-point correction=                           0.547288 (Hartree/Particle)
 Thermal correction to Energy=                   0.576828
 Thermal correction to Enthalpy=                 0.577789
 Thermal correction to Gibbs Free Energy=        0.483822
 Sum of electronic and zero-point Energies=          -5998.571652
 Sum of electronic and thermal Energies=             -5998.542111
 Sum of electronic and thermal Enthalpies=           -5998.541151
 Sum of electronic and thermal Free Energies=        -5998.635118
                    1                    2                    3
Frequencies --    11.5774              21.9624              26.8133
```

(*S*)-PhBOD-Rh(I)-Ph-CH-re-confD-close (20b)



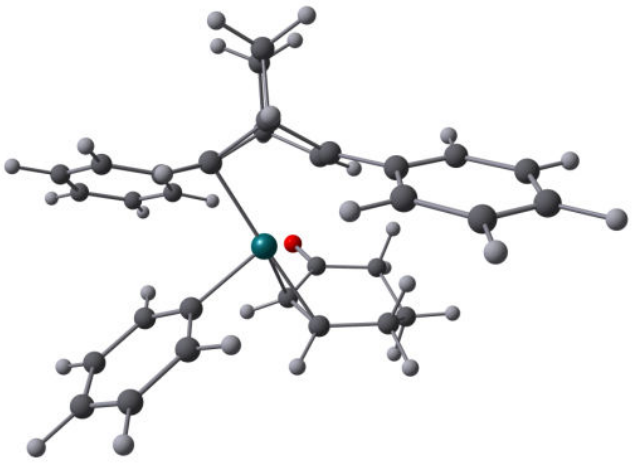
```
---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
```

Number	Number	Type	X	Y	Z
1	45	0	-0.179926	0.104241	-0.038447
2	6	0	-1.819910	-1.624948	0.083830
3	6	0	0.145011	-2.575011	-0.974645
4	6	0	3.047773	-1.541911	-1.411947
5	6	0	-3.191455	-1.097634	0.214577
6	6	0	-4.143754	-1.304378	-0.794227
7	6	0	-1.150176	-1.807364	-1.095755
8	6	0	-1.055606	-2.221534	1.262844
9	6	0	-4.855051	0.158000	1.463953
10	6	0	5.269718	-1.698795	-0.476329
11	6	0	-0.158601	-3.955578	-0.332736
12	6	0	0.319922	-1.576149	1.218391
13	6	0	-5.429344	-0.783365	-0.678243
14	6	0	1.003974	-1.791658	0.014721
15	6	0	3.329073	-1.950496	0.941886
16	6	0	-3.571578	-0.366072	1.349384
17	6	0	-0.899837	-3.742610	1.000339
18	6	0	-5.789914	-0.048049	0.450326
19	6	0	2.470903	-1.755281	-0.149940
20	6	0	4.712113	-1.919996	0.781690
21	6	0	4.428928	-1.510267	-1.574189
22	1	0	2.407644	-1.371718	-2.273833
23	1	0	6.348882	-1.675224	-0.601936
24	1	0	2.910354	-2.134282	1.927051
25	1	0	5.356164	-2.073385	1.643671
26	1	0	4.851896	-1.332443	-2.559657
27	1	0	-3.880437	-1.895450	-1.667459
28	1	0	-5.123475	0.737549	2.343009
29	1	0	-6.154759	-0.958573	-1.468431
30	1	0	-2.847654	-0.179467	2.138916
31	1	0	-6.792787	0.360418	0.539687
32	1	0	0.637092	-2.695896	-1.940829
33	1	0	-1.559741	-2.039830	2.213074
34	1	0	-0.761399	-4.544533	-1.031108
35	1	0	0.783231	-4.493415	-0.184325
36	1	0	-0.347785	-4.185090	1.835481
37	1	0	-1.890637	-4.208109	0.983867
38	1	0	0.827795	-1.297402	2.138125
39	1	0	-1.577317	-1.561153	-2.064784
40	6	0	1.043479	1.362336	0.946760
41	6	0	2.438391	1.472365	0.889148
42	6	0	0.369871	2.151327	1.897333
43	6	0	3.133232	2.342922	1.734630
44	1	0	3.008181	0.875780	0.179011
45	6	0	1.059972	3.014642	2.750173
46	1	0	-0.718474	2.119185	1.964418
47	6	0	2.449767	3.117126	2.670859
48	1	0	4.217057	2.410415	1.660320
49	1	0	0.507755	3.617250	3.468622
50	1	0	2.990414	3.794523	3.327336
51	6	0	0.030746	1.038360	-2.074618
52	1	0	-0.087314	0.150530	-2.693530
53	6	0	-1.109608	1.557004	-1.450000
54	1	0	-2.086358	1.089424	-1.571936
55	6	0	-1.158036	2.957475	-0.979903
56	8	0	-2.163175	3.415797	-0.445086
57	6	0	1.227113	1.904874	-2.395183
58	1	0	1.650953	1.579535	-3.352065
59	1	0	2.014834	1.770543	-1.648536
60	6	0	0.067391	3.812395	-1.224151
61	1	0	0.706395	3.730043	-0.336135

62	1	0	-0.265183	4.852644	-1.286174
63	6	0	0.839193	3.381190	-2.467162
64	1	0	1.735851	3.999016	-2.585113
65	1	0	0.218702	3.548402	-3.356853

```
SCF Done:  E(RPBE1PBE) =  -5999.08523336     A.U. after    1 cycles
             Convg  =    0.9801D-08             -V/T =  2.0047
Zero-point correction=                           0.544624 (Hartree/Particle)
 Thermal correction to Energy=                    0.575153
 Thermal correction to Enthalpy=                  0.576113
 Thermal correction to Gibbs Free Energy=         0.481811
 Sum of electronic and zero-point Energies=          -5998.540609
 Sum of electronic and thermal Energies=             -5998.510080
 Sum of electronic and thermal Enthalpies=           -5998.509120
 Sum of electronic and thermal Free Energies=        -5998.603423
                     1                      2                      3
Frequencies --    26.4689                31.2545                37.7159
```

(*S*)-PhBOD-Rh(I)-Ph-CH-re-confD-far (21b)

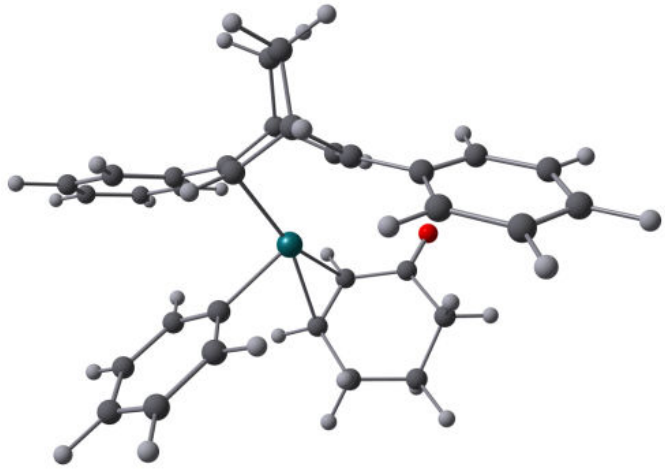


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.049949	0.436138	-0.105616
2	6	0	1.686615	-1.248415	-0.736473
3	6	0	-0.172525	-2.400808	0.308931
4	6	0	-2.987575	-1.467650	1.238872
5	6	0	3.053415	-0.718971	-0.907282
6	6	0	4.100332	-1.136430	-0.071885
7	6	0	1.138059	-1.664761	0.443848
8	6	0	0.801941	-1.606478	-1.925672
9	6	0	4.621560	0.735204	-2.063758
10	6	0	-5.301641	-1.493947	0.535610
11	6	0	0.056261	-3.628272	-0.616631
12	6	0	-0.557309	-1.002252	-1.619851
13	6	0	5.384132	-0.619633	-0.222999
14	6	0	-1.119955	-1.458144	-0.423843
15	6	0	-3.531950	-1.478770	-1.109136
16	6	0	3.338876	0.216692	-1.912992
17	6	0	0.662828	-3.152694	-1.949760
18	6	0	5.650270	0.320824	-1.218035
19	6	0	-2.559930	-1.463052	-0.098940
20	6	0	-4.888960	-1.491548	-0.795845

21	6	0	-4.343657	-1.480570	1.550585
22	1	0	-2.255507	-1.412282	2.041567
23	1	0	-6.360462	-1.504759	0.780968
24	1	0	-3.223922	-1.489331	-2.150929
25	1	0	-5.625640	-1.503995	-1.595081
26	1	0	-4.653629	-1.470090	2.592495
27	1	0	3.909077	-1.886824	0.690805
28	1	0	4.818677	1.467433	-2.842366
29	1	0	6.182226	-0.960238	0.431532
30	1	0	2.543792	0.560665	-2.570483
31	1	0	6.652904	0.722115	-1.338084
32	1	0	-0.565854	-2.703946	1.279353
33	1	0	1.209682	-1.237765	-2.868326
34	1	0	0.720308	-4.334820	-0.108860
35	1	0	-0.900089	-4.137706	-0.771634
36	1	0	0.026575	-3.430529	-2.795922
37	1	0	1.646628	-3.601290	-2.122566
38	1	0	-1.154000	-0.555714	-2.411362
39	1	0	1.669986	-1.639027	1.388931
40	6	0	-1.330184	1.786269	-0.664704
41	6	0	-2.663758	1.891490	-0.253042
42	6	0	-0.867634	2.705348	-1.622230
43	6	0	-3.507372	2.870919	-0.785350
44	1	0	-3.066137	1.198914	0.483736
45	6	0	-1.709491	3.679003	-2.163717
46	1	0	0.169891	2.669269	-1.959371
47	6	0	-3.037537	3.766872	-1.744424
48	1	0	-4.540396	2.928553	-0.448040
49	1	0	-1.324470	4.373577	-2.907929
50	1	0	-3.695595	4.527053	-2.158179
51	6	0	0.833320	1.973247	1.309128
52	1	0	0.497241	2.879131	0.805624
53	6	0	-0.130842	1.207401	1.969781
54	1	0	-1.177998	1.499157	1.979371
55	6	0	0.254481	0.254164	3.035963
56	8	0	-0.560023	-0.501448	3.558036
57	6	0	2.293888	1.910189	1.703338
58	1	0	2.766838	2.872991	1.484205
59	1	0	2.837364	1.164538	1.111091
60	6	0	1.696272	0.282147	3.517521
61	1	0	2.220241	-0.565680	3.058263
62	1	0	1.677015	0.077324	4.592203
63	6	0	2.428136	1.577331	3.187723
64	1	0	3.483489	1.492900	3.469268
65	1	0	2.003847	2.397519	3.779753

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5999.08420651     A.U. after    1 cycles
            Convg  =    0.6007D-08             -V/T =  2.0047
Zero-point correction=                           0.544411 (Hartree/Particle)
 Thermal correction to Energy=                    0.575067
 Thermal correction to Enthalpy=                  0.576027
 Thermal correction to Gibbs Free Energy=         0.481382
 Sum of electronic and zero-point Energies=          -5998.539795
 Sum of electronic and thermal Energies=             -5998.509140
 Sum of electronic and thermal Enthalpies=           -5998.508180
 Sum of electronic and thermal Free Energies=        -5998.602825
                    1                      2                      3
Frequencies --    29.3326               32.8174                40.0160
```

(*S*)-PhBOD-Rh(I)-Ph-CH-si-confD-anti (22b)

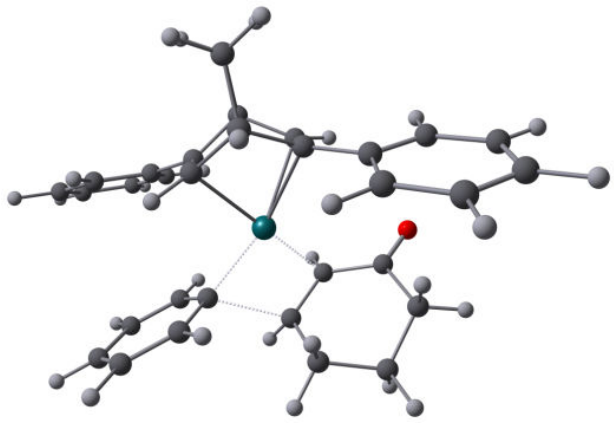


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.037616	0.228018	0.134028
2	6	0	1.393203	-1.522026	-0.469424
3	6	0	-0.502455	-2.476121	0.709539
4	6	0	-3.201630	-1.274069	1.643970
5	6	0	2.788023	-1.119403	-0.737879
6	6	0	3.836316	-1.522184	0.101678
7	6	0	0.854002	-1.807057	0.767554
8	6	0	0.462237	-1.932359	-1.603403
9	6	0	4.410942	0.039939	-2.131396
10	6	0	-5.524502	-1.106061	1.003630
11	6	0	-0.393370	-3.779943	-0.120035
12	6	0	-0.814266	-1.172452	-1.306891
13	6	0	5.149533	-1.146626	-0.168544
14	6	0	-1.383261	-1.494699	-0.059464
15	6	0	-3.806460	-1.304239	-0.684498
16	6	0	3.098944	-0.337231	-1.862580
17	6	0	0.204124	-3.455348	-1.501483
18	6	0	5.443676	-0.364949	-1.284823
19	6	0	-2.808468	-1.348060	0.298463
20	6	0	-5.149301	-1.183524	-0.336462
21	6	0	-4.542136	-1.151136	1.993954
22	1	0	-2.446346	-1.284601	2.425972
23	1	0	-6.572588	-1.012470	1.275353
24	1	0	-3.530701	-1.371081	-1.732891
25	1	0	-5.905782	-1.151628	-1.116240
26	1	0	-4.821846	-1.085988	3.042397
27	1	0	3.621878	-2.134950	0.971673
28	1	0	4.628101	0.653021	-3.002296
29	1	0	5.946325	-1.469453	0.496140
30	1	0	2.303024	-0.001030	-2.522637
31	1	0	6.469536	-0.074523	-1.495278
32	1	0	-0.891483	-2.681912	1.707493
33	1	0	0.868976	-1.672595	-2.581462
34	1	0	0.233962	-4.491433	0.426227
35	1	0	-1.387918	-4.228726	-0.210015
36	1	0	-0.477931	-3.747587	-2.306470
37	1	0	1.144501	-3.992189	-1.664467
38	1	0	-1.389981	-0.721788	-2.110364

39	1	0	1.416848	-1.734171	1.694528
40	6	0	-1.370709	1.613752	-0.617543
41	6	0	-2.633135	1.919594	-0.089809
42	6	0	-1.007103	2.254281	-1.814611
43	6	0	-3.493508	2.819478	-0.723261
44	1	0	-2.964789	1.447335	0.833738
45	6	0	-1.862812	3.154407	-2.455566
46	1	0	-0.037389	2.050550	-2.270464
47	6	0	-3.114265	3.442961	-1.911836
48	1	0	-4.466590	3.031162	-0.284013
49	1	0	-1.548660	3.629704	-3.383172
50	1	0	-3.782946	4.143176	-2.406706
51	6	0	0.291973	2.110699	1.443805
52	1	0	-0.722289	2.388040	1.709486
53	6	0	0.860026	1.019533	2.081322
54	1	0	0.282845	0.436562	2.796852
55	6	0	2.321439	0.833576	2.154982
56	8	0	2.812631	-0.064945	2.834082
57	6	0	1.142307	3.161644	0.762925
58	1	0	0.646110	4.132690	0.855477
59	1	0	1.208086	2.967091	-0.313944
60	6	0	3.177491	1.823980	1.398468
61	1	0	3.297800	1.441272	0.376051
62	1	0	4.170291	1.828701	1.856043
63	6	0	2.545515	3.212788	1.362576
64	1	0	3.176188	3.897932	0.786168
65	1	0	2.490210	3.612742	2.382756

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5999.08196398     A.U. after    1 cycles
             Convg  =    0.4847D-08             -V/T =  2.0047
Zero-point correction=                           0.544767 (Hartree/Particle)
 Thermal correction to Energy=                    0.575356
 Thermal correction to Enthalpy=                  0.576316
 Thermal correction to Gibbs Free Energy=         0.481750
 Sum of electronic and zero-point Energies=          -5998.537197
 Sum of electronic and thermal Energies=             -5998.506608
 Sum of electronic and thermal Enthalpies=           -5998.505648
 Sum of electronic and thermal Free Energies=        -5998.600214
                    1                      2                      3
Frequencies --    14.8789               37.3789                41.4127
```

(*S*)-PhBOD-Rh(I)-Ph-CH-re-confD-CR-TS (23b)



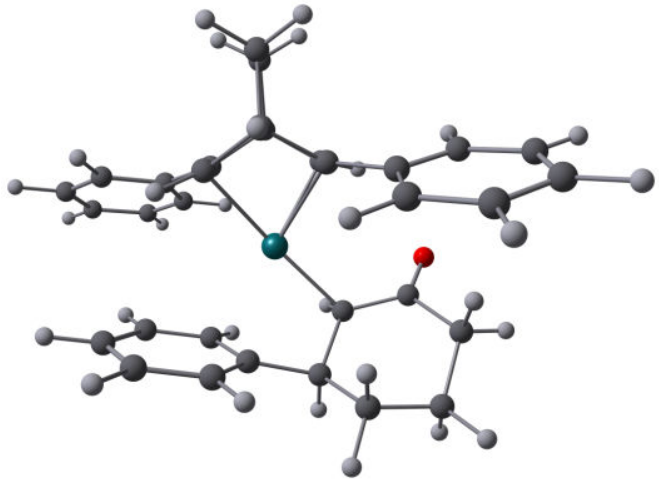
```
---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
```

1	45	0	0.177345	-0.256580	0.070336
2	6	0	1.746977	1.292634	0.067510
3	6	0	-0.065832	2.153765	-1.320493
4	6	0	-2.931944	1.029261	-1.741784
5	6	0	3.113988	0.826903	0.383640
6	6	0	4.090724	0.704045	-0.614196
7	6	0	1.144450	1.252130	-1.190532
8	6	0	0.983835	2.212195	1.019353
9	6	0	4.757586	0.073246	2.012514
10	6	0	-5.226809	1.242470	-1.016610
11	6	0	0.331382	3.610159	-0.973370
12	6	0	-0.425816	1.654557	1.010885
13	6	0	5.377405	0.272837	-0.305468
14	6	0	-1.021080	1.644076	-0.244571
15	6	0	-3.417541	1.863708	0.461155
16	6	0	3.472380	0.505959	1.703013
17	6	0	0.979760	3.641865	0.423247
18	6	0	5.718871	-0.043749	1.008005
19	6	0	-2.467132	1.509090	-0.506949
20	6	0	-4.780781	1.730438	0.210830
21	6	0	-4.293564	0.892723	-1.993398
22	1	0	-2.218022	0.738272	-2.508420
23	1	0	-6.290735	1.140300	-1.213115
24	1	0	-3.086090	2.256018	1.418278
25	1	0	-5.497954	2.014756	0.976618
26	1	0	-4.628337	0.510262	-2.954333
27	1	0	3.843712	0.949303	-1.641926
28	1	0	5.009785	-0.176071	3.040176
29	1	0	6.116389	0.182826	-1.097278
30	1	0	2.732195	0.573952	2.496289
31	1	0	6.724434	-0.379186	1.247927
32	1	0	-0.503356	2.099246	-2.318249
33	1	0	1.410368	2.210992	2.022750
34	1	0	1.021995	3.978106	-1.738905
35	1	0	-0.561379	4.242960	-1.012672
36	1	0	0.430250	4.304407	1.099683
37	1	0	2.009538	4.010701	0.375331
38	1	0	-0.982301	1.513329	1.933820
39	1	0	1.639973	0.844627	-2.068218
40	6	0	-1.150414	-1.457215	1.239989
41	6	0	-2.548409	-1.412197	1.173711
42	6	0	-0.555521	-1.682090	2.497416
43	6	0	-3.324097	-1.543233	2.326902
44	1	0	-3.049275	-1.251782	0.222323
45	6	0	-1.328005	-1.785991	3.651284
46	1	0	0.526225	-1.785514	2.572066
47	6	0	-2.721316	-1.720398	3.571127
48	1	0	-4.408024	-1.495889	2.248470
49	1	0	-0.843113	-1.938981	4.613029
50	1	0	-3.328369	-1.821447	4.467137
51	6	0	-0.235759	-2.530919	-0.223144
52	6	0	1.083911	-2.072532	-0.594725
53	1	0	-0.229807	-3.307053	0.536005
54	1	0	1.915907	-2.305573	0.071156
55	6	0	1.473049	-1.891909	-1.996087
56	8	0	2.631779	-1.641213	-2.331854
57	6	0	0.395007	-2.088511	-3.049038
58	1	0	-0.123265	-1.131393	-3.198714
59	1	0	0.895886	-2.336394	-3.988929
60	6	0	-0.609187	-3.156390	-2.627964
61	1	0	-1.371453	-3.293397	-3.403147
62	1	0	-0.094819	-4.118829	-2.513563

63	6	0	-1.274804	-2.757904	-1.314976
64	1	0	-1.854996	-1.847230	-1.493275
65	1	0	-1.987992	-3.519636	-0.984271

```
SCF Done:  E(RPBE1PBE) =  -5999.06907812     A.U. after    1 cycles
             Convg  =    0.2166D-08             -V/T =  2.0047
Zero-point correction=                           0.544803 (Hartree/Particle)
 Thermal correction to Energy=                    0.574396
 Thermal correction to Enthalpy=                  0.575356
 Thermal correction to Gibbs Free Energy=         0.482445
 Sum of electronic and zero-point Energies=          -5998.517088
 Sum of electronic and thermal Energies=             -5998.487495
 Sum of electronic and thermal Enthalpies=           -5998.486535
 Sum of electronic and thermal Free Energies=        -5998.579446
                     1                      2                      3
Frequencies --  -248.8396               3.5215                46.7092
```

(*S*)-PhBOD-Rh(I)-Ph-CH-si-confD-α-Rhketone (24b)

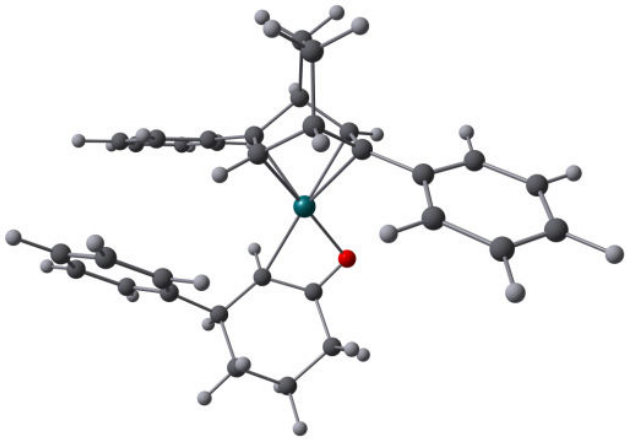


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.198418	0.215985	-0.236012
2	6	0	-0.979625	-1.547698	0.275665
3	6	0	1.046466	-2.324932	-0.849743
4	6	0	3.548081	-0.579943	-1.582798
5	6	0	-2.443161	-1.476806	0.473470
6	6	0	-3.328290	-2.021403	-0.467955
7	6	0	-0.332356	-1.701310	-0.966740
8	6	0	-0.083277	-1.983127	1.433140
9	6	0	-4.358297	-0.900640	1.861495
10	6	0	5.817184	-0.135468	-0.879926
11	6	0	0.948152	-3.684070	-0.116371
12	6	0	1.162893	-1.142622	1.255655
13	6	0	-4.704244	-2.006025	-0.249841
14	6	0	1.801238	-1.340124	0.040605
15	6	0	4.172857	-0.895405	0.720403
16	6	0	-2.984848	-0.915869	1.641900
17	6	0	0.264293	-3.480885	1.248945
18	6	0	-5.226592	-1.450262	0.916343
19	6	0	3.185608	-0.931331	-0.273845
20	6	0	5.474535	-0.499294	0.421854
21	6	0	4.846927	-0.180526	-1.882313

22	1	0	2.795780	-0.591905	-2.367991
23	1	0	6.832658	0.173064	-1.113832
24	1	0	3.918830	-1.189854	1.735207
25	1	0	6.226127	-0.481861	1.207180
26	1	0	5.103432	0.099743	-2.900837
27	1	0	-2.936494	-2.464324	-1.377908
28	1	0	-4.754309	-0.455545	2.770881
29	1	0	-5.369630	-2.432820	-0.995678
30	1	0	-2.322977	-0.468342	2.379279
31	1	0	-6.299831	-1.440910	1.087148
32	1	0	1.523233	-2.437911	-1.824745
33	1	0	-0.553917	-1.809288	2.401676
34	1	0	0.381429	-4.380288	-0.743049
35	1	0	1.953670	-4.101489	0.000693
36	1	0	0.918834	-3.793800	2.069062
37	1	0	-0.654101	-4.072165	1.325803
38	1	0	1.621071	-0.616657	2.090439
39	1	0	-0.870633	-1.679710	-1.912202
40	6	0	0.224549	2.548380	0.401065
41	6	0	1.494244	2.361536	-0.190343
42	6	0	0.168893	2.590507	1.809704
43	6	0	2.658418	2.288610	0.591587
44	1	0	1.595900	2.400478	-1.273438
45	6	0	1.323445	2.511746	2.579572
46	1	0	-0.787049	2.722956	2.306275
47	6	0	2.576922	2.369276	1.973427
48	1	0	3.621514	2.167727	0.103113
49	1	0	1.248231	2.572091	3.662668
50	1	0	3.477457	2.319639	2.579653
51	6	0	-0.993974	2.743673	-0.501717
52	1	0	-0.819746	3.648744	-1.106479
53	6	0	-1.040013	1.496354	-1.392880
54	1	0	-0.329842	1.541195	-2.231249
55	6	0	-2.314567	0.999018	-1.910288
56	8	0	-2.367791	0.171952	-2.830124
57	6	0	-2.299114	2.958516	0.257788
58	1	0	-2.269534	3.916787	0.790241
59	1	0	-2.432856	2.170563	1.010452
60	6	0	-3.605728	1.509668	-1.298103
61	1	0	-3.896201	0.799472	-0.514012
62	1	0	-4.379335	1.453295	-2.069606
63	6	0	-3.482688	2.906217	-0.699005
64	1	0	-4.408057	3.171974	-0.175792
65	1	0	-3.347704	3.649650	-1.495925

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5999.11258603     A.U. after    1 cycles
             Convg  =    0.5098D-08             -V/T =  2.0047
Zero-point correction=                           0.546850 (Hartree/Particle)
 Thermal correction to Energy=                    0.576324
 Thermal correction to Enthalpy=                  0.577284
 Thermal correction to Gibbs Free Energy=         0.486779
 Sum of electronic and zero-point Energies=          -5998.565736
 Sum of electronic and thermal Energies=             -5998.536262
 Sum of electronic and thermal Enthalpies=           -5998.535302
 Sum of electronic and thermal Free Energies=        -5998.625807
                    1                    2                    3
                    1                    2                    3
Frequencies --    29.5833               40.7323               49.8544
```

(*S*)-PhBOD-Rh(I)-Ph-CH-re-confD-Rh-oxa-π-allyl (25b)



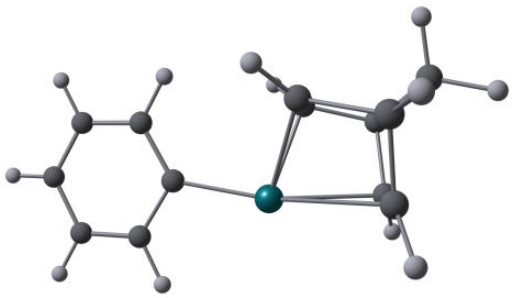
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.735081	-0.282715	-0.447270
2	6	0	2.506024	0.814420	0.271184
3	6	0	0.990412	2.452696	-0.709472
4	6	0	-1.905462	2.166598	-1.721965
5	6	0	3.743196	0.016896	0.406473
6	6	0	4.835842	0.226389	-0.446434
7	6	0	2.053583	1.395259	-0.912614
8	6	0	1.768413	1.370156	1.488188
9	6	0	5.022515	-1.714231	1.537045
10	6	0	-4.221454	2.437443	-1.091122
11	6	0	1.499011	3.549150	0.255021
12	6	0	0.318978	1.063103	1.160671
13	6	0	6.001526	-0.523660	-0.313579
14	6	0	-0.127585	1.663110	-0.030092
15	6	0	-2.553024	1.921284	0.581143
16	6	0	3.859284	-0.963321	1.403713
17	6	0	1.990385	2.898305	1.561895
18	6	0	6.100621	-1.497903	0.678363
19	6	0	-1.541630	1.909538	-0.389770
20	6	0	-3.876583	2.179980	0.234394
21	6	0	-3.227034	2.426894	-2.069896
22	1	0	-1.149278	2.141012	-2.502316
23	1	0	-5.254009	2.644233	-1.360161
24	1	0	-2.305832	1.729095	1.621149
25	1	0	-4.640628	2.181870	1.007250
26	1	0	-3.482514	2.618328	-3.109104
27	1	0	4.777809	0.994663	-1.212720
28	1	0	5.086703	-2.475808	2.309971
29	1	0	6.837951	-0.341933	-0.983555
30	1	0	3.019521	-1.158233	2.066164
31	1	0	7.010215	-2.083285	0.782967
32	1	0	0.670436	2.887160	-1.656927
33	1	0	2.086957	0.883360	2.411521
34	1	0	2.304012	4.105911	-0.235598
35	1	0	0.686918	4.258602	0.444994
36	1	0	1.448537	3.292232	2.427836
37	1	0	3.054027	3.097410	1.729899
38	1	0	-0.362238	0.706625	1.927847
39	1	0	2.570360	1.283133	-1.862667

40	6	0	-2.176824	-2.201708	-0.315716
41	6	0	-0.679052	-2.048705	-0.467982
42	1	0	-2.372067	-3.288765	-0.312103
43	1	0	-0.053992	-2.508547	0.301311
44	6	0	-0.054464	-1.977345	-1.731180
45	8	0	1.236714	-1.872050	-1.768115
46	6	0	-0.842415	-1.858020	-3.011538
47	1	0	-0.745039	-0.827474	-3.373113
48	1	0	-0.353288	-2.490814	-3.760116
49	6	0	-2.308246	-2.236350	-2.829238
50	1	0	-2.887443	-1.905423	-3.697920
51	1	0	-2.400989	-3.329518	-2.791124
52	6	0	-2.896906	-1.647202	-1.550464
53	1	0	-2.822138	-0.553577	-1.562361
54	1	0	-3.961638	-1.894754	-1.511692
55	6	0	-2.735591	-1.705892	1.013349
56	6	0	-4.110218	-1.487997	1.177899
57	6	0	-1.919712	-1.532964	2.137724
58	6	0	-4.644744	-1.097722	2.403887
59	1	0	-4.787218	-1.617013	0.338798
60	6	0	-2.447944	-1.143745	3.368771
61	1	0	-0.849813	-1.696318	2.058409
62	6	0	-3.815464	-0.918967	3.510062
63	1	0	-5.715861	-0.932689	2.493392
64	1	0	-1.784740	-1.019034	4.221812
65	1	0	-4.229714	-0.614821	4.467891

```
SCF Done:  E(RPBE1PBE) =  -5999.11909108     A.U. after    1 cycles
             Convg  =    0.2723D-08             -V/T =  2.0047
Zero-point correction=                           0.547016 (Hartree/Particle)
 Thermal correction to Energy=                    0.576536
 Thermal correction to Enthalpy=                  0.577496
 Thermal correction to Gibbs Free Energy=         0.484746
 Sum of electronic and zero-point Energies=          -5998.572075
 Sum of electronic and thermal Energies=             -5998.542555
 Sum of electronic and thermal Enthalpies=           -5998.541595
 Sum of electronic and thermal Free Energies=        -5998.634345
                     1                      2                      3
Frequencies --    21.0929               24.2204               36.7395
```

NBD-Rh pathway

NBD-Rh(I)-Ph (26)

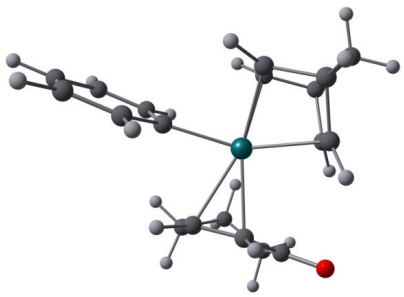


1	45	0	-0.282648	-0.637531	-0.000013
2	6	0	-2.442892	-0.925416	-0.687663

3	6	0	-2.549037	0.543515	1.127641
4	6	0	-2.442915	-0.925481	0.687558
5	6	0	-2.549007	0.543618	-1.127626
6	6	0	-1.173928	1.096911	-0.712761
7	6	0	-1.173943	1.096845	0.712875
8	6	0	-3.439325	1.109237	0.000042
9	1	0	-2.851865	0.718859	2.160167
10	1	0	-2.851832	0.719078	-2.160128
11	1	0	-0.570758	1.736420	-1.351299
12	1	0	-2.521986	-1.782547	1.349545
13	6	0	1.633294	-0.024083	-0.000001
14	6	0	2.152792	1.280327	-0.000019
15	6	0	2.560322	-1.080348	0.000018
16	6	0	3.528290	1.517650	-0.000012
17	1	0	1.478267	2.136409	-0.000045
18	6	0	3.939326	-0.856569	0.000023
19	1	0	2.207316	-2.116258	0.000043
20	6	0	4.427792	0.449639	0.000006
21	1	0	3.903121	2.539431	-0.000025
22	1	0	4.629987	-1.697529	0.000039
23	1	0	5.499262	0.634359	0.000006
24	1	0	-0.570785	1.736285	1.351491
25	1	0	-2.521938	-1.782426	-1.349729
26	1	0	-3.483139	2.203993	0.000067
27	1	0	-4.451110	0.687764	-0.000023

```
SCF Done:  E(RPBE1PBE) =  -5189.84905435     A.U. after    1 cycles
             Convg  =    0.4299D-08             -V/T =  2.0031
Zero-point correction=                           0.221282 (Hartree/Particle)
 Thermal correction to Energy=                    0.233079
 Thermal correction to Enthalpy=                  0.234039
 Thermal correction to Gibbs Free Energy=         0.181770
 Sum of electronic and zero-point Energies=          -5189.627773
 Sum of electronic and thermal Energies=             -5189.615975
 Sum of electronic and thermal Enthalpies=           -5189.615015
 Sum of electronic and thermal Free Energies=        -5189.667284
                     1                      2                      3
Frequencies --    46.5937               65.0260               71.0391
```

NBD-Rh(I)-Ph-CH-si-confU-anti (30a)

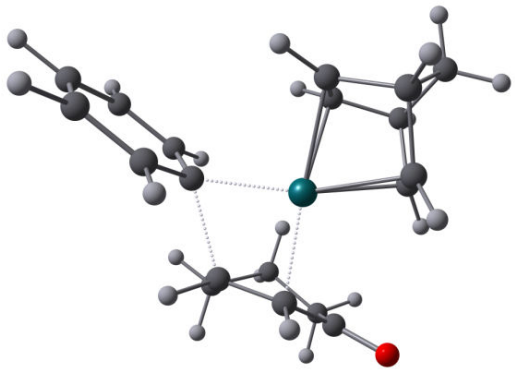


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.186224	0.223763	-0.223101
2	6	0	-1.996257	1.437411	-0.782022
3	6	0	-1.548210	2.110369	1.412160
4	6	0	-2.177963	1.029210	0.523184
5	6	0	-1.249586	2.779960	-0.716666
6	6	0	-1.857919	3.370330	0.574520

7	6	0	0.137354	2.361737	-0.200297
8	6	0	-0.051944	1.937515	1.116071
9	1	0	-1.838667	2.101703	2.462586
10	1	0	-1.264897	3.385898	-1.622301
11	1	0	1.080125	2.636079	-0.660874
12	1	0	-2.831793	0.237757	0.871671
13	6	0	1.871011	-0.015554	-0.112948
14	6	0	2.535879	-0.244299	1.102268
15	6	0	2.673624	0.199898	-1.246348
16	6	0	3.931402	-0.260478	1.184425
17	1	0	1.962536	-0.415805	2.012931
18	6	0	4.068280	0.190513	-1.171477
19	1	0	2.207035	0.376525	-2.215427
20	6	0	4.706980	-0.041423	0.047055
21	1	0	4.412116	-0.443989	2.143619
22	1	0	4.657549	0.362199	-2.070343
23	1	0	5.792389	-0.052531	0.108124
24	6	0	0.198480	-1.985566	-0.782126
25	6	0	-1.062531	-1.571609	-1.195915
26	1	0	1.011115	-1.978077	-1.502567
27	1	0	-1.217240	-1.197032	-2.207577
28	6	0	-2.287368	-1.978993	-0.482094
29	8	0	-3.402236	-1.704127	-0.917151
30	6	0	-2.113959	-2.817164	0.767745
31	1	0	-2.251438	-3.858906	0.444118
32	6	0	0.376760	-2.853451	0.432106
33	1	0	0.401299	-3.899725	0.089992
34	1	0	-2.475437	1.021890	-1.661969
35	1	0	0.719811	1.813424	1.867997
36	6	0	-0.752469	-2.661081	1.435831
37	1	0	1.350612	-2.656589	0.889658
38	1	0	-0.656385	-3.375594	2.260258
39	1	0	-0.670637	-1.655779	1.870620
40	1	0	-2.941999	-2.596220	1.447437
41	1	0	-2.931307	3.573810	0.487323
42	1	0	-1.326192	4.260656	0.928652

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5498.21193253     A.U. after    1 cycles
             Convg  =    0.4753D-08             -V/T =  2.0038
Zero-point correction=                           0.352386 (Hartree/Particle)
 Thermal correction to Energy=                    0.371489
 Thermal correction to Enthalpy=                  0.372449
 Thermal correction to Gibbs Free Energy=         0.304112
 Sum of electronic and zero-point Energies=          -5497.859546
 Sum of electronic and thermal Energies=             -5497.840444
 Sum of electronic and thermal Enthalpies=           -5497.839484
 Sum of electronic and thermal Free Energies=        -5497.907820
                    1                      2                      3
Frequencies --    31.7032               60.1284                61.9618
```

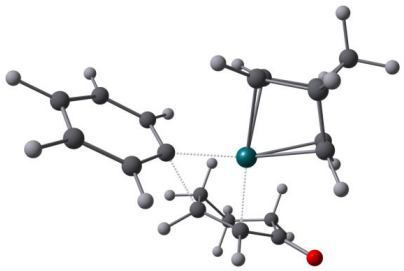
NBD-Rh(I)-Ph-CH-si-confU-CR-TS (31a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.305099	-0.219022	-0.270496
2	6	0	1.980896	-1.440204	-0.905443
3	6	0	1.813073	-1.928614	1.383064
4	6	0	2.287408	-0.901431	0.341621
5	6	0	1.315040	-2.801471	-0.633180
6	6	0	2.093590	-3.244483	0.624929
7	6	0	-0.022717	-2.384259	0.001981
8	6	0	0.285595	-1.845558	1.241139
9	1	0	2.213564	-1.817035	2.390801
10	1	0	1.257641	-3.490270	-1.476053
11	1	0	-1.004482	-2.679976	-0.353569
12	1	0	2.982721	-0.091614	0.537673
13	6	0	-1.772131	0.297274	-0.166089
14	6	0	-2.445209	0.289191	1.065191
15	6	0	-2.471541	-0.159576	-1.297650
16	6	0	-3.752684	-0.185550	1.167397
17	1	0	-1.941339	0.637533	1.964431
18	6	0	-3.771659	-0.650129	-1.195890
19	1	0	-1.993092	-0.124072	-2.275825
20	6	0	-4.421211	-0.662997	0.039693
21	1	0	-4.249510	-0.187693	2.135144
22	1	0	-4.284856	-1.008009	-2.085660
23	1	0	-5.440995	-1.030032	0.120367
24	6	0	-0.661623	1.938359	-0.629321
25	6	0	0.658002	1.681578	-1.158017
26	1	0	-1.416243	2.137515	-1.385222
27	1	0	0.760906	1.491396	-2.227799
28	6	0	1.867101	2.196696	-0.516349
29	8	0	2.972255	2.136374	-1.061692
30	6	0	1.730841	2.865373	0.840884
31	1	0	2.583061	2.562358	1.456834
32	6	0	-0.754991	2.849789	0.573841
33	1	0	-1.724633	2.748155	1.067188
34	1	0	2.388615	-1.124449	-1.860609
35	1	0	-0.406239	-1.633832	2.049206
36	6	0	0.398384	2.622249	1.539195
37	1	0	-0.708089	3.878896	0.188319
38	1	0	1.860302	3.939920	0.652064
39	1	0	0.304197	3.279333	2.410750
40	1	0	0.359112	1.588407	1.910332
41	1	0	3.160078	-3.406928	0.432115
42	1	0	1.654774	-4.122024	1.113377

```
 ----------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5498.19505886     A.U. after    1 cycles
             Convg  =    0.2462D-08             -V/T =  2.0038
Zero-point correction=                           0.351757 (Hartree/Particle)
 Thermal correction to Energy=                    0.370042
 Thermal correction to Enthalpy=                  0.371002
 Thermal correction to Gibbs Free Energy=         0.304771
 Sum of electronic and zero-point Energies=          -5497.843302
 Sum of electronic and thermal Energies=             -5497.825017
 Sum of electronic and thermal Enthalpies=           -5497.824057
 Sum of electronic and thermal Free Energies=        -5497.890287
                    1                    2                    3
Frequencies --  -296.3086               37.5871              59.5692
```

NBD-Rh(I)-Ph-CH-si-confD-CR-TS (31b)

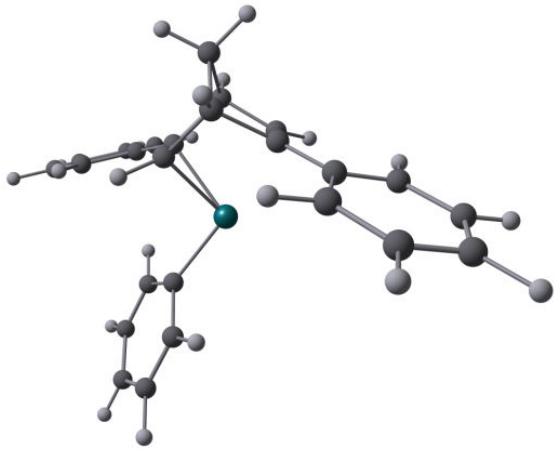


```
---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1         45           0        0.238814   -0.296698   -0.248822
      2          6           0        1.773858   -1.687445   -0.900541
      3          6           0        1.599821   -2.122369    1.398831
      4          6           0        2.155721   -1.164237    0.332385
      5          6           0        0.981774   -2.971899   -0.594149
      6          6           0        1.733948   -3.470774    0.658828
      7          6           0       -0.296497   -2.412561    0.053321
      8          6           0        0.085825   -1.885984    1.278748
      9          1           0        2.027207   -2.036031    2.397978
     10          1           0        0.841627   -3.664565   -1.424029
     11          1           0       -1.308524   -2.615983   -0.281559
     12          1           0        2.931283   -0.424063    0.502096
     13          6           0       -1.768321    0.438636   -0.106898
     14          6           0       -2.497452    0.464374    1.090001
     15          6           0       -2.464424    0.148234   -1.295462
     16          6           0       -3.861625    0.171632    1.106142
     17          1           0       -2.001093    0.701130    2.028388
     18          6           0       -3.821085   -0.167170   -1.277718
     19          1           0       -1.938623    0.173849   -2.249355
     20          6           0       -4.529125   -0.154405   -0.074210
     21          1           0       -4.404482    0.194045    2.048580
     22          1           0       -4.331348   -0.406940   -2.207958
     23          1           0       -5.591625   -0.382460   -0.059494
     24          6           0       -0.421951    1.946512   -0.362680
     25          6           0        0.780437    1.591238   -1.081278
     26          1           0       -1.202432    2.369391   -0.987882
     27          1           0        0.713593    1.477380   -2.165146
     28          6           0        2.116680    1.945609   -0.600361
     29          8           0        3.132669    1.724568   -1.261515
     30          6           0        2.207098    2.648298    0.743422
     31          1           0        2.310000    1.880701    1.523029
     32          1           0        3.129849    3.235019    0.746541
```

33	6	0	0.974489	3.501048	1.024991
34	1	0	1.061257	3.985462	2.003836
35	1	0	0.899915	4.301386	0.278336
36	6	0	-0.279896	2.633219	0.989284
37	1	0	-0.197674	1.893939	1.792291
38	1	0	-1.178949	3.221687	1.196693
39	1	0	2.190046	-1.422719	-1.867462
40	1	0	-0.567700	-1.603492	2.097378
41	1	0	2.775327	-3.742114	0.451633
42	1	0	1.218690	-4.292481	1.169261

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5498.19079476     A.U. after    1 cycles
             Convg  =    0.5630D-08             -V/T =  2.0038
Zero-point correction=                          0.351683 (Hartree/Particle)
 Thermal correction to Energy=                  0.370096
 Thermal correction to Enthalpy=                0.371056
 Thermal correction to Gibbs Free Energy=       0.304327
 Sum of electronic and zero-point Energies=          -5497.839112
 Sum of electronic and thermal Energies=             -5497.820699
 Sum of electronic and thermal Enthalpies=           -5497.819739
 Sum of electronic and thermal Free Energies=        -5497.886468
                    1                      2                      3
Frequencies --  -299.6022               39.7600                58.7007
```

(S)-PhNBD-Rh pathway
(*S*)-PhNBD-Rh(I)-Ph (34)

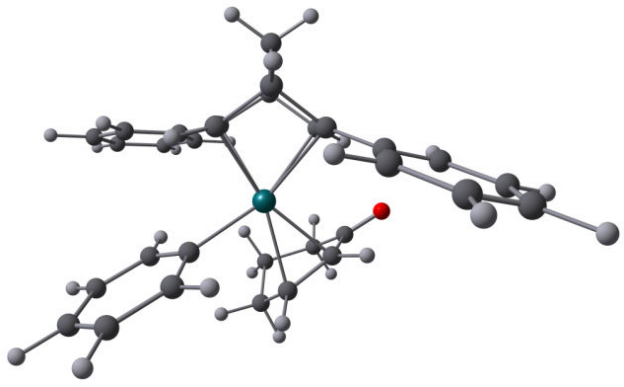


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.285214	0.230386	-0.392918
2	6	0	-1.911147	-1.262122	0.089729
3	6	0	0.013749	-2.547285	-0.282710
4	6	0	2.957797	-1.837680	-1.021047
5	6	0	-3.195791	-0.557211	0.009432
6	6	0	-3.952244	-0.555485	-1.175603
7	6	0	-1.146662	-1.793776	-0.934132
8	6	0	-1.199879	-1.677938	1.396675
9	6	0	-4.906149	0.837794	1.035337
10	6	0	5.151545	-1.352977	-0.131283
11	6	0	0.087165	-0.838359	1.343076
12	6	0	-5.158503	0.130855	-1.252924
13	6	0	0.883481	-1.402618	0.296937
14	6	0	3.175051	-0.909323	1.188587

15	6	0	-3.697514	0.150751	1.113921
16	6	0	-0.663284	-3.064652	0.999296
17	6	0	-5.643088	0.832735	-0.147559
18	6	0	2.347232	-1.379804	0.157768
19	6	0	4.559068	-0.896107	1.045980
20	6	0	4.342163	-1.823150	-1.165497
21	1	0	2.340666	-2.191452	-1.843197
22	1	0	6.232547	-1.342138	-0.242006
23	1	0	2.730952	-0.549000	2.111943
24	1	0	5.178768	-0.526299	1.858840
25	1	0	4.790773	-2.177493	-2.090154
26	1	0	-3.597017	-1.110337	-2.039921
27	1	0	-5.272421	1.381278	1.902435
28	1	0	-5.728288	0.113768	-2.178413
29	1	0	-3.130418	0.176708	2.040203
30	1	0	-6.587047	1.367366	-0.208565
31	1	0	0.531777	-3.273496	-0.908820
32	1	0	-1.788006	-1.607810	2.311803
33	1	0	0.465643	-0.284837	2.197915
34	1	0	-1.386141	-1.831810	-1.992439
35	6	0	0.925854	1.825607	-0.098056
36	6	0	2.252599	1.958313	-0.539628
37	6	0	0.305313	2.978511	0.422351
38	6	0	2.919565	3.184830	-0.487556
39	1	0	2.781958	1.094191	-0.937401
40	6	0	0.969319	4.205915	0.486013
41	1	0	-0.720159	2.927696	0.791671
42	6	0	2.282537	4.314098	0.027545
43	1	0	3.944013	3.257327	-0.848189
44	1	0	0.461825	5.077018	0.896330
45	1	0	2.804630	5.266874	0.074790
46	1	0	0.049259	-3.468264	1.727140
47	1	0	-1.457738	-3.792200	0.797465

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5651.43917355     A.U. after   17 cycles
             Convg  =    0.6219D-08             -V/T =  2.0041
Zero-point correction=                           0.384068 (Hartree/Particle)
 Thermal correction to Energy=                    0.406049
 Thermal correction to Enthalpy=                  0.407009
 Thermal correction to Gibbs Free Energy=         0.329516
 Sum of electronic and zero-point Energies=          -5651.055106
 Sum of electronic and thermal Energies=             -5651.033124
 Sum of electronic and thermal Enthalpies=           -5651.032164
 Sum of electronic and thermal Free Energies=        -5651.109657
                    1                    2                    3
Frequencies --    20.3262              25.0576              30.3455
```

(*S*)-PhNBD-Rh(I)-Ph-CH-si-confU-anti (37a)

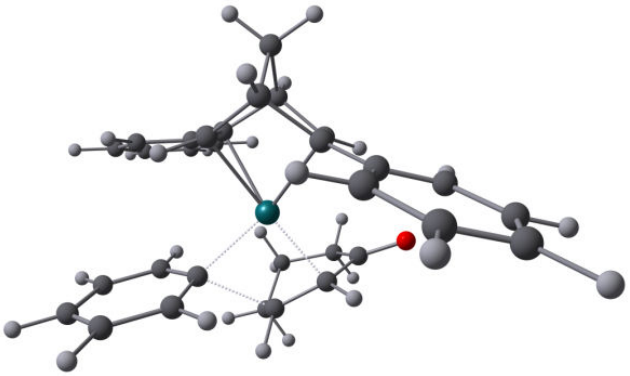


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.211591	0.166663	0.050661
2	6	0	1.830892	-0.979117	-1.081624
3	6	0	0.015969	-2.459731	-1.004732
4	6	0	-2.838430	-2.206044	0.225065
5	6	0	3.148731	-0.344165	-0.956210
6	6	0	4.091545	-0.807169	-0.024019
7	6	0	1.191057	-1.865791	-0.226514
8	6	0	1.009983	-1.001755	-2.387131
9	6	0	4.746436	1.347097	-1.664650
10	6	0	-5.146429	-1.747431	-0.319542
11	6	0	-0.315530	-0.351720	-1.971606
12	6	0	5.338824	-0.201701	0.084031
13	6	0	-0.969861	-1.277349	-1.139130
14	6	0	-3.370894	-0.805089	-1.661193
15	6	0	3.498163	0.740886	-1.775494
16	6	0	0.601888	-2.485853	-2.429277
17	6	0	5.673742	0.877391	-0.735354
18	6	0	-2.403046	-1.417578	-0.851820
19	6	0	-4.727447	-0.969128	-1.398244
20	6	0	-4.194498	-2.365285	0.492516
21	1	0	-2.105695	-2.686519	0.868800
22	1	0	-6.206081	-1.874933	-0.114725
23	1	0	-3.056891	-0.197148	-2.504534
24	1	0	-5.461025	-0.486411	-2.038643
25	1	0	-4.510086	-2.974030	1.335961
26	1	0	3.839333	-1.637892	0.628272
27	1	0	4.994846	2.189633	-2.304822
28	1	0	6.054232	-0.575437	0.811826
29	1	0	2.780990	1.126499	-2.495281
30	1	0	6.649593	1.347885	-0.649819
31	1	0	-0.403891	-3.384434	-0.609287
32	1	0	1.496985	-0.582809	-3.267344
33	1	0	-0.783462	0.464591	-2.511179
34	1	0	1.572860	-2.256379	0.709837
35	6	0	-1.143864	1.734926	-0.137344
36	6	0	-2.500394	1.701526	0.214083
37	6	0	-0.683151	2.896027	-0.784866
38	6	0	-3.358453	2.768349	-0.070753
39	1	0	-2.912697	0.831393	0.721704
40	6	0	-1.535117	3.962534	-1.079467
41	1	0	0.365870	2.978329	-1.069362
42	6	0	-2.883039	3.904504	-0.722544
43	1	0	-4.405761	2.704438	0.218959
44	1	0	-1.142394	4.842346	-1.585942
45	1	0	-3.549678	4.734093	-0.945488
46	6	0	0.464913	1.459912	1.968168
47	6	0	1.424969	0.456489	1.922047
48	1	0	0.724556	2.440092	1.574492
49	1	0	2.410374	0.648597	1.502448
50	6	0	1.326001	-0.731083	2.793062
51	8	0	2.230502	-1.562984	2.849330
52	6	0	0.116175	-0.849210	3.695797
53	1	0	-0.123339	-1.910858	3.806036
54	6	0	-0.676061	1.409453	2.943910
55	6	0	-1.086205	-0.021112	3.258963
56	1	0	0.461435	-0.510977	4.683447
57	1	0	-1.533333	-0.464064	2.360292
58	1	0	-1.853566	-0.036276	4.040450
59	1	0	-0.337760	1.913738	3.862851

60	1	0	-1.521313	1.989169	2.565370
61	1	0	-0.146494	-2.698397	-3.201281
62	1	0	1.455564	-3.166894	-2.524216

```
SCF Done:  E(RPBE1PBE) =  -5959.80038860     A.U. after   17 cycles
             Convg  =    0.6964D-08             -V/T =  2.0046
Zero-point correction=                           0.515336 (Hartree/Particle)
 Thermal correction to Energy=                    0.544468
 Thermal correction to Enthalpy=                  0.545428
 Thermal correction to Gibbs Free Energy=         0.454115
 Sum of electronic and zero-point Energies=          -5959.285053
 Sum of electronic and thermal Energies=             -5959.255920
 Sum of electronic and thermal Enthalpies=           -5959.254960
 Sum of electronic and thermal Free Energies=        -5959.346273
                     1                      2                      3
Frequencies --    24.2274                30.4227                39.5433
```

(*S*)-PhNBD-Rh(I)-Ph-CH-si-confU-CR-TS (38a)

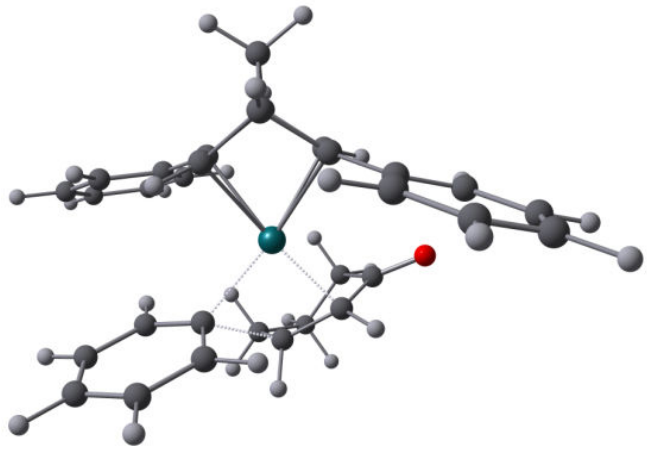


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.243970	0.089808	0.074031
2	6	0	1.773886	-1.097983	-0.951168
3	6	0	-0.060760	-2.564537	-0.812465
4	6	0	-2.906861	-2.145758	0.380785
5	6	0	3.117034	-0.507939	-0.858406
6	6	0	4.002785	-0.869523	0.169154
7	6	0	1.091376	-1.914082	-0.037783
8	6	0	0.987420	-1.227398	-2.275055
9	6	0	4.817844	0.999982	-1.728555
10	6	0	-5.198148	-1.563631	-0.117290
11	6	0	-0.346240	-0.541635	-1.950223
12	6	0	5.270527	-0.303547	0.245874
13	6	0	-1.025018	-1.384556	-1.071037
14	6	0	-3.407719	-0.788007	-1.544064
15	6	0	3.547618	0.435751	-1.805358
16	6	0	0.573503	-2.708979	-2.208109
17	6	0	5.687580	0.631160	-0.702767
18	6	0	-2.453855	-1.427619	-0.737658
19	6	0	-4.763112	-0.855413	-1.237749
20	6	0	-4.261977	-2.209011	0.691058
21	1	0	-2.187847	-2.648449	1.022790
22	1	0	-6.257227	-1.617672	0.120383
23	1	0	-3.083440	-0.239655	-2.423693
24	1	0	-5.484474	-0.356365	-1.879824
25	1	0	-4.588891	-2.765763	1.565582

26	1	0	3.686804	-1.578449	0.926862
27	1	0	5.128803	1.730273	-2.471359
28	1	0	5.937371	-0.594617	1.053271
29	1	0	2.876921	0.745888	-2.602089
30	1	0	6.680599	1.068772	-0.642212
31	1	0	-0.503935	-3.452909	-0.362445
32	1	0	1.498035	-0.885154	-3.174649
33	1	0	-0.767931	0.280234	-2.520352
34	1	0	1.466303	-2.270245	0.916825
35	6	0	-0.960195	1.873356	0.033040
36	6	0	-2.358115	1.857139	0.121693
37	6	0	-0.368706	2.828350	-0.816954
38	6	0	-3.137078	2.740640	-0.627434
39	1	0	-2.857383	1.135575	0.763966
40	6	0	-1.143562	3.694095	-1.584253
41	1	0	0.717057	2.900906	-0.871293
42	6	0	-2.537044	3.657592	-1.488579
43	1	0	-4.220828	2.699702	-0.543257
44	1	0	-0.659903	4.412033	-2.243026
45	1	0	-3.145641	4.344979	-2.070648
46	6	0	0.089660	1.766315	1.788347
47	6	0	1.219520	0.870874	1.814294
48	1	0	0.347644	2.804197	1.598311
49	1	0	2.189702	1.240859	1.483286
50	6	0	1.280012	-0.250637	2.752468
51	8	0	2.317289	-0.894817	2.940116
52	6	0	0.044658	-0.586476	3.570121
53	6	0	-0.962133	1.587105	2.858430
54	6	0	-1.234239	0.116678	3.133572
55	1	0	-0.065364	-1.675329	3.583313
56	1	0	0.295693	-0.297684	4.599880
57	1	0	-1.625868	-0.353566	2.222240
58	1	0	-2.006052	0.007302	3.903606
59	1	0	-0.561254	2.060506	3.767185
60	1	0	-1.876173	2.128438	2.603726
61	1	0	-0.148870	-2.984262	-2.985069
62	1	0	1.427230	-3.396245	-2.217231

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5959.78534216     A.U. after   17 cycles
             Convg  =    0.6233D-08             -V/T =  2.0046
Zero-point correction=                           0.514787 (Hartree/Particle)
 Thermal correction to Energy=                    0.543071
 Thermal correction to Enthalpy=                  0.544031
 Thermal correction to Gibbs Free Energy=         0.455075
 Sum of electronic and zero-point Energies=          -5959.270555
 Sum of electronic and thermal Energies=             -5959.242272
 Sum of electronic and thermal Enthalpies=           -5959.241312
 Sum of electronic and thermal Free Energies=        -5959.330267
                    1                      2                      3
Frequencies --  -294.1576               24.8744                37.8046
```

(*S*)-PhNBD-Rh(I)-Ph-CH-si-confD-CR-TS (38b)

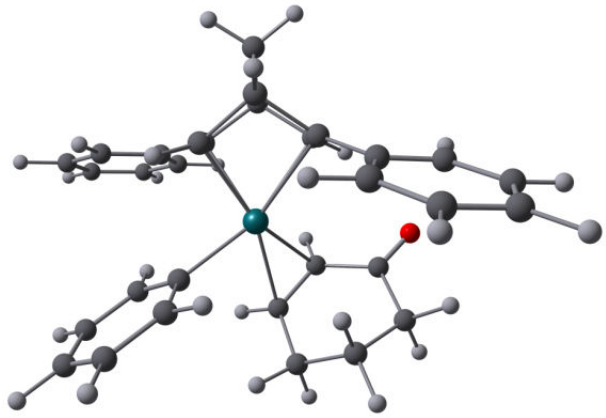


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.229478	0.010661	-0.084971
2	6	0	-1.762577	0.097297	1.485031
3	6	0	0.098897	-0.857403	2.559884
4	6	0	2.938010	-1.490890	1.396588
5	6	0	-3.094889	0.366394	0.925520
6	6	0	-3.945869	-0.677559	0.528063
7	6	0	-1.059390	-1.111045	1.588232
8	6	0	-0.993495	1.092664	2.382249
9	6	0	-4.808902	1.956290	0.247356
10	6	0	5.214783	-0.696345	1.246650
11	6	0	0.325482	1.277147	1.621209
12	6	0	-5.203169	-0.406869	0.000326
13	6	0	1.031544	0.078975	1.755233
14	6	0	3.400670	0.864524	1.589611
15	6	0	-3.548899	1.687115	0.774291
16	6	0	-0.545837	0.158311	3.520331
17	6	0	-5.644756	0.909790	-0.139848
18	6	0	2.464440	-0.180160	1.569357
19	6	0	4.759714	0.609255	1.430231
20	6	0	4.295801	-1.746444	1.231392
21	1	0	2.231660	-2.317270	1.378198
22	1	0	6.276061	-0.895162	1.123783
23	1	0	3.059465	1.884637	1.740244
24	1	0	5.467617	1.433857	1.454112
25	1	0	4.639243	-2.768430	1.092648
26	1	0	-3.609875	-1.706034	0.605597
27	1	0	-5.137943	2.986600	0.138124
28	1	0	-5.842579	-1.231184	-0.304546
29	1	0	-2.905829	2.516628	1.054731
30	1	0	-6.630021	1.117485	-0.548994
31	1	0	0.569358	-1.740660	2.992273
32	1	0	-1.523086	2.003787	2.657884
33	1	0	0.724677	2.235903	1.305850
34	1	0	-1.419159	-2.095720	1.306682
35	6	0	0.914227	1.152760	-1.499041
36	6	0	2.306360	1.293498	-1.521086
37	6	0	0.131583	2.260427	-1.881020
38	6	0	2.897816	2.510357	-1.866163
39	1	0	2.947794	0.457925	-1.254253

40	6	0	0.719931	3.482349	-2.197172
41	1	0	-0.952196	2.165212	-1.936992
42	6	0	2.111004	3.612961	-2.194067
43	1	0	3.982483	2.594506	-1.870610
44	1	0	0.092543	4.329301	-2.466218
45	1	0	2.574282	4.559355	-2.461026
46	6	0	0.203092	-0.591815	-2.310290
47	6	0	-1.030654	-1.094263	-1.755304
48	1	0	0.064691	0.040757	-3.181508
49	1	0	-1.961661	-0.610507	-2.053196
50	6	0	-1.181124	-2.496804	-1.361086
51	8	0	-2.264556	-2.976407	-1.017089
52	6	0	0.047442	-3.385634	-1.455776
53	6	0	1.403670	-1.522963	-2.411783
54	1	0	0.174189	0.630685	4.198250
55	1	0	-1.383665	-0.266096	4.085217
56	6	0	0.955570	-2.967100	-2.606422
57	1	0	-0.303091	-4.416579	-1.554938
58	1	0	0.597695	-3.319808	-0.507345
59	1	0	1.831647	-3.622747	-2.661571
60	1	0	0.417444	-3.072146	-3.556823
61	1	0	2.051060	-1.192918	-3.230202
62	1	0	2.007283	-1.478777	-1.499931

```
SCF Done:  E(RPBE1PBE) =  -5959.78147828     A.U. after    1 cycles
             Convg  =    0.5420D-08             -V/T =  2.0046
Zero-point correction=                           0.514715 (Hartree/Particle)
 Thermal correction to Energy=                    0.543103
 Thermal correction to Enthalpy=                  0.544063
 Thermal correction to Gibbs Free Energy=         0.454376
 Sum of electronic and zero-point Energies=          -5959.266763
 Sum of electronic and thermal Energies=             -5959.238376
 Sum of electronic and thermal Enthalpies=           -5959.237416
 Sum of electronic and thermal Free Energies=        -5959.327103
                     1                      2                      3
Frequencies --  -294.7001               21.8147                33.6511
```

(*S*)-PhNBD-Rh(I)-Ph-CH-re-confU-anti (44a)



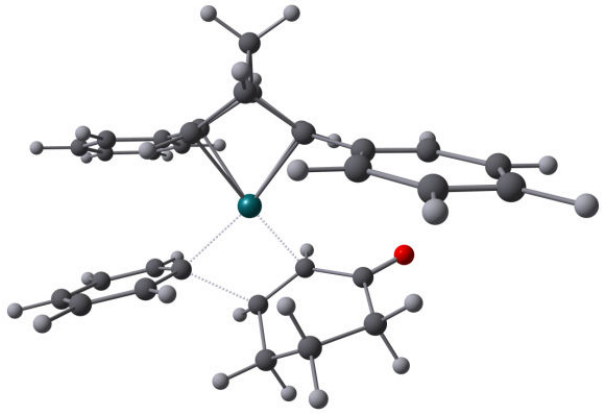
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.019863	0.036551	0.130618
2	6	0	1.403947	-1.594066	-0.704806
3	6	0	-0.502157	-2.744078	0.012944

4	6	0	-3.172325	-1.740569	1.310798
5	6	0	2.749400	-1.045491	-0.913910
6	6	0	3.815669	-1.381693	-0.066302
7	6	0	0.812114	-2.086697	0.443444
8	6	0	0.440662	-1.941628	-1.857014
9	6	0	4.276344	0.318187	-2.226556
10	6	0	-5.484685	-1.264969	0.799313
11	6	0	-0.753763	-1.025243	-1.574611
12	6	0	5.090731	-0.873277	-0.295680
13	6	0	-1.387741	-1.549803	-0.420007
14	6	0	-3.791299	-1.049706	-0.911984
15	6	0	3.002616	-0.194326	-2.002534
16	6	0	-0.100262	-3.296692	-1.368132
17	6	0	5.327448	-0.019975	-1.373580
18	6	0	-2.793173	-1.435550	-0.006064
19	6	0	-5.122400	-0.965988	-0.513645
20	6	0	-4.501573	-1.652107	1.711390
21	1	0	-2.412462	-2.030543	2.032771
22	1	0	-6.524048	-1.199133	1.109862
23	1	0	-3.522143	-0.814850	-1.937588
24	1	0	-5.880203	-0.664934	-1.232318
25	1	0	-4.772296	-1.885224	2.738060
26	1	0	3.644839	-2.046321	0.774587
27	1	0	4.450090	0.981681	-3.069764
28	1	0	5.904086	-1.148509	0.370601
29	1	0	2.189102	0.080563	-2.669525
30	1	0	6.324488	0.374392	-1.550907
31	1	0	-0.953234	-3.432110	0.727846
32	1	0	0.865966	-1.892372	-2.859469
33	1	0	-1.223055	-0.401622	-2.328161
34	1	0	1.262378	-2.163690	1.427567
35	6	0	-1.236625	1.602619	-0.457222
36	6	0	-2.529488	1.881476	0.006824
37	6	0	-0.727023	2.439189	-1.466646
38	6	0	-3.279319	2.943030	-0.505964
39	1	0	-2.971698	1.264227	0.787573
40	6	0	-1.472152	3.500697	-1.987286
41	1	0	0.274145	2.267908	-1.863271
42	6	0	-2.756072	3.759862	-1.507852
43	1	0	-4.279018	3.130101	-0.118210
44	1	0	-1.045765	4.125408	-2.770158
45	1	0	-3.338669	4.586026	-1.908243
46	6	0	0.100099	1.566183	1.894744
47	1	0	-0.942421	1.732030	2.150377
48	6	0	0.697211	0.377226	2.280566
49	1	0	0.117444	-0.391078	2.788217
50	6	0	2.157843	0.254546	2.425353
51	8	0	2.663268	-0.756486	2.910007
52	6	0	0.919751	2.780868	1.558872
53	1	0	0.989763	3.389847	2.473657
54	6	0	2.997800	1.455144	2.052812
55	6	0	2.315969	2.408756	1.077712
56	1	0	0.395327	3.393552	0.820250
57	1	0	2.248230	1.935570	0.089182
58	1	0	2.925851	3.309242	0.949397
59	1	0	3.962360	1.099250	1.682181
60	1	0	3.198513	1.975988	3.000652
61	1	0	-0.954160	-3.648541	-1.958006
62	1	0	0.668998	-4.075307	-1.304892

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5959.79773168     A.U. after   19 cycles
             Convg  =    0.5017D-08             -V/T =  2.0047
Zero-point correction=                          0.515058 (Hartree/Particle)
```

```
 Thermal correction to Energy=                    0.544195
 Thermal correction to Enthalpy=                  0.545155
 Thermal correction to Gibbs Free Energy=         0.454161
 Sum of electronic and zero-point Energies=          -5959.282674
 Sum of electronic and thermal Energies=             -5959.253536
 Sum of electronic and thermal Enthalpies=           -5959.252576
 Sum of electronic and thermal Free Energies=        -5959.343570
                     1                      2                      3
Frequencies --    19.6901                40.1496                43.1431
```

(*S*)-PhNBD-Rh(I)-Ph-CH-re-confU-CR-TS (45a)

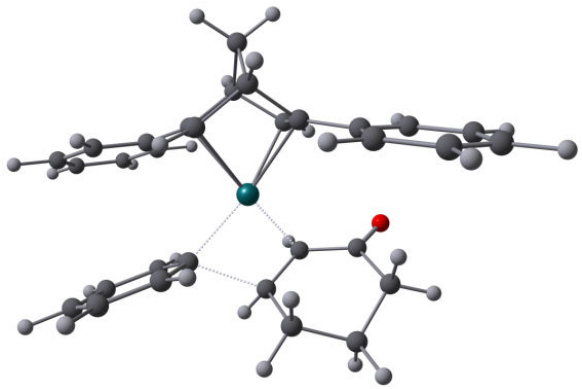


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.003226	-0.004261	-0.279423
2	6	0	-1.431394	-1.579296	0.346954
3	6	0	0.484298	-2.750600	-0.352255
4	6	0	3.211242	-1.651126	-1.410791
5	6	0	-2.839161	-1.202444	0.538149
6	6	0	-3.814847	-1.491941	-0.427077
7	6	0	-0.749910	-1.963384	-0.816133
8	6	0	-0.564550	-2.095646	1.517525
9	6	0	-4.587729	-0.282453	1.960541
10	6	0	5.499842	-1.189909	-0.790555
11	6	0	-0.064407	-3.424401	0.919827
12	6	0	0.700747	-1.239558	1.422474
13	6	0	-5.152939	-1.180400	-0.202791
14	6	0	1.382231	-1.664739	0.283802
15	6	0	3.758568	-1.168647	0.885016
16	6	0	-3.251054	-0.594419	1.736588
17	6	0	-5.547448	-0.577256	0.990831
18	6	0	2.792537	-1.480029	-0.082065
19	6	0	5.097381	-1.025176	0.534705
20	6	0	4.549223	-1.502953	-1.762862
21	1	0	2.477491	-1.884797	-2.178387
22	1	0	6.546252	-1.080678	-1.063172
23	1	0	3.456995	-1.043668	1.921307
24	1	0	5.830797	-0.785764	1.300392
25	1	0	4.852356	-1.633483	-2.798642
26	1	0	-3.524384	-1.963803	-1.360072
27	1	0	-4.882401	0.191858	2.893250
28	1	0	-5.890354	-1.409573	-0.967241
29	1	0	-2.512482	-0.352372	2.496857
30	1	0	-6.593209	-0.337547	1.164265

31	1	0	0.964386	-3.383113	-1.099147
32	1	0	-1.054527	-2.130133	2.490418
33	1	0	1.098807	-0.633520	2.229852
34	1	0	-1.160796	-2.000427	-1.820659
35	6	0	1.271577	1.689339	0.182041
36	6	0	2.545030	1.796605	-0.401458
37	6	0	1.118656	2.180508	1.490964
38	6	0	3.622063	2.339971	0.293953
39	1	0	2.700649	1.456221	-1.424240
40	6	0	2.195898	2.718001	2.194930
41	1	0	0.145830	2.141537	1.976346
42	6	0	3.454660	2.803328	1.599357
43	1	0	4.595216	2.401679	-0.187246
44	1	0	2.046708	3.080279	3.209971
45	1	0	4.291754	3.235291	2.141908
46	6	0	-0.139386	2.228597	-1.168925
47	1	0	0.675894	2.617971	-1.771646
48	6	0	-0.902071	1.185485	-1.811373
49	1	0	-0.467185	0.715434	-2.696814
50	6	0	-2.363071	1.185495	-1.827913
51	8	0	-2.992621	0.505110	-2.641026
52	6	0	-0.938693	3.303639	-0.462287
53	6	0	-3.092356	2.097067	-0.862701
54	6	0	-2.192330	2.735577	0.187493
55	1	0	-0.319020	3.849428	0.252723
56	1	0	-1.232503	4.025999	-1.238525
57	1	0	-1.910490	1.981654	0.933917
58	1	0	-2.735645	3.522789	0.721490
59	1	0	-3.556876	2.875939	-1.482800
60	1	0	-3.914933	1.530954	-0.415888
61	1	0	-0.872270	-4.134656	0.709595
62	1	0	0.714409	-3.898033	1.528630

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5959.78004895     A.U. after   17 cycles
             Convg  =    0.6515D-08             -V/T =  2.0046
Zero-point correction=                           0.514775 (Hartree/Particle)
 Thermal correction to Energy=                    0.542933
 Thermal correction to Enthalpy=                  0.543893
 Thermal correction to Gibbs Free Energy=         0.456186
 Sum of electronic and zero-point Energies=          -5959.265274
 Sum of electronic and thermal Energies=             -5959.237116
 Sum of electronic and thermal Enthalpies=           -5959.236156
 Sum of electronic and thermal Free Energies=        -5959.323863
                    1                    2                    3
Frequencies --  -300.0796               27.2548              45.5794
```

(*S*)-PhNBD-Rh(I)-Ph-CH-re-confD-CR-TS (45b)



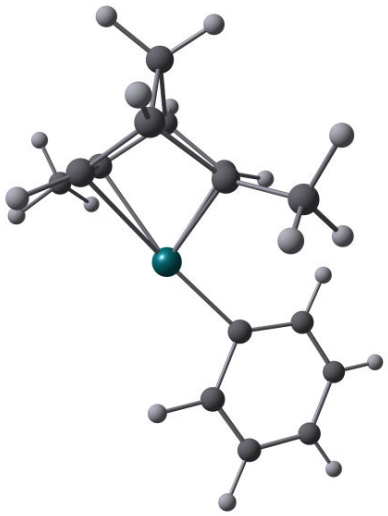
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.004643	-0.005925	-0.238258
2	6	0	-1.391701	-1.631850	0.319488
3	6	0	0.535263	-2.737499	-0.452337
4	6	0	3.241802	-1.564824	-1.471718
5	6	0	-2.800719	-1.276986	0.540349
6	6	0	-3.780621	-1.520912	-0.433120
7	6	0	-0.715041	-1.947413	-0.867235
8	6	0	-0.508105	-2.193250	1.455647
9	6	0	-4.545085	-0.439230	2.017925
10	6	0	5.520718	-1.061472	-0.848647
11	6	0	0.008334	-3.481818	0.788829
12	6	0	0.741103	-1.310739	1.391412
13	6	0	-5.118351	-1.224733	-0.186465
14	6	0	1.421204	-1.669807	0.228931
15	6	0	3.787208	-1.129046	0.833727
16	6	0	-3.207924	-0.732543	1.770788
17	6	0	-5.508827	-0.686594	1.039072
18	6	0	2.824746	-1.440061	-0.137268
19	6	0	5.119907	-0.941174	0.481901
20	6	0	4.574086	-1.373598	-1.824865
21	1	0	2.511926	-1.797298	-2.243217
22	1	0	6.562683	-0.917772	-1.122338
23	1	0	3.488819	-1.040806	1.874647
24	1	0	5.849988	-0.701528	1.250654
25	1	0	4.875551	-1.469368	-2.864930
26	1	0	-3.493094	-1.943554	-1.390307
27	1	0	-4.836714	-0.016112	2.975884
28	1	0	-5.859322	-1.417849	-0.957489
29	1	0	-2.465550	-0.525013	2.537396
30	1	0	-6.554521	-0.460761	1.230388
31	1	0	1.017166	-3.325507	-1.233594
32	1	0	-0.988269	-2.284036	2.429867
33	1	0	1.137611	-0.740369	2.224820
34	1	0	-1.132045	-1.936233	-1.869710
35	6	0	1.279112	1.667269	0.294320
36	6	0	2.463773	1.845123	-0.443326
37	6	0	1.281089	2.088498	1.633298
38	6	0	3.607750	2.382021	0.138575
39	1	0	2.490212	1.566740	-1.495872
40	6	0	2.426836	2.627476	2.221245
41	1	0	0.380767	1.992285	2.236217
42	6	0	3.596335	2.777835	1.477777
43	1	0	4.511243	2.493946	-0.456161
44	1	0	2.399844	2.938096	3.263710
45	1	0	4.485468	3.207720	1.931976
46	6	0	-0.338334	2.265980	-0.802483
47	1	0	0.389249	2.895430	-1.305215
48	6	0	-0.963570	1.280260	-1.648195
49	1	0	-0.431612	1.001821	-2.562485
50	6	0	-2.417361	1.192719	-1.808539
51	8	0	-2.923037	0.495091	-2.688731
52	6	0	-1.232340	3.013769	0.171178
53	6	0	-3.277022	2.054609	-0.906870
54	1	0	-0.789523	-4.194324	0.549805
55	1	0	0.799678	-3.972009	1.367664
56	6	0	-2.569165	3.340924	-0.490930
57	1	0	-0.725143	3.917003	0.522372
58	1	0	-1.435723	2.398817	1.053708
59	1	0	-3.195684	3.910020	0.204849

60	1	0	-2.407135	3.979949	-1.368251
61	1	0	-3.524092	1.462549	-0.016269
62	1	0	-4.217019	2.246422	-1.431463

```
SCF Done:  E(RPBE1PBE) =  -5959.77618496     A.U. after    1 cycles
            Convg  =    0.6800D-08             -V/T =  2.0046
Zero-point correction=                          0.514648 (Hartree/Particle)
 Thermal correction to Energy=                   0.542968
 Thermal correction to Enthalpy=                 0.543928
 Thermal correction to Gibbs Free Energy=        0.455426
 Sum of electronic and zero-point Energies=          -5959.261537
 Sum of electronic and thermal Energies=             -5959.233217
 Sum of electronic and thermal Enthalpies=           -5959.232257
 Sum of electronic and thermal Free Energies=        -5959.320759
                     1                      2                      3
Frequencies --  -298.1248               23.1811                44.4333
```

(S)-MeNBD-Rh pathway

(*S*)-MeNBD-Rh(I)-Ph (48)



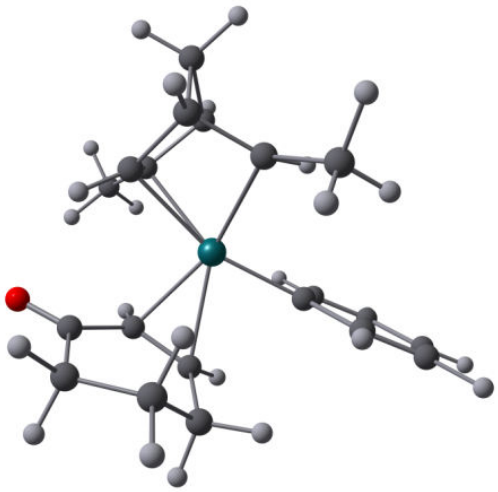
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.149402	-0.496189	-0.248601
2	6	0	2.295611	-1.017634	0.277167
3	6	0	2.399494	1.014551	-0.884710
4	6	0	2.286088	-0.512419	-1.006047
5	6	0	2.412977	0.203550	1.210245
6	6	0	1.038079	0.871267	1.032438
7	6	0	1.028568	1.405875	-0.292984
8	6	0	3.301217	1.133637	0.360099
9	1	0	2.694517	1.550821	-1.788365
10	1	0	2.719766	-0.011121	2.235391
11	1	0	3.354266	2.153767	0.758382
12	1	0	4.310820	0.738078	0.196605
13	1	0	0.450395	1.249959	1.865028
14	1	0	2.377121	-1.075842	-1.930870
15	6	0	-1.809815	-0.090081	0.053996
16	6	0	-2.464374	0.803709	0.916861
17	6	0	-2.625487	-0.943740	-0.710544

18	6	0	-3.856703	0.838936	1.014690
19	1	0	-1.885009	1.487719	1.536150
20	6	0	-4.019911	-0.915728	-0.627255
21	1	0	-2.167550	-1.659223	-1.401595
22	6	0	-4.641285	-0.019348	0.241525
23	1	0	-4.334706	1.537749	1.698791
24	1	0	-4.618967	-1.589131	-1.237265
25	1	0	-5.725616	0.010821	0.316424
26	6	0	2.446018	-2.429251	0.741897
27	1	0	1.743339	-2.659777	1.550404
28	1	0	2.283308	-3.141928	-0.071562
29	1	0	3.456543	-2.593817	1.139006
30	6	0	0.271227	2.591690	-0.803352
31	1	0	-0.672853	2.728904	-0.272496
32	1	0	0.874018	3.502994	-0.681498
33	1	0	0.047294	2.488433	-1.869629

SCF Done: E(RPBE1PBE) = -5268.39238060 A.U. after 16 cycles
Convg = 0.6362D-08 -V/T = 2.0033
Zero-point correction= 0.277180 (Hartree/Particle)
Thermal correction to Energy= 0.292527
Thermal correction to Enthalpy= 0.293487
Thermal correction to Gibbs Free Energy= 0.233866
Sum of electronic and zero-point Energies= -5268.115201
Sum of electronic and thermal Energies= -5268.099854
Sum of electronic and thermal Enthalpies= -5268.098894
Sum of electronic and thermal Free Energies= -5268.158515

	1	2	3
Frequencies --	35.6717	53.2007	65.9299

(*S*)-MeNBD-Rh(I)-Ph-CH-si-confU-anti (52a)

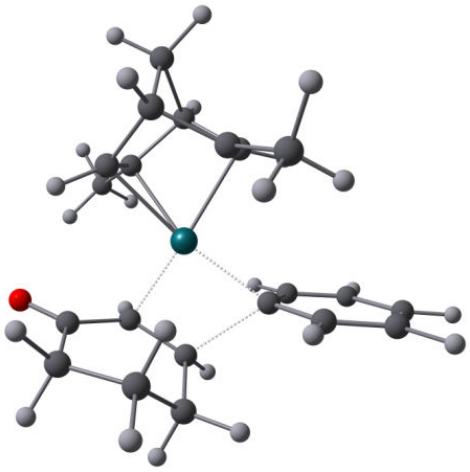


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.128468	-0.115879	-0.205422
2	6	0	1.943710	-1.333195	-0.838392
3	6	0	1.674758	-1.852223	1.431689
4	6	0	2.199204	-0.824954	0.422689
5	6	0	1.226764	-2.676142	-0.603530
6	6	0	-0.123816	-2.250531	-0.006888
7	6	0	0.146456	-1.758233	1.275666

8	6	0	1.953959	-3.162718	0.666627
9	1	0	2.049616	-1.757944	2.452023
10	1	0	1.181630	-3.342338	-1.466340
11	1	0	1.479493	-4.040652	1.121406
12	1	0	3.023671	-3.346955	0.510198
13	1	0	-1.087599	-2.603889	-0.358946
14	1	0	2.879286	-0.014399	0.659428
15	6	0	-1.946731	0.017850	-0.271823
16	6	0	-2.792147	0.335282	0.801416
17	6	0	-2.570954	-0.332920	-1.483558
18	6	0	-4.184866	0.299736	0.680368
19	1	0	-2.368189	0.616836	1.763994
20	6	0	-3.960659	-0.373236	-1.613437
21	1	0	-1.963562	-0.581990	-2.353567
22	6	0	-4.779242	-0.055800	-0.528752
23	1	0	-4.805563	0.553137	1.538038
24	1	0	-4.404849	-0.651809	-2.567329
25	1	0	-5.861733	-0.083046	-0.626277
26	6	0	-0.361181	2.103436	-0.645053
27	6	0	0.931250	1.788178	-1.051458
28	1	0	-1.152959	2.094803	-1.388234
29	1	0	1.123361	1.499884	-2.084030
30	6	0	2.107336	2.254933	-0.296234
31	8	0	3.247600	2.127108	-0.737757
32	6	0	1.860232	2.986270	1.006842
33	1	0	1.962486	4.053438	0.763338
34	6	0	-0.613855	2.910042	0.597084
35	1	0	-0.673126	3.967078	0.293641
36	6	0	-0.760239	-1.690352	2.459160
37	1	0	-0.561155	-2.551272	3.112212
38	1	0	-0.582317	-0.788446	3.054340
39	1	0	-1.811017	-1.715829	2.167380
40	6	0	2.534023	-0.949673	-2.154294
41	1	0	3.027822	0.023105	-2.105141
42	1	0	3.278253	-1.702100	-2.448147
43	1	0	1.773920	-0.929585	-2.942983
44	6	0	0.492022	2.728752	1.627671
45	1	0	2.680831	2.751334	1.690993
46	1	0	0.336078	3.400137	2.478940
47	1	0	0.451012	1.701801	2.013204
48	1	0	-1.593428	2.659396	1.013144

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5576.75439497     A.U. after   17 cycles
             Convg  =    0.5811D-08             -V/T =  2.0039
Zero-point correction=                           0.408601 (Hartree/Particle)
 Thermal correction to Energy=                    0.430992
 Thermal correction to Enthalpy=                  0.431952
 Thermal correction to Gibbs Free Energy=         0.357381
 Sum of electronic and zero-point Energies=          -5576.345794
 Sum of electronic and thermal Energies=             -5576.323403
 Sum of electronic and thermal Enthalpies=           -5576.322443
 Sum of electronic and thermal Free Energies=        -5576.397014
                     1                      2                      3
Frequencies --    21.2840                58.3919                59.6784
```

(*S*)-MeNBD-Rh(I)-Ph-CH-si-confU-CR-TS (53a)

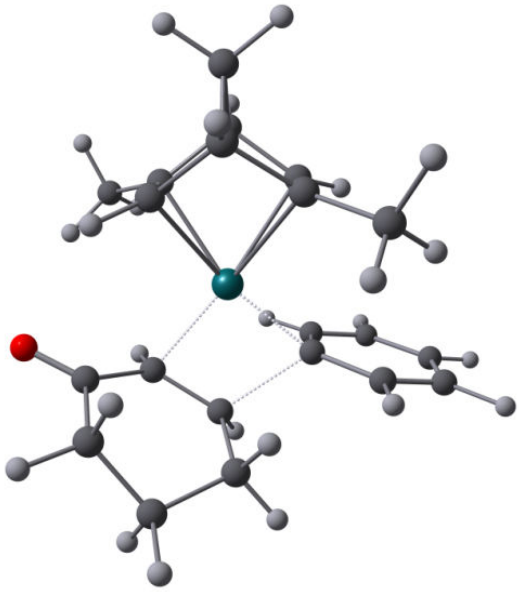


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.267809	-0.077481	-0.196940
2	6	0	2.094888	-1.075715	-0.830619
3	6	0	1.909477	-1.697920	1.431827
4	6	0	2.284986	-0.571364	0.458800
5	6	0	1.558891	-2.508060	-0.630785
6	6	0	2.352639	-2.933789	0.621627
7	6	0	0.170135	-2.270498	-0.013699
8	6	0	0.380110	-1.791432	1.272309
9	1	0	2.272133	-1.592974	2.455729
10	1	0	1.591783	-3.153087	-1.510234
11	1	0	3.435869	-2.969444	0.454790
12	1	0	2.002670	-3.880872	1.049799
13	1	0	-0.762056	-2.667178	-0.405155
14	1	0	2.884442	0.297118	0.715895
15	6	0	-1.865808	0.190247	-0.357418
16	6	0	-2.722702	0.132866	0.751143
17	6	0	-2.340575	-0.338584	-1.573484
18	6	0	-3.984347	-0.457479	0.661329
19	1	0	-2.403195	0.539341	1.708156
20	6	0	-3.589654	-0.947368	-1.662667
21	1	0	-1.723061	-0.265874	-2.468096
22	6	0	-4.422164	-1.007516	-0.542572
23	1	0	-4.625211	-0.491423	1.539880
24	1	0	-3.922743	-1.360192	-2.612374
25	1	0	-5.405726	-1.464759	-0.612665
26	6	0	-0.900048	1.959172	-0.662861
27	6	0	0.495404	1.880389	-1.019776
28	1	0	-1.572017	2.082132	-1.507715
29	1	0	0.754244	1.738430	-2.069257
30	6	0	1.538553	2.511552	-0.216249
31	8	0	2.701081	2.616557	-0.621714
32	6	0	1.158604	3.098375	1.132453
33	1	0	1.947788	2.844916	1.846933
34	6	0	-1.252139	2.829344	0.522293
35	1	0	-2.264075	2.619840	0.876315
36	6	0	-0.553344	-1.777811	2.436376
37	1	0	-1.592638	-1.887602	2.120575
38	1	0	-0.308804	-2.609920	3.110884

39	1	0	-0.461156	-0.855650	3.020327
40	6	0	2.692178	-0.589538	-2.111487
41	1	0	3.589958	-1.177200	-2.348860
42	1	0	1.996965	-0.710512	-2.949070
43	1	0	2.978277	0.462467	-2.034821
44	6	0	-0.223871	2.701455	1.636486
45	1	0	1.207861	4.187845	1.000810
46	1	0	-0.202348	1.661058	1.989461
47	1	0	-0.506159	3.324005	2.492784
48	1	0	-1.260119	3.865786	0.153786

```
SCF Done:  E(RPBE1PBE) =  -5576.73942499     A.U. after   17 cycles
            Convg  =    0.6302D-08             -V/T =  2.0039
Zero-point correction=                           0.407927 (Hartree/Particle)
 Thermal correction to Energy=                    0.429540
 Thermal correction to Enthalpy=                  0.430500
 Thermal correction to Gibbs Free Energy=         0.358025
 Sum of electronic and zero-point Energies=          -5576.331498
 Sum of electronic and thermal Energies=             -5576.309885
 Sum of electronic and thermal Enthalpies=           -5576.308925
 Sum of electronic and thermal Free Energies=        -5576.381400
                    1                      2                      3
Frequencies --  -295.8662               34.5998                52.1570
```

(*S*)-MeNBD-Rh(I)-Ph-CH-si-confD-CR-TS (53b)

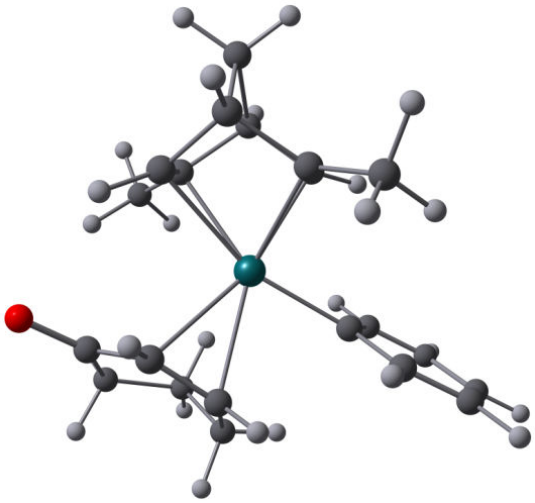


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.226402	-0.145876	-0.175064
2	6	0	1.937662	-1.313588	-0.842766
3	6	0	1.786917	-1.841545	1.444969
4	6	0	2.221490	-0.785842	0.419032
5	6	0	1.295067	-2.689285	-0.572810
6	6	0	2.094775	-3.137826	0.667594
7	6	0	-0.046558	-2.314466	0.079995
8	6	0	0.249801	-1.807435	1.339341
9	1	0	2.193633	-1.732862	2.451811

10	1	0	1.243115	-3.363493	-1.429150
11	1	0	3.164489	-3.271750	0.466768
12	1	0	1.681899	-4.036301	1.141963
13	1	0	-1.021642	-2.645835	-0.264630
14	1	0	2.905823	0.031904	0.625419
15	6	0	-1.880188	0.287357	-0.294093
16	6	0	-2.783784	0.264173	0.776319
17	6	0	-2.353406	-0.120696	-1.557303
18	6	0	-4.091484	-0.195247	0.607487
19	1	0	-2.472259	0.600302	1.762093
20	6	0	-3.648723	-0.603817	-1.722893
21	1	0	-1.698601	-0.056913	-2.425518
22	6	0	-4.528263	-0.642883	-0.638095
23	1	0	-4.770664	-0.205043	1.457404
24	1	0	-3.979538	-0.934581	-2.705012
25	1	0	-5.546089	-1.001223	-0.768064
26	6	0	-0.735125	1.974717	-0.394943
27	6	0	0.577817	1.810836	-0.972567
28	1	0	-1.495212	2.283876	-1.106144
29	1	0	0.646222	1.704716	-2.056482
30	6	0	1.781259	2.362543	-0.351250
31	8	0	2.882145	2.330273	-0.907387
32	6	0	1.621008	3.036872	0.999927
33	1	0	1.746424	2.275622	1.782027
34	1	0	2.441552	3.751137	1.110489
35	6	0	0.253735	3.698029	1.139534
36	1	0	0.157673	4.174252	2.121582
37	1	0	0.149324	4.491403	0.388907
38	6	0	-0.850115	2.660239	0.960795
39	1	0	-0.758438	1.931583	1.772676
40	1	0	-1.841549	3.113205	1.058224
41	6	0	-0.636071	-1.679942	2.533674
42	1	0	-1.691823	-1.725722	2.258774
43	1	0	-0.428456	-2.501301	3.233198
44	1	0	-0.456039	-0.744942	3.075393
45	6	0	2.503693	-0.917544	-2.167866
46	1	0	3.346198	-1.575293	-2.423612
47	1	0	1.759740	-1.023169	-2.964565
48	1	0	2.861942	0.114769	-2.151042

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5576.73542285     A.U. after   17 cycles
             Convg  =    0.6055D-08             -V/T =  2.0039
Zero-point correction=                           0.407974 (Hartree/Particle)
 Thermal correction to Energy=                    0.429684
 Thermal correction to Enthalpy=                  0.430644
 Thermal correction to Gibbs Free Energy=         0.357880
 Sum of electronic and zero-point Energies=          -5576.327449
 Sum of electronic and thermal Energies=             -5576.305739
 Sum of electronic and thermal Enthalpies=           -5576.304779
 Sum of electronic and thermal Free Energies=        -5576.377543
                     1                      2                      3
Frequencies --  -296.3657               36.0914                51.0827
```

(*S*)-MeNBD-Rh(I)-Ph-CH-re-confU-anti (59a)



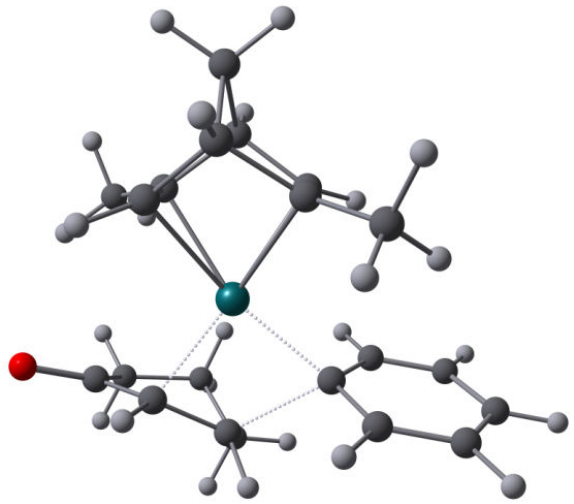
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.146103	-0.165220	-0.157074
2	6	0	-2.076848	-0.971208	0.845927
3	6	0	-1.516429	-2.544932	-0.794405
4	6	0	-2.156305	-1.176584	-0.516565
5	6	0	-1.365560	-2.208210	1.415916
6	6	0	-1.918712	-3.305947	0.486160
7	6	0	0.058534	-2.053554	0.867327
8	6	0	-0.019601	-2.305860	-0.514841
9	1	0	-1.748249	-2.995537	-1.760585
10	1	0	-1.455590	-2.345918	2.494561
11	1	0	-3.002680	-3.447353	0.575268
12	1	0	-1.399345	-4.264614	0.602466
13	1	0	0.957011	-2.138501	1.470235
14	1	0	-2.756137	-0.605581	-1.217871
15	6	0	1.912499	0.055218	0.035029
16	6	0	2.848454	-0.074694	-1.003654
17	6	0	2.432022	0.286361	1.321545
18	6	0	4.223944	0.015836	-0.777315
19	1	0	2.507159	-0.248151	-2.024143
20	6	0	3.806098	0.384628	1.557986
21	1	0	1.754391	0.393589	2.168101
22	6	0	4.713275	0.248333	0.507842
23	1	0	4.915022	-0.091769	-1.611459
24	1	0	4.166898	0.566231	2.568828
25	1	0	5.782998	0.322913	0.687354
26	6	0	0.349608	1.894949	-1.102928
27	1	0	1.102701	1.668788	-1.851750
28	6	0	-0.971341	1.559875	-1.368143
29	1	0	-1.231996	1.033842	-2.284569
30	6	0	-2.091195	2.248055	-0.704485
31	8	0	-3.253616	2.060093	-1.056889
32	6	0	0.700082	2.948986	-0.089434
33	1	0	0.799106	3.904069	-0.628127
34	6	0	-1.749322	3.263291	0.366123
35	1	0	-2.549325	3.263294	1.111878
36	6	0	1.039652	-2.830355	-1.426818
37	1	0	2.040484	-2.644468	-1.034474

38	1	0	0.907264	-3.914954	-1.544875
39	1	0	0.967697	-2.385159	-2.424560
40	6	0	-2.783192	0.009648	1.719454
41	1	0	-3.543451	-0.519077	2.309781
42	1	0	-2.095758	0.473871	2.434886
43	1	0	-3.284612	0.787787	1.143635
44	6	0	-0.370076	3.072026	0.986228
45	1	0	1.678827	2.735416	0.348635
46	1	0	-0.142755	3.906857	1.657462
47	1	0	-0.362688	2.161822	1.600772
48	1	0	-1.796914	4.241605	-0.133681

SCF Done: E(RPBE1PBE) = -5576.75168694 A.U. after 17 cycles
Convg = 0.6588D-08 -V/T = 2.0039
Zero-point correction= 0.408307 (Hartree/Particle)
Thermal correction to Energy= 0.430825
Thermal correction to Enthalpy= 0.431785
Thermal correction to Gibbs Free Energy= 0.356887
Sum of electronic and zero-point Energies= -5576.343380
Sum of electronic and thermal Energies= -5576.320862
Sum of electronic and thermal Enthalpies= -5576.319902
Sum of electronic and thermal Free Energies= -5576.394800

	1	2	3
Frequencies --	31.7259	38.7283	63.6199

(*S*)-MeNBD-Rh(I)-Ph-CH-re-confU-CR-TS (60a)

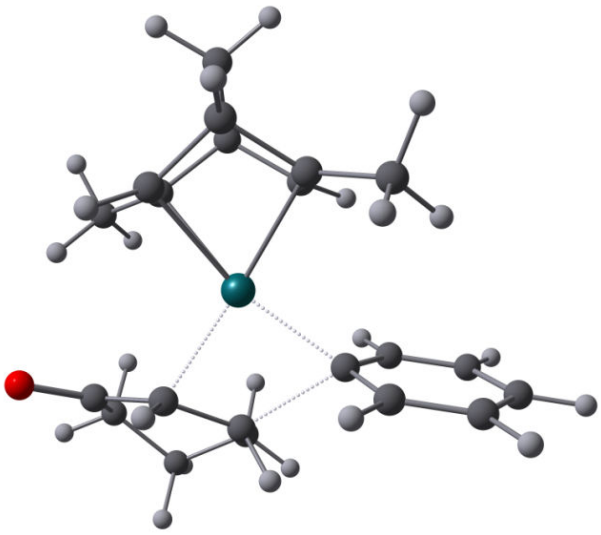


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.229216	0.199681	-0.253433
2	6	0	2.057615	1.157277	0.555795
3	6	0	1.026930	2.840280	-0.721289
4	6	0	1.850596	1.542183	-0.770296
5	6	0	1.316373	2.202328	1.407917
6	6	0	1.573079	3.475189	0.574469
7	6	0	-0.157118	1.934677	1.075122
8	6	0	-0.352167	2.356629	-0.234058
9	1	0	1.020820	3.442202	-1.631429
10	1	0	1.577942	2.215012	2.467327
11	1	0	2.634614	3.742098	0.506346
12	1	0	0.986521	4.336669	0.916036

13	1	0	-0.935674	1.742293	1.806957
14	1	0	2.429409	1.205301	-1.625573
15	6	0	-1.770736	-0.618817	-0.104600
16	6	0	-2.694430	-0.331270	-1.124762
17	6	0	-2.275317	-0.747391	1.201554
18	6	0	-4.047354	-0.140402	-0.853649
19	1	0	-2.350534	-0.264503	-2.156571
20	6	0	-3.627716	-0.552533	1.479945
21	1	0	-1.602640	-0.990519	2.021483
22	6	0	-4.522813	-0.246044	0.454217
23	1	0	-4.733403	0.085067	-1.667134
24	1	0	-3.983930	-0.644557	2.503764
25	1	0	-5.578967	-0.105543	0.669034
26	6	0	-0.482386	-2.031698	-0.764712
27	1	0	-1.202643	-2.222084	-1.554838
28	6	0	0.813544	-1.605753	-1.241786
29	1	0	0.888541	-1.275573	-2.280186
30	6	0	2.054065	-2.177822	-0.727408
31	8	0	3.127735	-2.039522	-1.320152
32	6	0	-0.491516	-3.084323	0.323810
33	1	0	-1.453718	-3.107398	0.840238
34	6	0	1.990390	-3.007073	0.541707
35	1	0	2.849309	-2.745149	1.166672
36	6	0	3.139691	0.308696	1.136758
37	1	0	3.924298	0.962415	1.543062
38	1	0	2.771521	-0.297933	1.971337
39	1	0	3.596605	-0.344725	0.392365
40	6	0	-1.621802	2.738662	-0.918724
41	1	0	-2.496557	2.330754	-0.409003
42	1	0	-1.707854	3.833996	-0.933904
43	1	0	-1.639306	2.398990	-1.959349
44	6	0	0.668638	-2.898141	1.290160
45	1	0	-0.383991	-4.054887	-0.182804
46	1	0	0.623778	-3.643170	2.091901
47	1	0	0.590861	-1.909798	1.764245
48	1	0	2.153010	-4.046362	0.224699

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5576.73520671     A.U. after   17 cycles
             Convg  =    0.6487D-08             -V/T =  2.0039
Zero-point correction=                           0.408011 (Hartree/Particle)
 Thermal correction to Energy=                    0.429611
 Thermal correction to Enthalpy=                  0.430571
 Thermal correction to Gibbs Free Energy=         0.357931
 Sum of electronic and zero-point Energies=          -5576.327195
 Sum of electronic and thermal Energies=             -5576.305595
 Sum of electronic and thermal Enthalpies=           -5576.304635
 Sum of electronic and thermal Free Energies=        -5576.377276
                     1                      2                      3
Frequencies --  -297.5250               23.5737                48.4967
```

(*S*)-MeNBD-Rh(I)-Ph-CH-re-confD-CR-TS (60b)



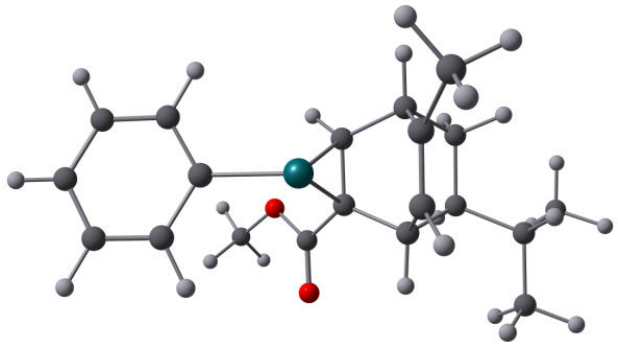
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.162299	0.261772	-0.212377
2	6	0	1.801001	1.592587	0.485034
3	6	0	0.364911	3.002678	-0.732733
4	6	0	1.439415	1.904741	-0.826072
5	6	0	0.905805	2.470788	1.376824
6	6	0	0.840313	3.756761	0.526480
7	6	0	-0.493912	1.893839	1.131241
8	6	0	-0.852584	2.249245	-0.163472
9	1	0	0.181757	3.575819	-1.643031
10	1	0	1.218316	2.554163	2.419112
11	1	0	1.816534	4.238899	0.394805
12	1	0	0.106810	4.481428	0.900325
13	1	0	-1.171046	1.553603	1.908768
14	1	0	2.022561	1.681672	-1.714900
15	6	0	-1.653898	-0.893432	-0.042016
16	6	0	-2.505144	-0.867278	-1.163031
17	6	0	-2.250490	-1.060013	1.217679
18	6	0	-3.887906	-0.950228	-1.029054
19	1	0	-2.075681	-0.789049	-2.161318
20	6	0	-3.636624	-1.145420	1.356574
21	1	0	-1.631467	-1.110134	2.110711
22	6	0	-4.464391	-1.086681	0.235826
23	1	0	-4.518472	-0.915586	-1.914790
24	1	0	-4.070560	-1.261204	2.347534
25	1	0	-5.543322	-1.160954	0.344066
26	6	0	-0.036567	-2.067649	-0.439063
27	1	0	-0.725812	-2.576011	-1.105711
28	6	0	1.085755	-1.452308	-1.107636
29	1	0	0.975860	-1.243767	-2.174893
30	6	0	2.468705	-1.751892	-0.735963
31	8	0	3.421992	-1.380081	-1.423357
32	6	0	0.234678	-2.828640	0.848063
33	1	0	-0.600122	-3.502976	1.060671
34	1	0	0.307263	-2.139776	1.695869
35	6	0	2.697894	-2.609153	0.496354
36	1	0	2.800266	-1.940410	1.361297

37	1	0	3.659414	-3.114286	0.370107
38	6	0	1.554298	-3.587768	0.741626
39	1	0	1.730951	-4.156928	1.661025
40	1	0	1.504865	-4.314846	-0.078564
41	6	0	3.073742	1.005168	0.997638
42	1	0	3.737331	1.820055	1.319486
43	1	0	2.900636	0.374649	1.875992
44	1	0	3.597309	0.425367	0.236113
45	6	0	-2.216427	2.355131	-0.760035
46	1	0	-2.947895	1.761834	-0.207456
47	1	0	-2.536776	3.406145	-0.741934
48	1	0	-2.229556	2.030368	-1.805068

```
SCF Done:  E(RPBE1PBE) =  -5576.73107252     A.U. after   17 cycles
             Convg  =    0.6711D-08             -V/T =  2.0039
Zero-point correction=                           0.407856 (Hartree/Particle)
 Thermal correction to Energy=                    0.429569
 Thermal correction to Enthalpy=                  0.430529
 Thermal correction to Gibbs Free Energy=         0.357690
 Sum of electronic and zero-point Energies=          -5576.323216
 Sum of electronic and thermal Energies=             -5576.301504
 Sum of electronic and thermal Enthalpies=           -5576.300544
 Sum of electronic and thermal Free Energies=        -5576.373382
                    1                    2                    3
Frequencies --  -293.6227               29.9062              54.1685
```

(S)-Diels-Alder methyl ester ligand-Rh pathway

(*S*)-DA-prox-Rh(I)-Ph (63)

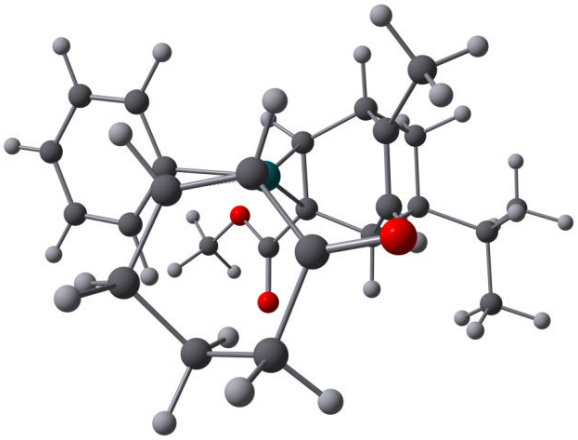


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.634521	-1.082535	-0.449271
2	6	0	1.512458	-1.908672	0.055684
3	6	0	1.693162	0.421376	-0.599399
4	6	0	1.635363	-1.042390	-0.997423
5	6	0	1.456178	-1.185414	1.396577
6	6	0	2.882992	0.661114	0.373296
7	6	0	0.252147	-0.273881	1.256963
8	6	0	0.399018	0.629171	0.168403
9	6	0	2.745316	-0.341291	1.546821
10	6	0	-0.324291	1.912929	0.029961
11	1	0	1.724904	1.088404	-1.460146
12	1	0	1.343059	-1.886212	2.227731
13	1	0	2.766607	1.684667	0.756389
14	1	0	2.731078	0.174803	2.512194

15	1	0	3.598986	-1.028892	1.566425
16	1	0	-0.390975	-0.051259	2.104474
17	1	0	1.842172	-1.373244	-2.013497
18	6	0	-2.524984	-0.479337	-0.166809
19	6	0	-3.298673	-0.871965	0.938875
20	6	0	-3.171765	0.241132	-1.186914
21	6	0	-4.664224	-0.586200	1.008274
22	1	0	-2.834002	-1.409887	1.764436
23	6	0	-4.536994	0.530487	-1.121452
24	1	0	-2.604926	0.594138	-2.048806
25	6	0	-5.290094	0.116008	-0.022610
26	1	0	-5.241196	-0.908533	1.873090
27	1	0	-5.011658	1.086393	-1.927852
28	1	0	-6.351845	0.343742	0.033279
29	8	0	-0.193964	2.670025	-0.917426
30	8	0	-1.143610	2.161337	1.063631
31	6	0	-1.991263	3.303254	0.912524
32	1	0	-2.581215	3.352614	1.826638
33	1	0	-1.398024	4.212062	0.789607
34	1	0	-2.646357	3.174115	0.048216
35	6	0	1.663218	-3.396194	-0.009759
36	1	0	2.610899	-3.700756	0.453340
37	1	0	0.863727	-3.904466	0.540715
38	1	0	1.660409	-3.757023	-1.041922
39	6	0	4.264292	0.584475	-0.301674
40	1	0	4.433089	-0.461491	-0.597603
41	6	0	5.364366	0.982050	0.684925
42	1	0	6.354827	0.868531	0.231746
43	1	0	5.253701	2.032428	0.980322
44	1	0	5.347173	0.377759	1.597191
45	6	0	4.364503	1.454051	-1.554823
46	1	0	3.717511	1.101929	-2.363337
47	1	0	4.091324	2.493089	-1.335457
48	1	0	5.390411	1.456035	-1.938253

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5613.87903261     A.U. after    1 cycles
             Convg  =    0.2682D-08             -V/T =  2.0039
Zero-point correction=                           0.407748 (Hartree/Particle)
 Thermal correction to Energy=                    0.431724
 Thermal correction to Enthalpy=                  0.432684
 Thermal correction to Gibbs Free Energy=         0.353147
 Sum of electronic and zero-point Energies=          -5613.471284
 Sum of electronic and thermal Energies=             -5613.447309
 Sum of electronic and thermal Enthalpies=           -5613.446349
 Sum of electronic and thermal Free Energies=        -5613.525885
                    1                      2                      3
Frequencies --    33.2681               38.3736                40.0296
```

(*S*)-DA-prox-Rh(I)-Ph-CH-si-confU-anti (67a)



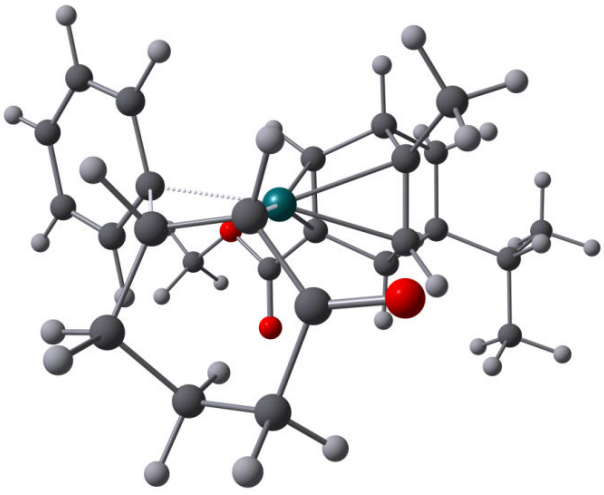
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.500280	0.564129	-0.457546
2	6	0	1.605083	0.884905	-1.415818
3	6	0	1.891362	-0.459897	0.585089
4	6	0	1.747872	0.908424	-0.047330
5	6	0	1.600490	-0.531741	-1.969454
6	6	0	3.119535	-1.194568	-0.033374
7	6	0	0.467884	-1.214765	-1.236737
8	6	0	0.642342	-1.200800	0.149288
9	6	0	2.940198	-1.201455	-1.571425
10	6	0	0.011496	-2.153223	1.094742
11	1	0	1.939861	-0.415771	1.672413
12	1	0	1.454457	-0.542211	-3.052013
13	1	0	3.082834	-2.228007	0.339048
14	1	0	2.967567	-2.219723	-1.972205
15	1	0	3.750885	-0.646356	-2.057465
16	1	0	-0.201211	-1.912558	-1.730304
17	1	0	1.973667	1.821798	0.496073
18	6	0	-2.298485	-0.452889	-0.484475
19	6	0	-2.914552	-1.006947	0.646705
20	6	0	-2.901478	-0.701770	-1.728969
21	6	0	-4.079358	-1.772612	0.543657
22	1	0	-2.484916	-0.847784	1.635116
23	6	0	-4.062072	-1.470442	-1.839418
24	1	0	-2.463714	-0.287712	-2.636969
25	6	0	-4.660643	-2.010227	-0.700498
26	1	0	-4.533935	-2.182695	1.443896
27	1	0	-4.502312	-1.643346	-2.819665
28	1	0	-5.567819	-2.603832	-0.782375
29	6	0	-2.167146	2.161449	-0.131983
30	6	0	-0.951243	2.747782	-0.458708
31	1	0	-2.887578	1.984323	-0.925786
32	1	0	-0.724654	3.003109	-1.492852
33	6	0	-0.142782	3.450290	0.559864
34	8	0	0.834490	4.124392	0.244304
35	6	0	-0.614245	3.391495	1.997258
36	1	0	0.267745	3.375389	2.644048
37	6	0	-2.700240	2.203534	1.271133
38	6	0	-1.579754	2.251612	2.299895
39	1	0	-1.107888	4.356878	2.178721

40	1	0	-1.039903	1.295911	2.282086
41	1	0	-1.990234	2.368643	3.308351
42	1	0	-3.327330	3.105049	1.353838
43	1	0	-3.363584	1.352448	1.443941
44	6	0	1.782857	2.050024	-2.335863
45	1	0	1.746289	2.999110	-1.797072
46	1	0	2.758599	1.971087	-2.833800
47	1	0	1.024024	2.053198	-3.125951
48	6	0	-1.241858	-4.120172	1.323742
49	1	0	-2.035447	-3.629997	1.890294
50	1	0	-1.663781	-4.871765	0.658387
51	1	0	-0.527607	-4.574872	2.013767
52	6	0	4.475042	-0.604272	0.395228
53	1	0	4.565682	0.391799	-0.062566
54	6	0	5.623141	-1.472000	-0.124808
55	1	0	6.591846	-1.024075	0.120087
56	1	0	5.591934	-2.466999	0.335370
57	1	0	5.586959	-1.607652	-1.210025
58	6	0	4.602090	-0.442624	1.909725
59	1	0	4.412237	-1.392125	2.424427
60	1	0	5.614157	-0.119763	2.175378
61	1	0	3.909275	0.301940	2.311695
62	8	0	-0.583380	-3.179016	0.470612
63	8	0	0.064302	-2.043362	2.307193

SCF Done: E(RPBE1PBE) = -5922.24114257 A.U. after 1 cycles
Convg = 0.5582D-08 -V/T = 2.0045
Zero-point correction= 0.538911 (Hartree/Particle)
Thermal correction to Energy= 0.569998
Thermal correction to Enthalpy= 0.570958
Thermal correction to Gibbs Free Energy= 0.476116
Sum of electronic and zero-point Energies= -5921.702231
Sum of electronic and thermal Energies= -5921.671144
Sum of electronic and thermal Enthalpies= -5921.670184
Sum of electronic and thermal Free Energies= -5921.765027

	1	2	3
Frequencies --	10.9762	38.7662	42.2844

(*S*)-DA-prox-Rh(I)-Ph-CH-si-confU-CR-TS (68a)

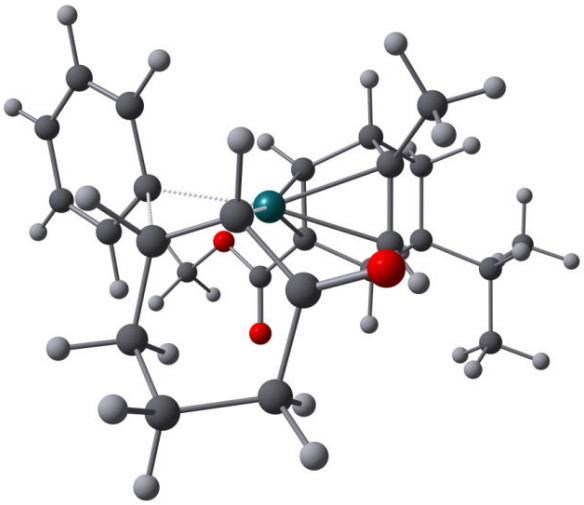


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	45	0	-0.441849	0.582493	-0.412314
2	6	0	1.511843	0.921525	-1.398318
3	6	0	1.965917	-0.412534	0.588249
4	6	0	1.696273	0.948682	-0.021052
5	6	0	1.597820	-0.493057	-1.957205
6	6	0	3.222499	-1.050189	-0.075046
7	6	0	0.537131	-1.249276	-1.188149
8	6	0	0.751626	-1.226738	0.182049
9	6	0	2.991607	-1.071823	-1.606325
10	1	0	2.045526	-0.377308	1.674049
11	1	0	1.416342	-0.513636	-3.034317
12	1	0	3.281493	-2.082695	0.297241
13	1	0	3.074714	-2.086601	-2.008560
14	1	0	3.745709	-0.463923	-2.119384
15	1	0	-0.143036	-1.949497	-1.663910
16	1	0	1.907111	1.872788	0.512563
17	6	0	-2.448469	-0.179828	-0.443641
18	6	0	-2.968107	-1.013927	0.556047
19	6	0	-2.871996	-0.404076	-1.767829
20	6	0	-3.862646	-2.038703	0.245726
21	1	0	-2.666887	-0.876432	1.592632
22	6	0	-3.740129	-1.445196	-2.084378
23	1	0	-2.525952	0.257649	-2.561137
24	6	0	-4.248172	-2.265329	-1.074163
25	1	0	-4.256755	-2.666660	1.041925
26	1	0	-4.040364	-1.602915	-3.117876
27	1	0	-4.947158	-3.062487	-1.313649
28	6	0	-2.462648	1.809286	-0.016514
29	6	0	-1.274558	2.534718	-0.390031
30	1	0	-3.273989	1.874543	-0.735810
31	1	0	-1.198594	2.917739	-1.408517
32	6	0	-0.483895	3.275819	0.597271
33	8	0	0.390727	4.077015	0.257155
34	6	0	-0.797875	3.084221	2.069995
35	6	0	-2.913857	1.925063	1.421541
36	6	0	-1.733368	1.921368	2.380787
37	1	0	0.150047	3.008623	2.611243
38	1	0	-1.256362	4.028585	2.393685
39	1	0	-1.190642	0.970721	2.287405
40	1	0	-2.081215	1.987112	3.417374
41	1	0	-3.444888	2.885308	1.501172
42	1	0	-3.642075	1.149027	1.667179
43	6	0	0.139381	-2.152313	1.157224
44	8	0	0.283489	-2.066486	2.365122
45	8	0	-0.569657	-3.130270	0.571070
46	6	0	1.625048	2.106499	-2.306616
47	1	0	1.463280	3.039501	-1.761278
48	1	0	2.627925	2.135586	-2.754771
49	1	0	0.905747	2.045333	-3.130137
50	6	0	-1.185796	-4.058598	1.466620
51	1	0	-1.838544	-3.541633	2.172390
52	1	0	-1.764935	-4.732890	0.837554
53	1	0	-0.425391	-4.612499	2.022362
54	6	0	4.541552	-0.353066	0.305336
55	1	0	4.540133	0.641535	-0.164261
56	6	0	5.736361	-1.135934	-0.243382
57	1	0	6.675361	-0.613628	-0.032113
58	1	0	5.794950	-2.125845	0.225259
59	1	0	5.677749	-1.285202	-1.325920
60	6	0	4.703096	-0.163981	1.813304
61	1	0	4.603909	-1.119095	2.343116
62	1	0	5.694791	0.239531	2.043485

```
     63          1           0        3.966897    0.529446    2.229368
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5922.22627907     A.U. after    1 cycles
             Convg  =    0.3689D-08             -V/T =  2.0045
Zero-point correction=                           0.538551 (Hartree/Particle)
 Thermal correction to Energy=                    0.568760
 Thermal correction to Enthalpy=                  0.569720
 Thermal correction to Gibbs Free Energy=         0.477600
 Sum of electronic and zero-point Energies=          -5921.687728
 Sum of electronic and thermal Energies=             -5921.657519
 Sum of electronic and thermal Enthalpies=           -5921.656559
 Sum of electronic and thermal Free Energies=        -5921.748679
                     1                    2                    3
Frequencies --  -293.2688               22.9077              33.9885
```

(*S*)-DA-prox-Rh(I)-Ph-CH-si-confD-CR-TS (68b)



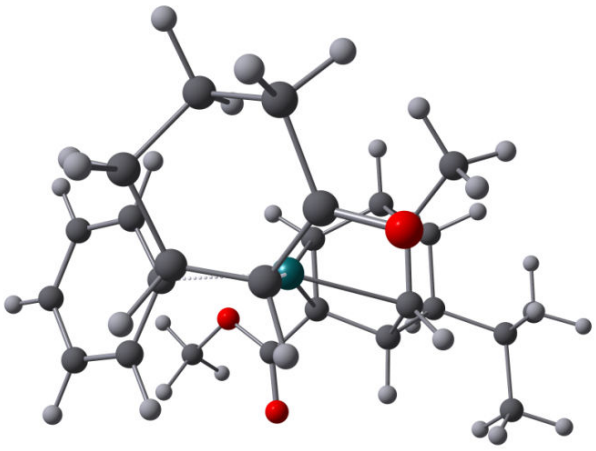
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.457243	0.505543	-0.435457
2	6	0	1.479685	0.829570	-1.465704
3	6	0	1.975287	-0.374899	0.593376
4	6	0	1.677644	0.942201	-0.095216
5	6	0	1.593648	-0.614123	-1.940117
6	6	0	3.238429	-1.030556	-0.038375
7	6	0	0.551239	-1.342037	-1.120696
8	6	0	0.773026	-1.233427	0.245419
9	6	0	3.001573	-1.140501	-1.565148
10	1	0	2.060462	-0.272638	1.674699
11	1	0	1.406451	-0.701743	-3.012786
12	1	0	3.312676	-2.039843	0.390521
13	1	0	3.107613	-2.173424	-1.911968
14	1	0	3.739089	-0.543667	-2.114234
15	1	0	-0.120456	-2.079753	-1.549110
16	1	0	1.877659	1.899727	0.380791
17	6	0	-2.443980	-0.297750	-0.419426
18	6	0	-2.984495	-1.167612	0.535938
19	6	0	-2.881822	-0.429298	-1.752114
20	6	0	-3.901149	-2.154619	0.171143
21	1	0	-2.692696	-1.082805	1.580173
22	6	0	-3.770529	-1.434942	-2.122415

23	1	0	-2.526516	0.268273	-2.509448
24	6	0	-4.291227	-2.301835	-1.158536
25	1	0	-4.310543	-2.814617	0.933067
26	1	0	-4.075141	-1.529421	-3.162382
27	1	0	-5.004743	-3.071700	-1.440476
28	6	0	-2.393014	1.642318	0.207427
29	6	0	-1.355417	2.440453	-0.397735
30	1	0	-3.346404	1.687045	-0.309785
31	1	0	-1.500272	2.764167	-1.429978
32	6	0	-0.505769	3.339939	0.391694
33	8	0	0.273977	4.132581	-0.139387
34	6	0	-0.661094	3.302590	1.900387
35	6	0	-2.514285	1.631152	1.725285
36	1	0	-0.327124	4.268295	2.289508
37	1	0	-3.541565	1.381277	2.007541
38	6	0	0.181322	-2.113727	1.273677
39	8	0	0.324885	-1.958409	2.474764
40	8	0	-0.513315	-3.132959	0.743066
41	6	0	1.545629	1.958403	-2.446615
42	1	0	1.344409	2.917405	-1.963368
43	1	0	2.546414	1.998511	-2.898819
44	1	0	0.829235	1.813815	-3.261953
45	6	0	-1.119962	-4.018696	1.686920
46	1	0	-1.785351	-3.473336	2.358974
47	1	0	-1.684723	-4.736670	1.094170
48	1	0	-0.354639	-4.528253	2.277145
49	6	0	4.549145	-0.296332	0.298540
50	1	0	4.533041	0.672007	-0.222666
51	6	0	5.752565	-1.091193	-0.212601
52	1	0	6.684988	-0.545386	-0.034155
53	1	0	5.826701	-2.053378	0.308569
54	1	0	5.691435	-1.299302	-1.285208
55	6	0	4.712638	-0.026353	1.794166
56	1	0	4.622785	-0.953080	2.373735
57	1	0	5.701132	0.397431	2.000434
58	1	0	3.971241	0.681545	2.175294
59	6	0	-2.092522	2.975117	2.311999
60	1	0	0.022120	2.539439	2.297310
61	1	0	-2.176381	2.942942	3.403575
62	1	0	-2.767127	3.766950	1.963045
63	1	0	-1.871594	0.857979	2.158177

SCF Done: E(RPBE1PBE) = -5922.22230298 A.U. after 1 cycles
Convg = 0.2385D-08 -V/T = 2.0045
Zero-point correction= 0.538589 (Hartree/Particle)
Thermal correction to Energy= 0.568932
Thermal correction to Enthalpy= 0.569892
Thermal correction to Gibbs Free Energy= 0.477366
Sum of electronic and zero-point Energies= -5921.683714
Sum of electronic and thermal Energies= -5921.653371
Sum of electronic and thermal Enthalpies= -5921.652411
Sum of electronic and thermal Free Energies= -5921.744937

	1	2	3
Frequencies --	-298.8898	24.4421	33.5618

(*S*)-DA-prox-Rh(I)-Ph-CH-re-confU-CR-TS (75a)



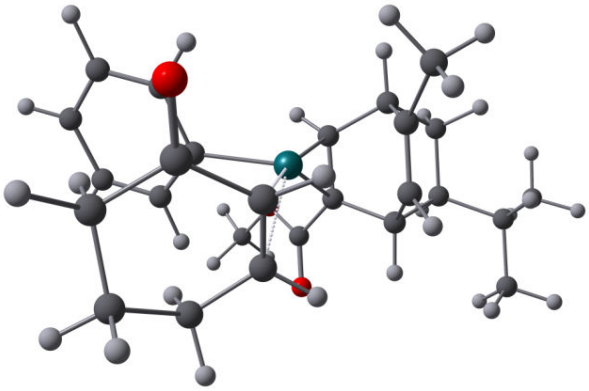
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.476866	-0.465170	-0.206525
2	6	0	1.290957	-1.594705	0.646537
3	6	0	2.143233	0.329313	-0.573751
4	6	0	1.595947	-1.084449	-0.607476
5	6	0	1.533019	-0.579776	1.752894
6	6	0	3.413754	0.381455	0.325849
7	6	0	0.689129	0.606775	1.353694
8	6	0	1.046287	1.120667	0.113743
9	6	0	3.031152	-0.180639	1.717073
10	6	0	0.769385	2.501105	-0.342810
11	1	0	2.328075	0.733676	-1.568063
12	1	0	1.251130	-0.976600	2.731229
13	1	0	3.680027	1.443268	0.424054
14	1	0	3.230654	0.546183	2.511099
15	1	0	3.622170	-1.074317	1.949529
16	1	0	0.099905	1.170935	2.070270
17	1	0	1.713016	-1.726414	-1.477921
18	6	0	-2.220474	0.795601	-0.168327
19	6	0	-2.348827	1.746310	-1.197916
20	6	0	-2.740931	1.132813	1.092380
21	6	0	-2.958783	2.977803	-0.977322
22	1	0	-1.986953	1.508862	-2.197386
23	6	0	-3.346096	2.368360	1.318836
24	1	0	-2.674755	0.424264	1.915328
25	6	0	-3.464872	3.295690	0.284432
26	1	0	-3.050784	3.686417	-1.797466
27	1	0	-3.734454	2.602454	2.307705
28	1	0	-3.954362	4.251060	0.455634
29	6	0	-2.713487	-1.020836	-0.881710
30	1	0	-3.191770	-0.497109	-1.703689
31	6	0	-1.631896	-1.887472	-1.287570
32	1	0	-1.236033	-1.763081	-2.298463
33	6	0	-1.522086	-3.261310	-0.793913
34	8	0	-0.822426	-4.098267	-1.367241
35	6	0	-3.694836	-1.586065	0.122580
36	6	0	-2.346854	-3.660276	0.414180
37	6	0	-3.004869	-2.490081	1.133272
38	1	0	-4.265141	-0.790013	0.606144
39	1	0	-4.417872	-2.180807	-0.455274

40	1	0	-2.244601	-1.914329	1.679515
41	1	0	-3.723262	-2.856715	1.874296
42	1	0	-3.117249	-4.344320	0.033314
43	1	0	-1.714898	-4.259917	1.076266
44	6	0	1.204257	-3.045169	0.999255
45	1	0	1.012641	-3.673041	0.128269
46	1	0	2.158799	-3.359306	1.444233
47	1	0	0.429124	-3.230549	1.750093
48	6	0	-0.100017	4.600209	0.217568
49	1	0	0.853684	5.122064	0.105098
50	1	0	-0.661808	4.667106	-0.714992
51	1	0	-0.674807	5.028834	1.037212
52	6	0	4.630136	-0.339095	-0.283297
53	1	0	4.418238	-1.418375	-0.273616
54	6	0	5.878682	-0.092585	0.566113
55	1	0	6.733425	-0.655011	0.175845
56	1	0	6.147929	0.970532	0.553190
57	1	0	5.738854	-0.386328	1.611034
58	6	0	4.904583	0.075552	-1.728703
59	1	0	4.110003	-0.237806	-2.411767
60	1	0	5.010467	1.163748	-1.813186
61	1	0	5.836165	-0.375903	-2.086008
62	8	0	0.123914	3.234515	0.576994
63	8	0	1.137818	2.948505	-1.414951

SCF Done: E(RPBE1PBE) = -5922.22211064 A.U. after 1 cycles
Convg = 0.3516D-08 -V/T = 2.0045
Zero-point correction= 0.538591 (Hartree/Particle)
Thermal correction to Energy= 0.568717
Thermal correction to Enthalpy= 0.569677
Thermal correction to Gibbs Free Energy= 0.477917
Sum of electronic and zero-point Energies= -5921.683520
Sum of electronic and thermal Energies= -5921.653393
Sum of electronic and thermal Enthalpies= -5921.652433
Sum of electronic and thermal Free Energies= -5921.744194

	1	2	3
Frequencies --	-298.1182	20.6875	39.7046

(*S*)-DA-prox-Rh(I)-Ph-CH-re-confD-close (72b)



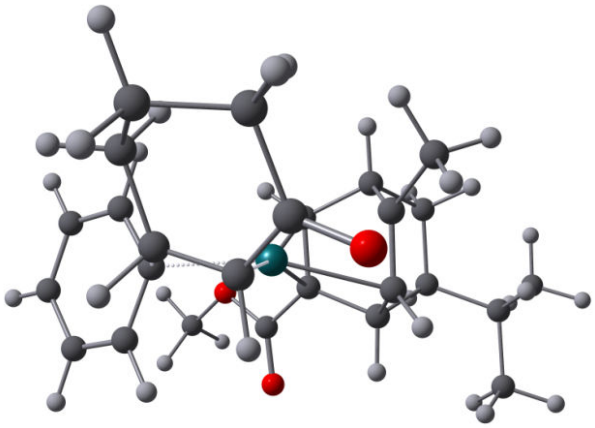
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.398811	-0.513788	-0.260781
2	6	0	-1.576935	-1.616728	-1.069263
3	6	0	-2.256923	-0.003257	0.605948

4	6	0	-1.769343	-1.395254	0.263006
5	6	0	-1.891929	-0.383988	-1.907445
6	6	0	-3.603701	0.261518	-0.135333
7	6	0	-1.002463	0.713536	-1.352429
8	6	0	-1.222320	0.934863	0.012134
9	6	0	-3.373300	-0.010435	-1.641911
10	6	0	-0.921293	2.197461	0.725490
11	1	0	-2.339626	0.162118	1.679527
12	1	0	-1.710771	-0.559734	-2.970372
13	1	0	-3.832645	1.326447	0.009820
14	1	0	-3.640123	0.859462	-2.250270
15	1	0	-3.998829	-0.843498	-1.983329
16	1	0	-0.544829	1.459892	-1.994972
17	1	0	-1.738062	-2.193334	1.001599
18	6	0	1.963321	0.699276	-0.599293
19	6	0	2.375206	1.833478	0.110426
20	6	0	2.687030	0.360657	-1.755491
21	6	0	3.476228	2.589021	-0.301522
22	1	0	1.843324	2.144449	1.007975
23	6	0	3.785400	1.113962	-2.174762
24	1	0	2.410444	-0.518839	-2.339546
25	6	0	4.188472	2.233590	-1.445611
26	1	0	3.776916	3.460683	0.276973
27	1	0	4.331217	0.818714	-3.068500
28	1	0	5.046700	2.819146	-1.765511
29	6	0	1.118989	-1.283178	1.780479
30	1	0	0.145745	-1.366072	2.260093
31	6	0	1.442898	-2.197209	0.777746
32	1	0	0.762779	-3.002653	0.504602
33	6	0	2.839554	-2.397727	0.335209
34	8	0	3.113035	-3.210087	-0.543388
35	6	0	2.180115	-0.554868	2.565941
36	6	0	3.906065	-1.584635	1.033775
37	1	0	2.280790	0.476487	2.218343
38	1	0	4.040113	-0.658375	0.461180
39	6	0	-1.323775	-2.939633	-1.718832
40	1	0	-1.126258	-3.723134	-0.983055
41	1	0	-2.201411	-3.238836	-2.306132
42	1	0	-0.477403	-2.893146	-2.412134
43	6	0	-4.791293	-0.538096	0.430416
44	1	0	-4.624797	-1.598198	0.189216
45	6	0	-6.095632	-0.098795	-0.238260
46	1	0	-6.936381	-0.708288	0.109084
47	1	0	-6.320450	0.946242	0.006823
48	1	0	-6.054996	-0.182083	-1.328571
49	6	0	-4.925948	-0.412000	1.947763
50	1	0	-4.978780	0.639911	2.252754
51	1	0	-5.842560	-0.902354	2.291950
52	1	0	-4.091281	-0.874061	2.482667
53	8	0	-1.066027	2.355843	1.925683
54	8	0	-0.503196	3.169856	-0.098916
55	6	0	-0.183654	4.414552	0.529655
56	1	0	0.592958	4.279431	1.285055
57	1	0	0.174531	5.061753	-0.269244
58	1	0	-1.071595	4.842028	1.000828
59	6	0	3.531254	-1.263503	2.477579
60	1	0	1.853311	-0.490629	3.609682
61	1	0	4.308604	-0.644767	2.937882
62	1	0	3.486101	-2.195764	3.054781
63	1	0	4.844143	-2.143088	0.966440

SCF Done: E(RPBE1PBE) = -5922.23580478 A.U. after 1 cycles
Convg = 0.2275D-08 -V/T = 2.0045

```
Zero-point correction=                           0.537968 (Hartree/Particle)
 Thermal correction to Energy=                    0.569518
 Thermal correction to Enthalpy=                  0.570478
 Thermal correction to Gibbs Free Energy=         0.474099
 Sum of electronic and zero-point Energies=          -5921.697837
 Sum of electronic and thermal Energies=             -5921.666287
 Sum of electronic and thermal Enthalpies=           -5921.665327
 Sum of electronic and thermal Free Energies=        -5921.761706
                     1                      2                      3
Frequencies --    19.4545                31.6798                36.7056
```

(*S*)-DA-prox-Rh(I)-Ph-CH-re-confD-CR-TS (75b)

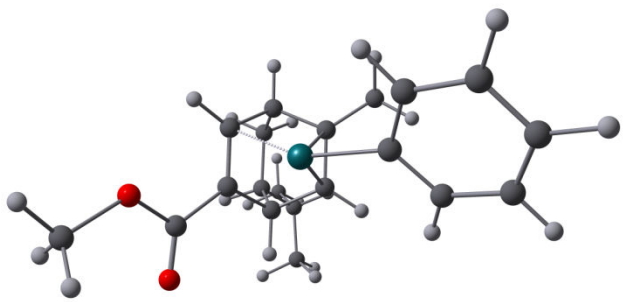


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.485865	-0.408123	-0.162037
2	6	0	1.229658	-1.638803	0.663152
3	6	0	2.171869	0.234793	-0.568366
4	6	0	1.542755	-1.145145	-0.595305
5	6	0	1.542320	-0.639397	1.766142
6	6	0	3.454954	0.213205	0.313712
7	6	0	0.758910	0.591451	1.376695
8	6	0	1.130181	1.086639	0.132237
9	6	0	3.059522	-0.324241	1.710924
10	6	0	0.917225	2.477045	-0.327285
11	1	0	2.366542	0.628710	-1.564951
12	1	0	1.251556	-1.020136	2.748223
13	1	0	3.783456	1.257879	0.406758
14	1	0	3.308481	0.392227	2.500428
15	1	0	3.603203	-1.248533	1.939480
16	1	0	0.211240	1.186712	2.101135
17	1	0	1.606597	-1.791726	-1.467712
18	6	0	-2.141218	0.965360	-0.107555
19	6	0	-2.242520	1.817269	-1.224894
20	6	0	-2.639374	1.437140	1.115731
21	6	0	-2.798704	3.087809	-1.117624
22	1	0	-1.899205	1.471262	-2.198783
23	6	0	-3.201363	2.709755	1.225245
24	1	0	-2.592100	0.809438	2.002429
25	6	0	-3.289472	3.540277	0.110038
26	1	0	-2.862793	3.722601	-1.998663
27	1	0	-3.578274	3.048533	2.187903
28	1	0	-3.741462	4.525520	0.191630

29	6	0	-2.751589	-0.906066	-0.585885
30	1	0	-3.367915	-0.391918	-1.316510
31	6	0	-1.762759	-1.784177	-1.161878
32	1	0	-1.487068	-1.605681	-2.205053
33	6	0	-1.680169	-3.203805	-0.801670
34	8	0	-0.977109	-3.990291	-1.435924
35	6	0	-3.529784	-1.411360	0.617416
36	6	0	-2.556629	-3.694877	0.334903
37	1	0	-4.438393	-0.816210	0.745961
38	1	0	-2.738348	-4.760965	0.174060
39	6	0	1.071951	-3.083607	1.015233
40	1	0	0.819130	-3.695546	0.148356
41	1	0	2.021655	-3.453013	1.426894
42	1	0	0.314447	-3.229358	1.792031
43	6	0	0.130289	4.611812	0.221216
44	1	0	1.101969	5.098001	0.102574
45	1	0	-0.432202	4.691544	-0.709790
46	1	0	-0.426688	5.066328	1.039219
47	6	0	4.619730	-0.575763	-0.311327
48	1	0	4.347611	-1.641438	-0.297829
49	6	0	5.891739	-0.400772	0.520822
50	1	0	6.707397	-1.011631	0.119864
51	1	0	6.221514	0.645067	0.502907
52	1	0	5.749571	-0.685504	1.567953
53	6	0	4.897513	-0.177405	-1.760673
54	1	0	4.078319	-0.447136	-2.433158
55	1	0	5.061633	0.903306	-1.847813
56	1	0	5.798205	-0.679502	-2.129347
57	8	0	0.304848	3.241248	0.589828
58	8	0	1.304149	2.903593	-1.401506
59	6	0	-3.849929	-2.894705	0.452021
60	1	0	-2.941928	-1.293797	1.533157
61	1	0	-4.437890	-3.244925	1.307449
62	1	0	-4.465572	-3.050392	-0.442612
63	1	0	-1.984494	-3.605199	1.268158

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5922.21802016     A.U. after    1 cycles
             Convg  =    0.2219D-08             -V/T =  2.0045
Zero-point correction=                           0.538639 (Hartree/Particle)
 Thermal correction to Energy=                    0.568858
 Thermal correction to Enthalpy=                  0.569818
 Thermal correction to Gibbs Free Energy=         0.477874
 Sum of electronic and zero-point Energies=          -5921.679381
 Sum of electronic and thermal Energies=             -5921.649162
 Sum of electronic and thermal Enthalpies=           -5921.648202
 Sum of electronic and thermal Free Energies=        -5921.740146
                    1                      2                      3
Frequencies --  -297.4695               25.4579                36.3675
```

(*S*)-DA-dist-Rh(I)-Ph (64)

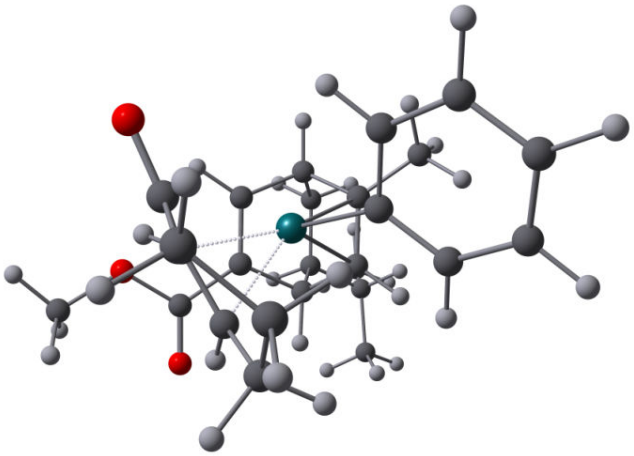


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.917529	0.526010	-0.217097
2	6	0	-0.000985	-1.252410	-0.919492
3	6	0	-1.613583	-0.207405	0.612059
4	6	0	-0.341409	-1.020504	0.437980
5	6	0	-1.002013	-0.591466	-1.862666
6	6	0	-2.809776	-0.904122	-0.094286
7	6	0	-0.930738	0.862943	-1.454547
8	6	0	-1.283641	1.072774	-0.134297
9	6	0	-2.413107	-1.155833	-1.569868
10	6	0	-1.559074	2.387902	0.468098
11	1	0	-1.830509	0.015320	1.656231
12	1	0	-0.724055	-0.736100	-2.909509
13	1	0	-3.644098	-0.189741	-0.061145
14	1	0	-3.135857	-0.706921	-2.258779
15	1	0	-2.394795	-2.230177	-1.787205
16	1	0	-0.834794	1.669308	-2.176852
17	1	0	0.019437	-1.673039	1.231683
18	8	0	-2.081163	2.550046	1.556931
19	8	0	-1.170196	3.412743	-0.319156
20	6	0	-1.421784	4.717345	0.212602
21	1	0	-1.056977	5.415616	-0.539367
22	1	0	-2.490632	4.864027	0.381324
23	1	0	-0.886980	4.858515	1.154146
24	6	0	0.812989	-2.414924	-1.402041
25	1	0	0.147776	-3.237695	-1.700063
26	1	0	1.414428	-2.146007	-2.275367
27	1	0	1.487141	-2.781068	-0.624699
28	6	0	-3.281404	-2.189186	0.610708
29	1	0	-2.494609	-2.947706	0.483632
30	6	0	-4.560480	-2.717932	-0.041232
31	1	0	-4.868834	-3.664248	0.415420
32	1	0	-5.381666	-2.003023	0.090657
33	1	0	-4.442080	-2.892563	-1.115040
34	6	0	-3.513482	-1.995298	2.109153
35	1	0	-2.588079	-1.786262	2.653273
36	1	0	-4.207213	-1.167097	2.296709
37	1	0	-3.950679	-2.898266	2.548254
38	6	0	2.737227	-0.228271	0.215583
39	6	0	3.785118	0.148057	-0.643767
40	6	0	3.076536	-0.980103	1.352462
41	6	0	5.111945	-0.198325	-0.377911
42	1	0	3.572545	0.722385	-1.547762
43	6	0	4.401995	-1.323038	1.629562
44	1	0	2.299881	-1.299441	2.045641
45	6	0	5.425436	-0.936621	0.763575
46	1	0	5.900646	0.105316	-1.063563
47	1	0	4.637022	-1.895666	2.524738
48	1	0	6.456434	-1.209722	0.974758

SCF Done: E(RPBE1PBE) = -5613.87935719 A.U. after 1 cycles
Convg = 0.2224D-08 -V/T = 2.0039
Zero-point correction= 0.407912 (Hartree/Particle)
Thermal correction to Energy= 0.431808
Thermal correction to Enthalpy= 0.432768
Thermal correction to Gibbs Free Energy= 0.352710
Sum of electronic and zero-point Energies= -5613.471445
Sum of electronic and thermal Energies= -5613.447549
Sum of electronic and thermal Enthalpies= -5613.446589
Sum of electronic and thermal Free Energies= -5613.526647

	1	2	3
Frequencies --	17.9709	33.9786	39.8232

(*S*)-DA-dist-Rh(I)-Ph-CH-si-confU-close (78a)

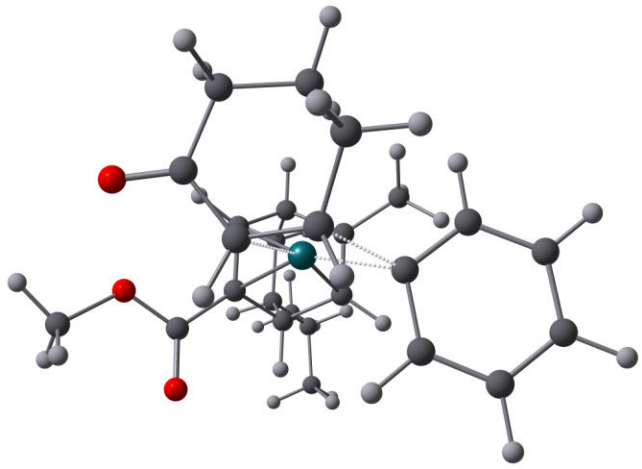


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.457347	-0.010158	-0.267820
2	6	0	-1.637395	1.085559	-0.224602
3	6	0	-1.760060	-0.702776	-1.829544
4	6	0	-1.338754	0.714201	-1.514446
5	6	0	-2.248130	-0.027298	0.599814
6	6	0	-3.278491	-0.844281	-1.539704
7	6	0	-1.267003	-1.176209	0.486157
8	6	0	-1.015715	-1.576737	-0.822155
9	6	0	-3.593293	-0.431182	-0.081241
10	1	0	-1.522249	-0.981793	-2.858337
11	1	0	-2.395795	0.303605	1.627073
12	1	0	-3.553460	-1.890658	-1.714009
13	1	0	-4.216799	0.473532	-0.087118
14	1	0	-1.053426	-1.819549	1.336322
15	1	0	-1.049936	1.423423	-2.284850
16	6	0	1.885217	-1.386507	0.071408
17	6	0	2.799299	-1.627517	-0.967137
18	6	0	1.963698	-2.203588	1.209610
19	6	0	3.754153	-2.642958	-0.872382
20	1	0	2.785647	-1.007403	-1.863449
21	6	0	2.922950	-3.213592	1.312265
22	1	0	1.276953	-2.050718	2.040593
23	6	0	3.822844	-3.440419	0.270206
24	1	0	4.452541	-2.803420	-1.691394
25	1	0	2.966894	-3.826416	2.210723
26	1	0	4.569650	-4.226568	0.348783
27	6	0	1.416949	1.505688	1.168855
28	6	0	1.682434	1.857062	-0.152683
29	1	0	0.500220	1.861660	1.637656
30	1	0	1.000172	2.488515	-0.719017
31	6	0	3.056751	1.810633	-0.699495
32	8	0	3.273823	2.008722	-1.890507
33	6	0	4.180141	1.652644	0.298704
34	1	0	5.070454	1.300018	-0.228396
35	6	0	2.502049	1.121319	2.134461

36	6	0	3.841023	0.766578	1.493370
37	1	0	4.398439	2.676178	0.638977
38	1	0	3.825301	-0.275271	1.170066
39	1	0	2.623683	1.993468	2.796797
40	1	0	2.163481	0.307510	2.784579
41	1	0	4.634470	0.849705	2.244163
42	6	0	-1.669282	2.472700	0.272296
43	8	0	-2.065233	2.792610	1.379855
44	8	0	-1.220417	3.363032	-0.632032
45	6	0	-1.224012	4.729682	-0.201150
46	1	0	-0.827212	5.300512	-1.039065
47	1	0	-2.240199	5.052196	0.034185
48	1	0	-0.591997	4.856161	0.680108
49	6	0	-0.534816	-2.932037	-1.244196
50	1	0	0.159006	-2.870421	-2.087926
51	1	0	-0.030243	-3.454100	-0.429052
52	1	0	-1.392218	-3.539141	-1.566145
53	6	0	-4.371748	-1.517771	0.682147
54	1	0	-3.814659	-2.460875	0.582920
55	6	0	-5.755336	-1.716511	0.059382
56	1	0	-5.703516	-1.949670	-1.008551
57	1	0	-6.290764	-2.535231	0.551281
58	1	0	-6.360481	-0.809050	0.172441
59	6	0	-4.520317	-1.210064	2.171913
60	1	0	-4.971506	-0.223004	2.328162
61	1	0	-5.169798	-1.949876	2.651549
62	1	0	-3.563016	-1.228574	2.700727
63	1	0	-3.844571	-0.242247	-2.257521

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5922.23601619     A.U. after    1 cycles
             Convg  =    0.5206D-08             -V/T =  2.0045
Zero-point correction=                           0.538131 (Hartree/Particle)
 Thermal correction to Energy=                    0.569586
 Thermal correction to Enthalpy=                  0.570546
 Thermal correction to Gibbs Free Energy=         0.474896
 Sum of electronic and zero-point Energies=          -5921.697885
 Sum of electronic and thermal Energies=             -5921.666430
 Sum of electronic and thermal Enthalpies=           -5921.665470
 Sum of electronic and thermal Free Energies=        -5921.761120
                     1                      2                      3
Frequencies --    21.7406                36.2432                41.9014
```

(*S*)-DA-dist-Rh(I)-Ph-CH-si-confU-CR-TS (81a)

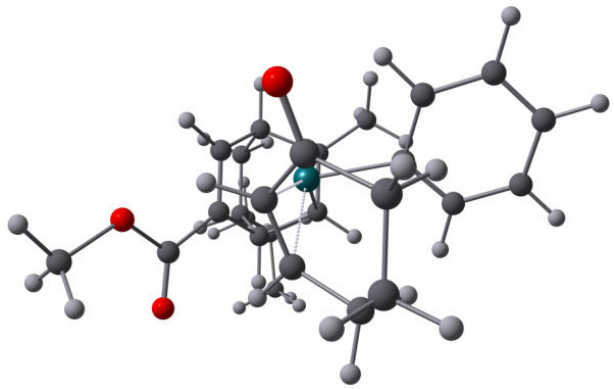


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.607079	0.036913	0.022625
2	6	0	-1.309783	1.042559	0.243861
3	6	0	-1.397413	0.047501	-1.955338
4	6	0	-0.902196	1.178609	-1.082844
5	6	0	-2.103684	-0.223305	0.503069
6	6	0	-2.941529	-0.043010	-1.855653
7	6	0	-1.180210	-1.322993	0.015446
8	6	0	-0.810224	-1.199576	-1.308727
9	6	0	-3.385911	-0.178540	-0.378302
10	1	0	-1.071315	0.156300	-2.992582
11	1	0	-2.334652	-0.309001	1.564178
12	1	0	-3.266812	-0.913076	-2.438065
13	1	0	-3.934155	0.726417	-0.081018
14	1	0	-1.028071	-2.239913	0.580174
15	1	0	-0.556428	2.123452	-1.492011
16	6	0	1.988560	-1.489477	0.597299
17	6	0	2.470108	-2.466667	-0.284409
18	6	0	1.751899	-1.870361	1.932567
19	6	0	2.676671	-3.780534	0.138820
20	1	0	2.676217	-2.213933	-1.322020
21	6	0	1.936411	-3.185310	2.351130
22	1	0	1.423956	-1.125313	2.656162
23	6	0	2.403955	-4.149531	1.455103
24	1	0	3.047719	-4.519409	-0.568203
25	1	0	1.732022	-3.454595	3.384925
26	1	0	2.566983	-5.172326	1.784543
27	6	0	2.917141	0.326278	0.517675
28	6	0	2.066368	1.491784	0.567413
29	1	0	3.349015	0.045405	1.474054
30	1	0	1.788014	1.878458	1.548999
31	6	0	2.156148	2.523535	-0.473524
32	8	0	1.759345	3.673042	-0.285004
33	6	0	2.820238	2.170476	-1.794312
34	6	0	3.884076	0.231587	-0.640951
35	6	0	3.240197	0.711831	-1.932322
36	1	0	2.151439	2.484761	-2.602046
37	1	0	3.700138	2.822823	-1.862320
38	1	0	2.359012	0.088987	-2.144092
39	1	0	3.927693	0.594518	-2.777115
40	1	0	4.734782	0.883387	-0.392698
41	1	0	4.287142	-0.779241	-0.733952
42	6	0	-1.307623	2.130797	1.249386
43	8	0	-1.562084	1.969541	2.431437
44	8	0	-1.004219	3.314270	0.708249
45	6	0	-0.832704	4.396778	1.625983
46	1	0	-0.496321	5.237636	1.023051
47	1	0	-1.777349	4.626791	2.124613
48	1	0	-0.077312	4.147313	2.373078
49	6	0	-0.261186	-2.295387	-2.164706
50	1	0	0.119719	-3.125004	-1.565620
51	1	0	-1.056565	-2.680767	-2.817458
52	1	0	0.541371	-1.936570	-2.817847
53	6	0	-4.329594	-1.375143	-0.159656
54	1	0	-3.835105	-2.268589	-0.568579
55	6	0	-5.640329	-1.166686	-0.921242
56	1	0	-5.479519	-0.986093	-1.988570
57	1	0	-6.290211	-2.043106	-0.827588
58	1	0	-6.185434	-0.305225	-0.517098
59	6	0	-4.631468	-1.635506	1.316049

60	1	0	-5.017313	-0.733015	1.805042
61	1	0	-5.391988	-2.416859	1.418510
62	1	0	-3.750039	-1.967269	1.872101
63	1	0	-3.387040	0.838878	-2.327004

```
SCF Done:  E(RPBE1PBE) =  -5922.22387896     A.U. after    1 cycles
            Convg  =    0.3557D-08             -V/T =  2.0045
Zero-point correction=                           0.538219 (Hartree/Particle)
 Thermal correction to Energy=                    0.568602
 Thermal correction to Enthalpy=                  0.569562
 Thermal correction to Gibbs Free Energy=         0.476627
 Sum of electronic and zero-point Energies=          -5921.685660
 Sum of electronic and thermal Energies=             -5921.655277
 Sum of electronic and thermal Enthalpies=           -5921.654317
 Sum of electronic and thermal Free Energies=        -5921.747252
                     1                      2                      3
Frequencies --  -283.4193               27.5671                32.7396
```

(*S*)-DA-dist-Rh(I)-Ph-CH-si-confD-close (78b)



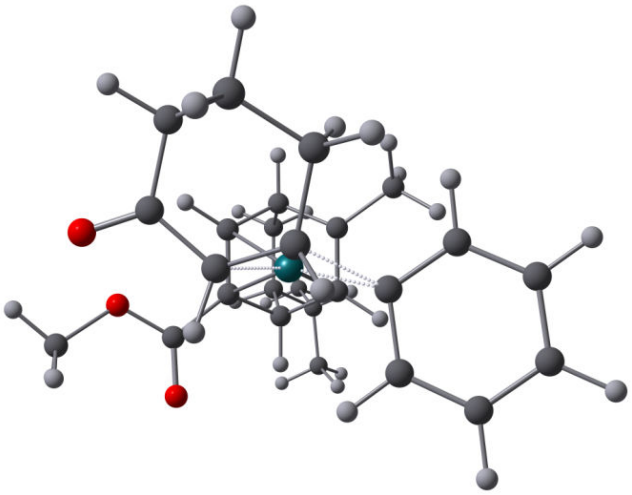
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.458406	-0.027174	-0.289562
2	6	0	-1.639105	1.081394	-0.284689
3	6	0	-1.780908	-0.779183	-1.803113
4	6	0	-1.354303	0.649609	-1.557297
5	6	0	-2.238871	0.008351	0.598907
6	6	0	-3.295528	-0.904910	-1.487689
7	6	0	-1.257647	-1.144754	0.526750
8	6	0	-1.021684	-1.604915	-0.766803
9	6	0	-3.591709	-0.429130	-0.044551
10	1	0	-1.556664	-1.104943	-2.821187
11	1	0	-2.374110	0.386912	1.611354
12	1	0	-3.573546	-1.957302	-1.614567
13	1	0	-4.219480	0.471820	-0.081474
14	1	0	-1.040275	-1.752591	1.401893
15	1	0	-1.068636	1.321927	-2.361315
16	6	0	1.888544	-1.399357	0.062884
17	6	0	2.725703	-1.714806	-1.020104
18	6	0	2.041872	-2.147708	1.238938
19	6	0	3.682152	-2.728404	-0.929250
20	1	0	2.650187	-1.153949	-1.952039
21	6	0	3.001398	-3.159157	1.337006
22	1	0	1.402718	-1.951863	2.098986
23	6	0	3.826825	-3.455692	0.252752

24	1	0	4.321245	-2.943257	-1.783351
25	1	0	3.099525	-3.720206	2.264467
26	1	0	4.573273	-4.242507	0.327390
27	6	0	1.357246	1.557918	1.122062
28	6	0	1.717194	1.826249	-0.198097
29	1	0	0.420850	1.960436	1.502379
30	1	0	1.098524	2.453990	-0.837503
31	6	0	3.107198	1.639146	-0.666986
32	8	0	3.416137	1.862793	-1.833726
33	6	0	4.131541	1.198642	0.355712
34	1	0	5.104580	1.579636	0.032183
35	6	0	2.378092	1.183989	2.168137
36	1	0	2.386993	0.102925	2.336235
37	6	0	-1.663876	2.492629	0.139524
38	8	0	-2.073638	2.872579	1.222930
39	8	0	-1.188677	3.329349	-0.800989
40	6	0	-1.185373	4.717076	-0.443640
41	1	0	-0.768495	5.238391	-1.303763
42	1	0	-2.201772	5.061858	-0.243429
43	1	0	-0.566316	4.884053	0.440018
44	6	0	-0.557378	-2.983662	-1.128182
45	1	0	0.116054	-2.971376	-1.990240
46	1	0	-0.034704	-3.464073	-0.298783
47	1	0	-1.424792	-3.602758	-1.395608
48	6	0	-4.353497	-1.482949	0.779432
49	1	0	-3.788564	-2.424904	0.722392
50	6	0	-5.741780	-1.725238	0.183235
51	1	0	-5.699828	-2.016923	-0.870626
52	1	0	-6.265614	-2.519412	0.725361
53	1	0	-6.353135	-0.817511	0.252657
54	6	0	-4.490309	-1.100791	2.253118
55	1	0	-4.948332	-0.110596	2.362494
56	1	0	-5.129439	-1.819894	2.776141
57	1	0	-3.528549	-1.084682	2.773677
58	1	0	-3.870385	-0.333347	-2.223241
59	6	0	3.777067	1.651209	1.768719
60	1	0	4.183813	0.103783	0.311863
61	1	0	2.082581	1.640576	3.119234
62	1	0	4.516870	1.271070	2.480929
63	1	0	3.819376	2.746444	1.821383

SCF Done: E(RPBE1PBE) = -5922.23629364 A.U. after 1 cycles
Convg = 0.4899D-08 -V/T = 2.0045
Zero-point correction= 0.538252 (Hartree/Particle)
Thermal correction to Energy= 0.569675
Thermal correction to Enthalpy= 0.570635
Thermal correction to Gibbs Free Energy= 0.475217
Sum of electronic and zero-point Energies= -5921.698041
Sum of electronic and thermal Energies= -5921.666619
Sum of electronic and thermal Enthalpies= -5921.665659
Sum of electronic and thermal Free Energies= -5921.761076

	1	2	3
Frequencies --	23.1905	37.5691	42.9467

(*S*)-DA-dist-Rh(I)-Ph-CH-si-confD-CR-TS (81b)

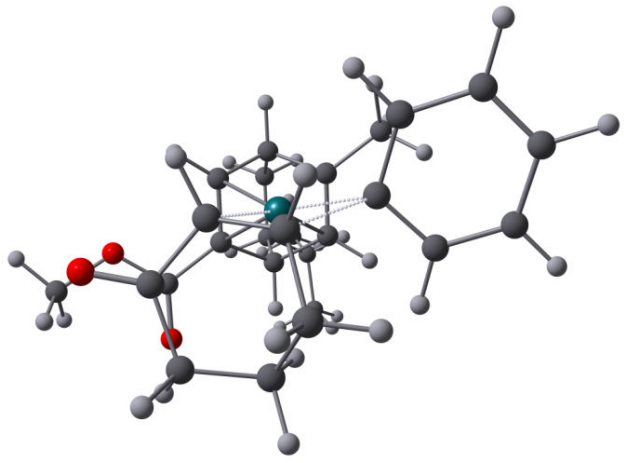


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.589802	-0.045826	0.014551
2	6	0	-1.258354	1.083526	0.254635
3	6	0	-1.396504	0.148593	-1.967969
4	6	0	-0.837933	1.225819	-1.066519
5	6	0	-2.130122	-0.137154	0.480552
6	6	0	-2.943840	0.148906	-1.876065
7	6	0	-1.275207	-1.280773	-0.029901
8	6	0	-0.888586	-1.147079	-1.349781
9	6	0	-3.403779	0.005755	-0.404128
10	1	0	-1.059500	0.262383	-3.001191
11	1	0	-2.369481	-0.232985	1.538965
12	1	0	-3.317573	-0.686361	-2.480078
13	1	0	-3.898372	0.934720	-0.087455
14	1	0	-1.188292	-2.220169	0.511125
15	1	0	-0.436471	2.158280	-1.453381
16	6	0	1.859413	-1.675064	0.547948
17	6	0	2.246951	-2.734333	-0.282112
18	6	0	1.674929	-1.943038	1.918845
19	6	0	2.401689	-4.024968	0.227025
20	1	0	2.427797	-2.564672	-1.340452
21	6	0	1.802776	-3.235572	2.420829
22	1	0	1.429039	-1.131688	2.602241
23	6	0	2.170283	-4.286069	1.576476
24	1	0	2.702320	-4.830895	-0.439093
25	1	0	1.632117	-3.420259	3.479035
26	1	0	2.290370	-5.291781	1.970492
27	6	0	2.899906	0.054614	0.212896
28	6	0	2.193026	1.271345	0.537018
29	1	0	3.502159	-0.334232	1.028065
30	1	0	2.091033	1.519245	1.595429
31	6	0	2.292505	2.459540	-0.322418
32	8	0	1.980848	3.578672	0.078920
33	6	0	2.889405	2.268680	-1.704410
34	6	0	3.561759	-0.077829	-1.152729
35	1	0	2.109347	1.891686	-2.379298
36	1	0	4.385098	-0.795932	-1.090123
37	6	0	-1.194242	2.144302	1.287621

38	8	0	-1.437540	1.960786	2.468541
39	8	0	-0.856538	3.330385	0.772509
40	6	0	-0.627901	4.377852	1.719697
41	1	0	-0.331940	5.243156	1.130027
42	1	0	-1.538898	4.584879	2.285937
43	1	0	0.177197	4.100327	2.401509
44	6	0	-0.412235	-2.255752	-2.232287
45	1	0	-0.093670	-3.124651	-1.653120
46	1	0	-1.229608	-2.568287	-2.896554
47	1	0	0.416488	-1.937362	-2.873735
48	6	0	-4.415966	-1.138233	-0.215818
49	1	0	-3.970355	-2.050160	-0.639827
50	6	0	-5.707265	-0.839956	-0.981043
51	1	0	-5.529243	-0.649550	-2.043935
52	1	0	-6.407503	-1.678733	-0.907670
53	1	0	-6.204166	0.044198	-0.563981
54	6	0	-4.742986	-1.410392	1.252302
55	1	0	-5.080983	-0.497395	1.756972
56	1	0	-5.547420	-2.149028	1.333781
57	1	0	-3.886022	-1.802805	1.806758
58	1	0	-3.333607	1.066445	-2.328460
59	6	0	4.049289	1.275523	-1.660384
60	1	0	3.198887	3.250455	-2.071979
61	1	0	4.491607	1.159543	-2.655909
62	1	0	4.838896	1.662435	-1.004228
63	1	0	2.853460	-0.476832	-1.886118

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5922.21976431     A.U. after    1 cycles
             Convg  =    0.3924D-08             -V/T =  2.0045
Zero-point correction=                           0.538612 (Hartree/Particle)
 Thermal correction to Energy=                    0.569014
 Thermal correction to Enthalpy=                  0.569974
 Thermal correction to Gibbs Free Energy=         0.476844
 Sum of electronic and zero-point Energies=          -5921.681153
 Sum of electronic and thermal Energies=             -5921.650750
 Sum of electronic and thermal Enthalpies=           -5921.649790
 Sum of electronic and thermal Free Energies=        -5921.742920
                    1                    2                    3
Frequencies --  -289.4572               22.1642              31.6268
```

(*S*)-DA-dist-Rh(I)-Ph-CH-re-confU-CR-TS (88a)

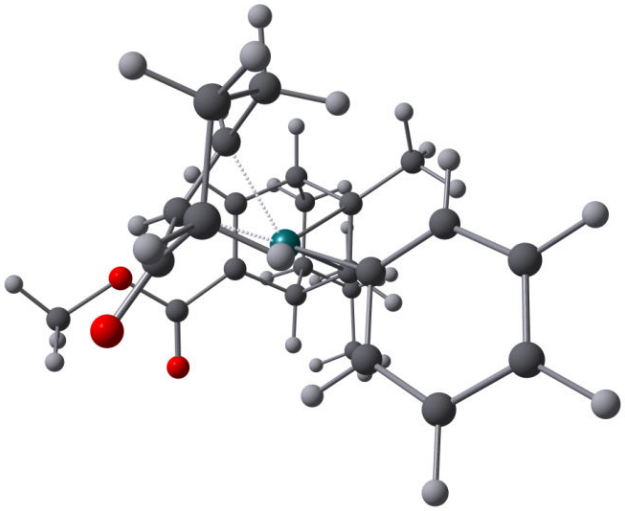


```
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
```

Number	Number	Type	X	Y	Z
1	45	0	0.663867	0.080619	-0.416081
2	6	0	-1.464715	0.684072	-0.282465
3	6	0	-1.409217	-1.220832	-1.770132
4	6	0	-1.181487	0.261956	-1.578135
5	6	0	-1.851198	-0.452390	0.645402
6	6	0	-2.864228	-1.568817	-1.363013
7	6	0	-0.701132	-1.428394	0.522846
8	6	0	-0.469626	-1.870667	-0.765693
9	6	0	-3.153584	-1.099888	0.085081
10	1	0	-1.193183	-1.542009	-2.791840
11	1	0	-1.980478	-0.078517	1.660582
12	1	0	-2.985672	-2.655037	-1.448712
13	1	0	-3.909216	-0.301895	0.061877
14	1	0	-0.279486	-1.929965	1.390630
15	1	0	-1.137304	0.952431	-2.415575
16	6	0	2.512228	-0.910382	0.013218
17	6	0	3.135067	-1.525786	-1.087829
18	6	0	2.673903	-1.514890	1.271591
19	6	0	3.855343	-2.709569	-0.947568
20	1	0	3.069657	-1.061368	-2.071071
21	6	0	3.396912	-2.698273	1.415878
22	1	0	2.220637	-1.066483	2.153049
23	6	0	3.990348	-3.304482	0.307449
24	1	0	4.321991	-3.162773	-1.819298
25	1	0	3.496801	-3.148886	2.400932
26	1	0	4.561165	-4.222092	0.422816
27	6	0	2.809766	1.091499	-0.106291
28	1	0	3.661707	0.845134	-0.732638
29	6	0	1.787170	1.861264	-0.773808
30	1	0	1.847972	1.951273	-1.860113
31	6	0	1.210545	3.045774	-0.126580
32	8	0	0.664269	3.932227	-0.784380
33	6	0	3.191576	1.516227	1.294724
34	6	0	1.361317	3.205182	1.374067
35	6	0	1.981995	2.005178	2.076165
36	1	0	3.722220	0.715231	1.814543
37	1	0	3.908893	2.343007	1.182850
38	1	0	1.242321	1.196010	2.149721
39	1	0	2.265596	2.271790	3.099929
40	1	0	1.993469	4.091991	1.514010
41	1	0	0.379246	3.457027	1.784334
42	6	0	-1.845738	2.068624	0.088660
43	8	0	-1.968598	2.455450	1.238831
44	8	0	-2.104292	2.830577	-0.980405
45	6	0	-2.451791	4.193068	-0.700865
46	1	0	-2.662971	4.642016	-1.670386
47	1	0	-3.334836	4.234098	-0.059347
48	1	0	-1.612720	4.701410	-0.225500
49	6	0	-3.713874	-2.231094	0.966648
50	1	0	-3.019818	-3.081889	0.899162
51	6	0	-5.077418	-2.688659	0.444982
52	1	0	-5.040898	-2.995931	-0.604551
53	1	0	-5.452856	-3.537568	1.026019
54	1	0	-5.812272	-1.878889	0.528080
55	6	0	-3.835308	-1.834579	2.437761
56	1	0	-2.862633	-1.654824	2.904644
57	1	0	-4.435866	-0.924181	2.551643
58	1	0	-4.328170	-2.628673	3.008640
59	1	0	-3.559869	-1.114509	-2.075818
60	6	0	0.272424	-3.115408	-1.132792
61	1	0	0.857332	-2.981981	-2.047114

```
     62          1           0        0.946832   -3.436787   -0.335739
     63          1           0       -0.448298   -3.923433   -1.320278
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5922.22250646     A.U. after    1 cycles
             Convg  =    0.1614D-08             -V/T =  2.0045
Zero-point correction=                          0.538735 (Hartree/Particle)
 Thermal correction to Energy=                   0.568805
 Thermal correction to Enthalpy=                 0.569765
 Thermal correction to Gibbs Free Energy=        0.478217
 Sum of electronic and zero-point Energies=          -5921.683771
 Sum of electronic and thermal Energies=             -5921.653701
 Sum of electronic and thermal Enthalpies=           -5921.652741
 Sum of electronic and thermal Free Energies=        -5921.744290
                    1                    2                    3
Frequencies --  -287.7828               20.8730              36.7240
```

(*S*)-DA-dist-Rh(I)-Ph-CH-re-confD-close (85b)

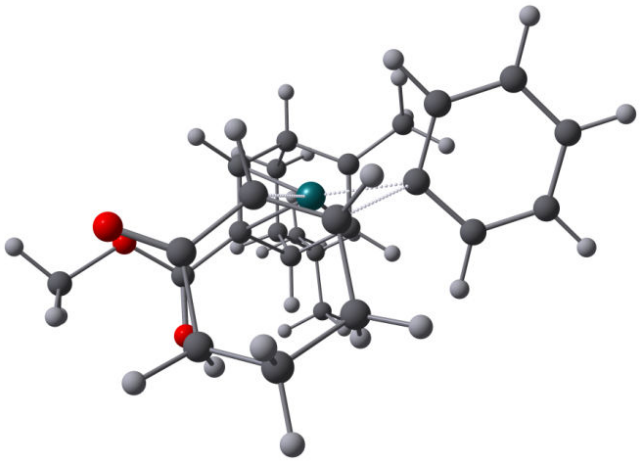


```
---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
 ---------------------------------------------------------------------
      1         45           0        0.420598   -0.006347   -0.178965
      2          6           0       -1.569707    1.182800    0.002055
      3          6           0       -1.820007   -0.237349   -1.924605
      4          6           0       -1.319662    1.060871   -1.341397
      5          6           0       -2.269201   -0.025078    0.596313
      6          6           0       -3.342400   -0.356690   -1.647823
      7          6           0       -1.356496   -1.190938    0.248574
      8          6           0       -1.124497   -1.327948   -1.120188
      9          6           0       -3.633889   -0.194160   -0.136385
     10          1           0       -1.600886   -0.319098   -2.991926
     11          1           0       -2.394895    0.106190    1.670049
     12          1           0       -3.669541   -1.340501   -2.003243
     13          1           0       -4.191797    0.738433    0.026431
     14          1           0       -1.191416   -2.010518    0.943927
     15          1           0       -0.974818    1.887181   -1.956357
     16          6           0        1.679652   -1.414164    0.527489
     17          6           0        2.200952   -2.560361   -0.083691
     18          6           0        1.982842   -1.211697    1.886282
     19          6           0        3.006802   -3.460166    0.621302
     20          1           0        1.988361   -2.769960   -1.130177
```

21	6	0	2.784403	-2.107455	2.595657
22	1	0	1.607152	-0.331161	2.409690
23	6	0	3.303999	-3.238823	1.964371
24	1	0	3.401237	-4.338696	0.114160
25	1	0	3.008276	-1.915176	3.642914
26	1	0	3.932169	-3.936159	2.512842
27	6	0	1.866172	0.778231	-1.760165
28	1	0	1.146125	0.972837	-2.553282
29	6	0	1.865149	1.629194	-0.651785
30	1	0	1.185040	2.477031	-0.592416
31	6	0	3.026335	1.709361	0.258206
32	8	0	3.029587	2.480311	1.213821
33	6	0	3.095415	0.001496	-2.167826
34	6	0	4.217203	0.835089	-0.065781
35	1	0	3.015979	-1.046480	-1.866472
36	1	0	4.075890	-0.122598	0.450386
37	6	0	-0.736441	-2.601377	-1.801090
38	1	0	-0.301267	-3.315018	-1.099173
39	1	0	-1.628480	-3.064326	-2.245646
40	1	0	-0.026047	-2.425346	-2.615360
41	6	0	-4.491616	-1.343944	0.422251
42	1	0	-3.987598	-2.288533	0.169951
43	6	0	-5.872120	-1.350984	-0.237679
44	1	0	-5.814408	-1.409545	-1.328846
45	1	0	-6.464598	-2.204356	0.108246
46	1	0	-6.425146	-0.438899	0.017239
47	6	0	-4.651092	-1.283498	1.941329
48	1	0	-5.044729	-0.310158	2.257636
49	1	0	-5.354657	-2.050433	2.281683
50	1	0	-3.708702	-1.452271	2.469639
51	1	0	-3.879398	0.389734	-2.241458
52	6	0	-1.419985	2.421503	0.797181
53	8	0	-1.758932	2.521579	1.961387
54	8	0	-0.877974	3.430330	0.093644
55	6	0	-0.638214	4.633712	0.837291
56	1	0	-0.205969	5.334493	0.124923
57	1	0	-1.573910	5.025248	1.240530
58	1	0	0.061100	4.440263	1.652588
59	6	0	4.364630	0.605800	-1.567420
60	1	0	3.159359	0.002319	-3.262005
61	1	0	5.220121	-0.048614	-1.765014
62	1	0	4.576773	1.562881	-2.060663
63	1	0	5.102965	1.308546	0.367031

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5922.23640500     A.U. after    1 cycles
            Convg  =    0.3806D-08             -V/T =  2.0045
Zero-point correction=                           0.538216 (Hartree/Particle)
 Thermal correction to Energy=                    0.569634
 Thermal correction to Enthalpy=                  0.570594
 Thermal correction to Gibbs Free Energy=         0.474990
 Sum of electronic and zero-point Energies=          -5921.698189
 Sum of electronic and thermal Energies=             -5921.666771
 Sum of electronic and thermal Enthalpies=           -5921.665811
 Sum of electronic and thermal Free Energies=        -5921.761415
                    1                      2                      3
Frequencies --    21.2698               30.5414                38.6608
```

(*S*)-DA-prox-Rh(I)-Ph-CH-re-confD-CR-TS (88b)



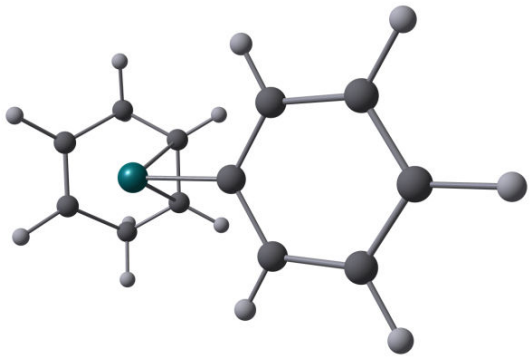
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.642718	-0.045827	-0.390758
2	6	0	-1.392079	0.820815	-0.256018
3	6	0	-1.570628	-1.066556	-1.754773
4	6	0	-1.162450	0.376447	-1.554883
5	6	0	-1.924300	-0.262481	0.663402
6	6	0	-3.059081	-1.233468	-1.354494
7	6	0	-0.902338	-1.372183	0.541028
8	6	0	-0.722807	-1.833184	-0.750222
9	6	0	-3.294526	-0.738483	0.093884
10	1	0	-1.390911	-1.407237	-2.777089
11	1	0	-2.011250	0.119968	1.679811
12	1	0	-3.313753	-2.295764	-1.445978
13	1	0	-3.945391	0.146918	0.071955
14	1	0	-0.551790	-1.928393	1.407556
15	1	0	-1.025452	1.061086	-2.386740
16	6	0	2.330816	-1.270408	0.068559
17	6	0	2.912339	-1.882624	-1.057750
18	6	0	2.434946	-1.935690	1.299869
19	6	0	3.525014	-3.129549	-0.966866
20	1	0	2.896114	-1.369338	-2.018261
21	6	0	3.057394	-3.180769	1.394151
22	1	0	2.018903	-1.487230	2.199061
23	6	0	3.601146	-3.788067	0.262122
24	1	0	3.955314	-3.584138	-1.856447
25	1	0	3.117420	-3.678024	2.359862
26	1	0	4.091044	-4.755143	0.338821
27	6	0	2.791740	0.715158	0.118631
28	1	0	3.720644	0.366591	-0.321174
29	6	0	2.009050	1.565659	-0.745080
30	1	0	2.228592	1.520441	-1.814446
31	6	0	1.601335	2.911751	-0.316743
32	8	0	1.204425	3.748478	-1.126235
33	6	0	2.914046	1.088313	1.587203
34	6	0	1.772527	3.265930	1.147790
35	1	0	3.781715	0.583719	2.022593
36	1	0	1.811132	4.356158	1.221627
37	6	0	-1.578232	2.239028	0.132245
38	8	0	-1.664180	2.623132	1.287228

39	8	0	-1.697173	3.047749	-0.926536
40	6	0	-1.850099	4.440882	-0.629238
41	1	0	-1.922168	4.937024	-1.595630
42	1	0	-2.757798	4.604266	-0.043824
43	1	0	-0.980520	4.809428	-0.084929
44	6	0	-3.994260	-1.795337	0.967901
45	1	0	-3.406720	-2.723064	0.903310
46	6	0	-5.399680	-2.084814	0.436473
47	1	0	-5.394485	-2.396374	-0.612496
48	1	0	-5.879626	-2.880783	1.015563
49	1	0	-6.031100	-1.191552	0.514432
50	6	0	-4.077966	-1.388960	2.439164
51	1	0	-3.095254	-1.336823	2.916401
52	1	0	-4.557497	-0.409098	2.550265
53	1	0	-4.674462	-2.113997	3.002941
54	1	0	-3.689694	-0.693618	-2.068111
55	6	0	-0.133285	-3.155690	-1.123867
56	1	0	0.464847	-3.087160	-2.036883
57	1	0	0.497746	-3.559329	-0.328735
58	1	0	-0.944476	-3.871514	-1.316376
59	6	0	3.010285	2.602919	1.745144
60	1	0	2.035843	0.747528	2.144909
61	1	0	3.103230	2.858892	2.806184
62	1	0	3.912721	2.977939	1.246004
63	1	0	0.876771	2.934141	1.688442

```
SCF Done:  E(RPBE1PBE) =  -5922.21834098     A.U. after    1 cycles
             Convg  =    0.7862D-08             -V/T =  2.0045
Zero-point correction=                           0.538427 (Hartree/Particle)
 Thermal correction to Energy=                    0.568746
 Thermal correction to Enthalpy=                  0.569706
 Thermal correction to Gibbs Free Energy=         0.477308
 Sum of electronic and zero-point Energies=          -5921.679914
 Sum of electronic and thermal Energies=             -5921.649595
 Sum of electronic and thermal Enthalpies=           -5921.648634
 Sum of electronic and thermal Free Energies=        -5921.741033
                     1                      2                      3
Frequencies --  -281.8160               23.8379                32.2096
```

CHD-Rh pathway

CHD-Rh(I)-Ph (91)

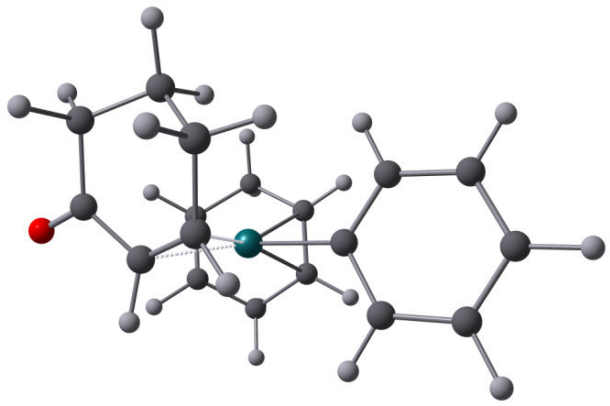


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.517055	-0.000387	-0.571150

2	6	0	2.788619	-0.685511	-0.533973
3	6	0	2.453868	1.419073	0.742272
4	6	0	2.790069	0.680450	-0.537253
5	6	0	2.451322	-1.417839	0.748684
6	6	0	1.221711	-0.705398	1.270082
7	6	0	1.223041	0.711153	1.266899
8	1	0	2.235970	2.470222	0.537150
9	1	0	2.231463	-2.469460	0.548092
10	1	0	0.517209	-1.246604	1.898525
11	1	0	3.120800	1.232270	-1.414541
12	6	0	-1.430020	0.000277	-0.121699
13	6	0	-2.155867	1.200983	-0.015841
14	6	0	-2.155617	-1.200662	-0.016711
15	6	0	-3.542828	1.203528	0.151780
16	1	0	-1.634301	2.156467	-0.065561
17	6	0	-3.542583	-1.203579	0.150829
18	1	0	-1.633948	-2.156058	-0.067150
19	6	0	-4.243486	-0.000131	0.234992
20	1	0	-4.077407	2.148876	0.224127
21	1	0	-4.076987	-2.149072	0.222569
22	1	0	-5.322163	-0.000300	0.371766
23	1	0	3.118182	-1.242160	-1.408663
24	1	0	0.519448	1.256421	1.892866
25	1	0	3.291176	-1.392502	1.464277
26	1	0	3.293715	1.395248	1.457922

```
SCF Done:  E(RPBE1PBE) =  -5151.79986189     A.U. after    1 cycles
             Convg  =    0.3699D-08             -V/T =  2.0031
Zero-point correction=                           0.214685 (Hartree/Particle)
 Thermal correction to Energy=                    0.226883
 Thermal correction to Enthalpy=                  0.227843
 Thermal correction to Gibbs Free Energy=         0.173850
 Sum of electronic and zero-point Energies=          -5151.585177
 Sum of electronic and thermal Energies=             -5151.572979
 Sum of electronic and thermal Enthalpies=           -5151.572019
 Sum of electronic and thermal Free Energies=        -5151.626012
                     1                      2                      3
Frequencies --    20.1037               53.0769               58.7072
```

CHD-Rh(I)-Ph-CH-si-confU-anti (95a)

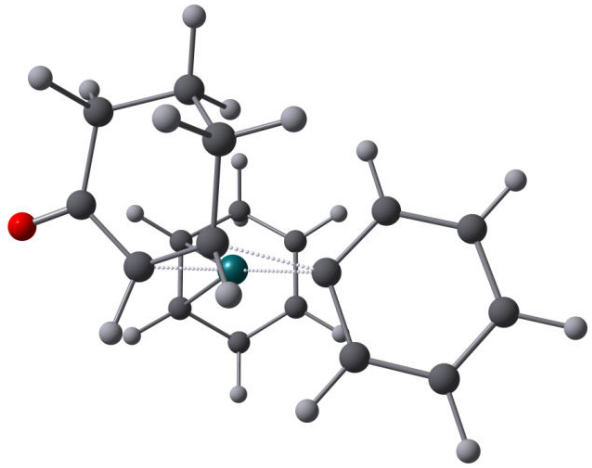


1	45	0	-0.193832	0.403728	-0.172458
2	6	0	-1.799478	2.001445	-0.578585

3	6	0	-1.219114	2.005897	1.843773
4	6	0	-2.050397	1.516923	0.680274
5	6	0	-0.699664	3.023641	-0.768853
6	6	0	0.453542	2.489214	0.052461
7	6	0	0.198163	1.985938	1.320140
8	1	0	-1.324492	1.338788	2.702890
9	1	0	-0.419108	3.102185	-1.821866
10	1	0	1.475994	2.661024	-0.271812
11	1	0	-2.917985	0.887044	0.855582
12	6	0	1.782403	-0.162066	-0.119310
13	6	0	2.397022	-0.608330	1.061206
14	6	0	2.610501	0.035584	-1.236980
15	6	0	3.772965	-0.846766	1.125036
16	1	0	1.797803	-0.776580	1.955414
17	6	0	3.986564	-0.196320	-1.178180
18	1	0	2.179599	0.375438	-2.178370
19	6	0	4.577217	-0.640592	0.005177
20	1	0	4.216021	-1.194005	2.056630
21	1	0	4.598628	-0.031315	-2.062918
22	1	0	5.647664	-0.824409	0.052590
23	6	0	-0.174098	-1.771915	-0.900948
24	6	0	-1.353641	-1.123187	-1.254124
25	1	0	0.619604	-1.840279	-1.639373
26	1	0	-1.456977	-0.653447	-2.232034
27	6	0	-2.623089	-1.387531	-0.548326
28	8	0	-3.683064	-0.903864	-0.936469
29	6	0	-2.581594	-2.350929	0.619302
30	1	0	-2.898256	-3.319893	0.207188
31	6	0	-0.133692	-2.767372	0.224610
32	1	0	-0.283032	-3.766621	-0.213266
33	1	0	-2.462487	1.744181	-1.400783
34	1	0	1.023262	1.760413	1.990438
35	6	0	-1.208763	-2.493612	1.268339
36	1	0	0.862779	-2.776575	0.675849
37	1	0	-1.230614	-3.297446	2.012023
38	1	0	-0.956238	-1.568471	1.803709
39	1	0	-3.354536	-2.056648	1.335016
40	1	0	-1.526720	3.011721	2.174203
41	1	0	-1.013035	4.027928	-0.438810

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5460.16722228     A.U. after    1 cycles
             Convg  =    0.6574D-08             -V/T =  2.0037
Zero-point correction=                           0.345759 (Hartree/Particle)
 Thermal correction to Energy=                    0.365128
 Thermal correction to Enthalpy=                  0.366088
 Thermal correction to Gibbs Free Energy=         0.297266
 Sum of electronic and zero-point Energies=          -5459.821463
 Sum of electronic and thermal Energies=             -5459.802094
 Sum of electronic and thermal Enthalpies=           -5459.801134
 Sum of electronic and thermal Free Energies=        -5459.869956
                     1                      2                      3
Frequencies --    26.0715               56.3296               63.6119
```

CHD-Rh(I)-Ph-CH-si-confU-CR-TS (96a)



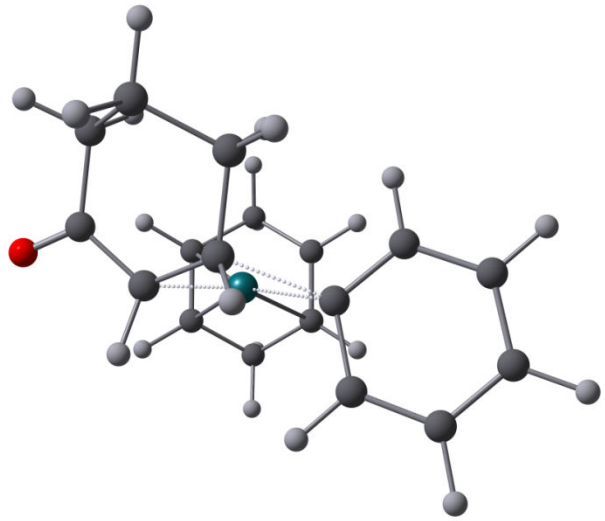
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.289011	0.446242	-0.199375
2	6	0	-1.638191	2.117054	-0.667693
3	6	0	-1.290741	2.040513	1.804003
4	6	0	-2.023014	1.595152	0.556901
5	6	0	-0.495810	3.110342	-0.709250
6	6	0	0.554717	2.502023	0.196560
7	6	0	0.169607	1.981429	1.411645
8	1	0	-1.497819	1.364435	2.637370
9	1	0	-0.112472	3.217098	-1.726997
10	1	0	1.608681	2.591322	-0.054647
11	1	0	-2.943690	1.022481	0.637199
12	6	0	1.579735	-0.573170	-0.208398
13	6	0	2.225501	-0.841105	1.009312
14	6	0	2.380284	-0.210906	-1.307575
15	6	0	3.608916	-0.715952	1.132784
16	1	0	1.643995	-1.129138	1.882403
17	6	0	3.760558	-0.071204	-1.182655
18	1	0	1.915795	-0.043073	-2.278462
19	6	0	4.383875	-0.325129	0.040534
20	1	0	4.082945	-0.920242	2.090394
21	1	0	4.353520	0.221834	-2.046176
22	1	0	5.462319	-0.231708	0.137702
23	6	0	0.104639	-1.822343	-0.772008
24	6	0	-1.119771	-1.195986	-1.220583
25	1	0	0.764545	-2.133271	-1.577596
26	1	0	-1.195574	-0.893506	-2.266614
27	6	0	-2.410101	-1.457340	-0.578457
28	8	0	-3.470937	-1.064296	-1.069718
29	6	0	-2.426507	-2.280245	0.696787
30	1	0	-3.164828	-1.842805	1.375659
31	6	0	-0.017802	-2.852564	0.329790
32	1	0	0.952740	-3.046934	0.792806
33	1	0	-2.255549	1.952783	-1.547492
34	1	0	0.916652	1.656484	2.131065
35	6	0	-1.065456	-2.456992	1.360110
36	1	0	-0.324171	-3.790775	-0.155702
37	1	0	-2.827086	-3.260773	0.404731
38	1	0	-1.128122	-3.212527	2.151056

39	1	0	-0.763928	-1.515060	1.838724
40	1	0	-0.804075	4.113583	-0.370613
41	1	0	-1.593492	3.051781	2.123968

SCF Done: E(RPBE1PBE) = -5460.14996033 A.U. after 1 cycles
Convg = 0.4679D-08 -V/T = 2.0037
Zero-point correction= 0.345233 (Hartree/Particle)
Thermal correction to Energy= 0.363766
Thermal correction to Enthalpy= 0.364726
Thermal correction to Gibbs Free Energy= 0.298037
Sum of electronic and zero-point Energies= -5459.804728
Sum of electronic and thermal Energies= -5459.786194
Sum of electronic and thermal Enthalpies= -5459.785234
Sum of electronic and thermal Free Energies= -5459.851923

	1	2	3
Frequencies --	-299.2395	33.2135	58.8343

CHD-Rh(I)-Ph-CH-si-confD-CR-TS (96b)



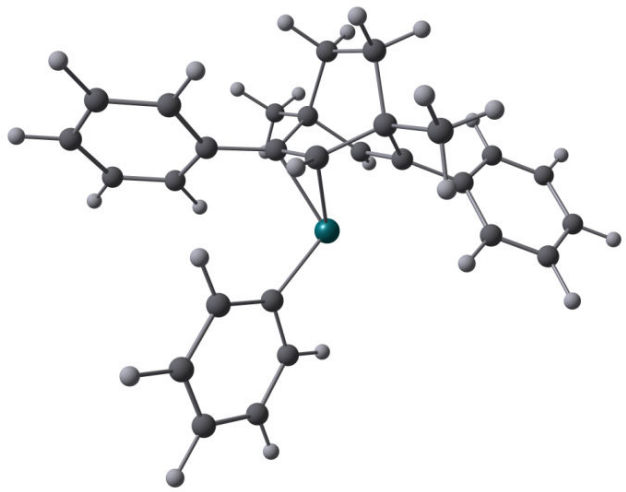
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.200729	0.497592	-0.163769
2	6	0	-1.356338	2.295238	-0.688372
3	6	0	-1.102922	2.198521	1.794707
4	6	0	-1.835245	1.826000	0.524096
5	6	0	-0.114367	3.162293	-0.693452
6	6	0	0.834324	2.450459	0.248805
7	6	0	0.354374	1.978860	1.451812
8	1	0	-1.409692	1.552060	2.620776
9	1	0	0.311979	3.220290	-1.697902
10	1	0	1.899738	2.426228	0.034258
11	1	0	-2.815536	1.357758	0.574870
12	6	0	1.564582	-0.693607	-0.142495
13	6	0	2.263289	-0.978579	1.039872
14	6	0	2.315531	-0.484536	-1.315502
15	6	0	3.658020	-1.007596	1.060589
16	1	0	1.722100	-1.163326	1.964749
17	6	0	3.707968	-0.493038	-1.290925
18	1	0	1.802687	-0.316625	-2.261542
19	6	0	4.388810	-0.756513	-0.100348

20	1	0	4.175914	-1.223146	1.992668
21	1	0	4.264153	-0.308446	-2.207314
22	1	0	5.475199	-0.779359	-0.081662
23	6	0	-0.087336	-1.802558	-0.476225
24	6	0	-1.174527	-1.106191	-1.131019
25	1	0	0.555926	-2.351226	-1.158094
26	1	0	-1.092552	-0.928359	-2.205292
27	6	0	-2.559108	-1.186738	-0.653631
28	8	0	-3.495115	-0.686233	-1.277906
29	6	0	-2.808613	-1.961198	0.628308
30	1	0	-2.723873	-1.261271	1.471159
31	1	0	-3.843788	-2.312705	0.605395
32	6	0	-1.811421	-3.101642	0.804376
33	1	0	-2.007745	-3.639163	1.738629
34	1	0	-1.931800	-3.826111	-0.010850
35	6	0	-0.386766	-2.556243	0.813529
36	1	0	-0.286725	-1.894306	1.679285
37	1	0	0.345378	-3.358718	0.947072
38	1	0	-1.956051	2.188768	-1.589094
39	1	0	1.039212	1.585169	2.198446
40	1	0	-0.326428	4.194991	-0.369633
41	1	0	-1.305870	3.238116	2.102188

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5460.14570214     A.U. after    1 cycles
             Convg  =    0.4149D-08             -V/T =  2.0037
Zero-point correction=                           0.345397 (Hartree/Particle)
 Thermal correction to Energy=                    0.363967
 Thermal correction to Enthalpy=                  0.364927
 Thermal correction to Gibbs Free Energy=         0.298145
 Sum of electronic and zero-point Energies=          -5459.800305
 Sum of electronic and thermal Energies=             -5459.781736
 Sum of electronic and thermal Enthalpies=           -5459.780776
 Sum of electronic and thermal Free Energies=        -5459.847557
                     1                      2                      3
Frequencies --  -301.0155               37.4575                60.8988
```

(S)-1,4-Me$_2$PhBOD (Carnell ligand)-Rh pathway

(*S*)-1,4-Me$_2$BOD-Rh(I)-Ph (48)



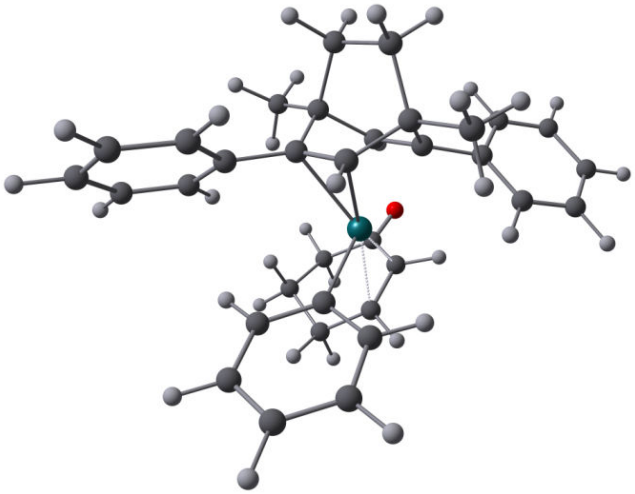
```
 ---------------------------------------------------------------------
 Center     Atomic      Atomic             Coordinates (Angstroms)
 Number     Number       Type              X           Y           Z
```

1	45	0	-0.132464	0.660444	-0.425948
2	6	0	-1.913552	-0.711840	0.032114
3	6	0	-0.063748	-2.093429	-0.811114
4	6	0	3.101811	-0.905963	-1.110279
5	6	0	-3.255095	-0.079897	-0.047409
6	6	0	-4.311138	-0.768787	-0.660768
7	6	0	-1.270936	-1.213901	-1.076316
8	6	0	-1.249266	-1.150085	1.350542
9	6	0	-4.770652	1.776306	0.363887
10	6	0	5.109734	-1.744345	-0.054150
11	6	0	-0.505500	-3.250222	0.121571
12	6	0	0.173697	-0.646204	1.156551
13	6	0	-5.579034	-0.196101	-0.760278
14	6	0	0.846977	-1.153775	0.008338
15	6	0	2.968883	-1.964838	1.045714
16	6	0	-3.506093	1.201607	0.465051
17	6	0	-1.220779	-2.701421	1.366153
18	6	0	-5.814013	1.078787	-0.247193
19	6	0	2.323392	-1.328671	-0.024050
20	6	0	4.349274	-2.170169	1.033421
21	6	0	4.478525	-1.110143	-1.126878
22	1	0	2.620957	-0.385725	-1.934169
23	1	0	6.185290	-1.900474	-0.065794
24	1	0	2.382695	-2.302681	1.897262
25	1	0	4.828944	-2.662981	1.875481
26	1	0	5.064552	-0.765170	-1.975153
27	1	0	-4.134581	-1.765052	-1.058654
28	1	0	-4.940979	2.775085	0.757710
29	1	0	-6.383860	-0.748284	-1.238732
30	1	0	-2.697455	1.763080	0.926602
31	1	0	-6.800615	1.527802	-0.325215
32	1	0	-1.162744	-3.918022	-0.446686
33	1	0	0.380120	-3.834217	0.397703
34	1	0	-0.714040	-3.022204	2.283488
35	1	0	-2.251288	-3.069930	1.426304
36	1	0	0.731963	-0.291667	2.023115
37	1	0	-1.693856	-1.137860	-2.077045
38	6	0	1.272228	2.059462	-0.042443
39	6	0	2.389375	2.041398	0.810449
40	6	0	1.004709	3.268820	-0.712241
41	6	0	3.191468	3.170760	0.990706
42	1	0	2.650414	1.127638	1.342236
43	6	0	1.803709	4.404271	-0.545172
44	1	0	0.147308	3.338718	-1.387848
45	6	0	2.903605	4.358484	0.312784
46	1	0	4.048001	3.125696	1.661170
47	1	0	1.568803	5.321738	-1.081633
48	1	0	3.530566	5.236208	0.450755
49	6	0	0.543618	-2.626596	-2.098129
50	1	0	1.431744	-3.234003	-1.899660
51	1	0	-0.186549	-3.256041	-2.618228
52	1	0	0.830245	-1.815804	-2.775004
53	6	0	-1.889667	-0.609300	2.618313
54	1	0	-2.941002	-0.904713	2.692557
55	1	0	-1.365097	-1.008156	3.493024
56	1	0	-1.837869	0.481784	2.669003

SCF Done: E(RPBE1PBE) = -5769.27144984 A.U. after 1 cycles
Convg = 0.1935D-08 -V/T = 2.0044
Zero-point correction= 0.468953 (Hartree/Particle)
Thermal correction to Energy= 0.494399
Thermal correction to Enthalpy= 0.495344

```
 Thermal correction to Gibbs Free Energy=          0.412962
 Sum of electronic and zero-point Energies=          -5768.802497
 Sum of electronic and thermal Energies=             -5768.777050
 Sum of electronic and thermal Enthalpies=           -5768.776106
 Sum of electronic and thermal Free Energies=        -5768.858487
                     1                      2                      3
Frequencies --     25.3928                35.4212                38.8627
```

(*S*)-1,4-Me$_2$BOD-Rh(I)-Ph-CH-si-confU-anti (103a)



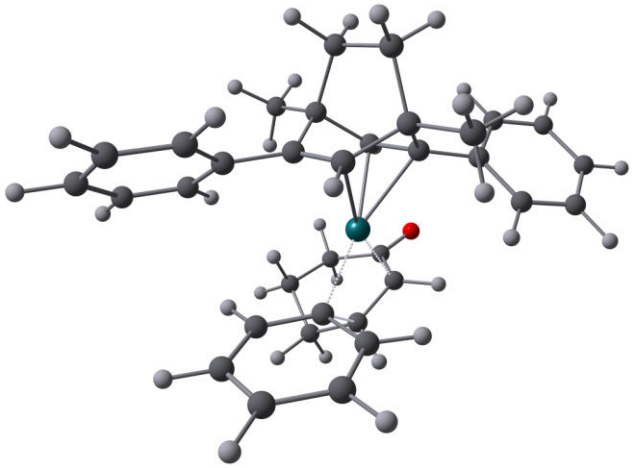
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.106936	-0.483256	-0.060690
2	6	0	-1.780212	1.075955	-0.274275
3	6	0	-0.016201	2.096054	1.110107
4	6	0	3.085824	0.998484	1.461764
5	6	0	-3.164460	0.595158	-0.508307
6	6	0	-4.214813	1.139223	0.243922
7	6	0	-1.236413	1.204267	0.988470
8	6	0	-0.983165	1.854559	-1.331684
9	6	0	-4.782542	-0.796877	-1.670997
10	6	0	5.240320	1.766137	0.678620
11	6	0	-0.391789	3.487074	0.524139
12	6	0	0.421174	1.310839	-1.147579
13	6	0	-5.530650	0.724408	0.041789
14	6	0	0.982575	1.462568	0.125907
15	6	0	3.245370	2.197587	-0.615472
16	6	0	-3.470378	-0.377099	-1.472285
17	6	0	-0.977283	3.343305	-0.886637
18	6	0	-5.819653	-0.245562	-0.916532
19	6	0	2.449924	1.535356	0.332231
20	6	0	4.624604	2.309976	-0.447475
21	6	0	4.462260	1.109845	1.633459
22	1	0	2.502061	0.463829	2.203548
23	1	0	6.315282	1.853105	0.812511
24	1	0	2.776299	2.641691	-1.489337
25	1	0	5.217104	2.829149	-1.196421
26	1	0	4.930296	0.675700	2.513203
27	1	0	-3.996791	1.899812	0.989195
28	1	0	-4.996078	-1.560613	-2.414298
29	1	0	-6.330035	1.160925	0.634871

30	1	0	-2.670736	-0.828834	-2.052887
31	1	0	-6.844063	-0.572451	-1.073676
32	1	0	-1.113158	3.954322	1.203242
33	1	0	0.503012	4.119814	0.521983
34	1	0	-0.389059	3.909693	-1.616944
35	1	0	-2.002574	3.727295	-0.933963
36	1	0	1.043313	1.131421	-2.021087
37	1	0	-1.776537	0.887660	1.877812
38	6	0	1.368210	-1.447224	-1.155116
39	6	0	2.711764	-1.617797	-0.793015
40	6	0	1.005260	-1.852523	-2.453603
41	6	0	3.650736	-2.155627	-1.680273
42	1	0	3.050529	-1.324338	0.197942
43	6	0	1.937087	-2.383296	-3.348789
44	1	0	-0.028714	-1.754084	-2.784768
45	6	0	3.271168	-2.538966	-2.966143
46	1	0	4.684805	-2.272739	-1.360657
47	1	0	1.618080	-2.679392	-4.346522
48	1	0	3.999784	-2.955338	-3.657636
49	6	0	-0.309815	-2.723869	0.456842
50	6	0	-1.376087	-1.997640	0.979614
51	1	0	-0.443890	-3.203189	-0.510049
52	1	0	-2.309378	-1.906316	0.427628
53	6	0	-1.472153	-1.727169	2.425504
54	8	0	-2.485691	-1.226922	2.917322
55	6	0	-0.338217	-2.187790	3.313957
56	6	0	0.759530	-3.293570	1.344888
57	6	0	-1.460941	1.720872	-2.768080
58	1	0	-1.376651	0.692971	-3.131149
59	1	0	-2.501284	2.041165	-2.877310
60	1	0	-0.843721	2.352099	-3.415851
61	6	0	0.429847	2.226273	2.557282
62	1	0	0.604177	1.249451	3.017423
63	1	0	1.342188	2.822034	2.649394
64	1	0	-0.357108	2.725058	3.132590
65	6	0	0.975975	-2.444688	2.588011
66	1	0	-0.227599	-1.468947	4.131208
67	1	0	-0.696285	-3.120307	3.773287
68	1	0	1.418890	-1.489118	2.284100
69	1	0	1.687167	-2.929063	3.264982
70	1	0	1.690394	-3.414183	0.784944
71	1	0	0.436800	-4.305833	1.633687

SCF Done: E(RPBE1PBE) = -6077.62726308 A.U. after 1 cycles
Convg = 0.4460D-08 -V/T = 2.0049
Zero-point correction= 0.600337 (Hartree/Particle)
Thermal correction to Energy= 0.632668
Thermal correction to Enthalpy= 0.633613
Thermal correction to Gibbs Free Energy= 0.537079
Sum of electronic and zero-point Energies= -6077.026927
Sum of electronic and thermal Energies= -6076.994595
Sum of electronic and thermal Enthalpies= -6076.993650
Sum of electronic and thermal Free Energies= -6077.090184

	1	2	3
Frequencies --	24.8692	25.7683	37.9218

(*S*)-1,4-Me$_2$BOD-Rh(I)-Ph-CH-si-confU-CR-TS (104a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.154795	-0.464841	0.027350
2	6	0	1.729879	1.067161	0.162139
3	6	0	-0.037620	2.024870	-1.277794
4	6	0	-3.139762	0.856255	-1.505421
5	6	0	3.144718	0.679348	0.392715
6	6	0	4.148156	1.244952	-0.406427
7	6	0	1.161548	1.107880	-1.110173
8	6	0	0.951115	1.935464	1.165572
9	6	0	4.866583	-0.525392	1.613778
10	6	0	-5.309807	1.581343	-0.722797
11	6	0	0.382960	3.443706	-0.798249
12	6	0	-0.463989	1.406516	1.027053
13	6	0	5.491342	0.929715	-0.202609
14	6	0	-1.032727	1.481854	-0.236202
15	6	0	-3.308337	2.186123	0.489075
16	6	0	3.527286	-0.206152	1.410056
17	6	0	0.967340	3.389728	0.620263
18	6	0	5.855981	0.042280	0.808325
19	6	0	-2.503374	1.492307	-0.428799
20	6	0	-4.694374	2.226901	0.348662
21	6	0	-4.523383	0.897980	-1.651144
22	1	0	-2.550728	0.301908	-2.228067
23	1	0	-6.390236	1.612520	-0.835825
24	1	0	-2.840316	2.710091	1.318119
25	1	0	-5.292876	2.771003	1.074876
26	1	0	-4.990183	0.387418	-2.489616
27	1	0	3.871249	1.942603	-1.192907
28	1	0	5.140073	-1.223822	2.400603
29	1	0	6.252567	1.379176	-0.835223
30	1	0	2.763807	-0.666444	2.031232
31	1	0	6.901681	-0.207238	0.967748
32	1	0	1.117630	3.835501	-1.510350
33	1	0	-0.490750	4.103772	-0.844419
34	1	0	0.389878	4.016358	1.308923
35	1	0	1.998937	3.759372	0.639574
36	6	0	-1.272320	-1.685590	1.069851
37	6	0	-2.634802	-1.716397	0.742500
38	6	0	-0.924458	-1.793321	2.430616

39	6	0	-3.613270	-1.810993	1.734184
40	1	0	-2.951730	-1.645358	-0.294755
41	6	0	-1.898177	-1.867059	3.424049
42	1	0	0.125747	-1.828970	2.717890
43	6	0	-3.252662	-1.878103	3.079804
44	1	0	-4.663434	-1.823530	1.450350
45	1	0	-1.599395	-1.933764	4.467892
46	1	0	-4.015267	-1.951404	3.850922
47	6	0	-0.031047	-2.842097	-0.073938
48	6	0	1.220894	-2.244841	-0.471890
49	1	0	0.039756	-3.475599	0.805442
50	1	0	2.065942	-2.309500	0.213058
51	6	0	1.589717	-2.119621	-1.879171
52	8	0	2.748964	-1.862353	-2.231590
53	6	0	0.536832	-2.384504	-2.938361
54	6	0	-0.899848	-3.415303	-1.169476
55	6	0	-0.508997	2.066507	-2.722320
56	1	0	-0.693159	1.063620	-3.118608
57	1	0	-1.422432	2.657560	-2.835060
58	1	0	0.267657	2.526987	-3.342085
59	6	0	1.435864	1.889279	2.605392
60	1	0	1.359478	0.883188	3.027783
61	1	0	2.475545	2.218986	2.689922
62	1	0	0.820069	2.555412	3.219036
63	1	0	-1.068992	1.239107	1.915888
64	1	0	1.709911	0.763933	-1.985978
65	6	0	-0.883342	-2.534972	-2.408636
66	1	0	0.849481	-3.313940	-3.433233
67	1	0	0.610548	-1.597880	-3.696116
68	1	0	-1.534524	-2.948355	-3.185920
69	1	0	-1.283434	-1.547271	-2.145557
70	1	0	-1.916865	-3.591648	-0.812555
71	1	0	-0.480611	-4.402067	-1.414785

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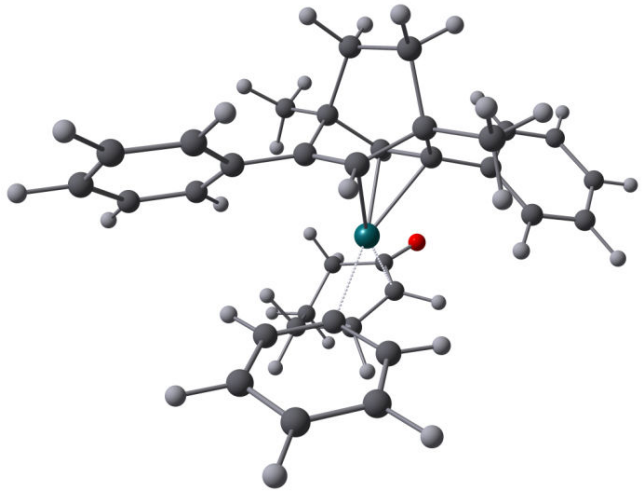
SCF Done:  E(RPBE1PBE) =  -6077.61272607     A.U. after    1 cycles
             Convg  =    0.2267D-08             -V/T =  2.0049
Zero-point correction=                           0.599648 (Hartree/Particle)
 Thermal correction to Energy=                    0.631142
 Thermal correction to Enthalpy=                  0.632086
 Thermal correction to Gibbs Free Energy=         0.537957
 Sum of electronic and zero-point Energies=          -6077.013078
 Sum of electronic and thermal Energies=             -6076.981584
 Sum of electronic and thermal Enthalpies=           -6076.980640
 Sum of electronic and thermal Free Energies=        -6077.074769
                    1                      2                      3
Frequencies --  -290.3070               22.8014                32.0937
```

(*S*)-1,4-Me$_2$BOD-Rh(I)-Ph-CH-si-confD-CR-TS (104b)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.122542	0.425872	0.055363
2	6	0	-1.713071	-1.094260	0.102643
3	6	0	0.052181	-1.997110	-1.370908
4	6	0	3.110968	-0.717791	-1.538483
5	6	0	-3.122472	-0.696238	0.349924
6	6	0	-4.136391	-1.240483	-0.450616
7	6	0	-1.143043	-1.082448	-1.168358
8	6	0	-0.946334	-2.015823	1.069546
9	6	0	-4.823863	0.505858	1.601215
10	6	0	5.309487	-1.450537	-0.848253
11	6	0	-0.371767	-3.434481	-0.954767
12	6	0	0.473337	-1.489197	0.964445
13	6	0	-5.475217	-0.916860	-0.231538
14	6	0	1.040965	-1.494414	-0.303290
15	6	0	3.342785	-2.202525	0.338520
16	6	0	-3.488903	0.178243	1.382228
17	6	0	-0.971136	-3.442357	0.458115
18	6	0	-5.824242	-0.041726	0.795594
19	6	0	2.508570	-1.459522	-0.510585
20	6	0	4.727344	-2.196590	0.175322
21	6	0	4.492689	-0.711338	-1.705480
22	1	0	2.494951	-0.116964	-2.200296
23	1	0	6.388439	-1.444512	-0.978087
24	1	0	2.899353	-2.799986	1.130751
25	1	0	5.350931	-2.781097	0.846975
26	1	0	4.934454	-0.119554	-2.503129
27	1	0	-3.871130	-1.927562	-1.250376
28	1	0	-5.085257	1.194823	2.400385
29	1	0	-6.245177	-1.349770	-0.865095
30	1	0	-2.716676	0.622107	2.004310
31	1	0	-6.866500	0.214089	0.967123
32	1	0	-1.097614	-3.797360	-1.690769
33	1	0	0.503973	-4.090206	-1.019792
34	1	0	-0.407090	-4.106205	1.122524
35	1	0	-2.006330	-3.802305	0.448850
36	6	0	1.253228	1.567281	1.238988
37	6	0	2.647342	1.545866	1.108467

38	6	0	0.716001	1.730572	2.531440
39	6	0	3.475234	1.631204	2.230484
40	1	0	3.106015	1.440787	0.129190
41	6	0	1.539262	1.791926	3.653446
42	1	0	-0.361508	1.819223	2.663256
43	6	0	2.928553	1.743317	3.508587
44	1	0	4.555120	1.603820	2.101419
45	1	0	1.096508	1.896336	4.641589
46	1	0	3.574949	1.808018	4.380060
47	6	0	0.261824	2.716247	-0.133099
48	6	0	-1.069747	2.272014	-0.473577
49	1	0	0.284106	3.443188	0.672376
50	1	0	-1.866677	2.459497	0.246778
51	6	0	-1.523955	2.188022	-1.860011
52	8	0	-2.706678	1.975432	-2.154082
53	6	0	-0.500180	2.450916	-2.947831
54	1	0	0.007706	1.507133	-3.186804
55	1	0	-1.041257	2.761668	-3.846051
56	6	0	0.526637	3.490069	-2.508055
57	1	0	1.253012	3.669230	-3.307836
58	1	0	0.022989	4.445051	-2.313321
59	6	0	1.250415	3.014494	-1.252772
60	1	0	1.825006	2.120654	-1.512451
61	1	0	1.974597	3.759047	-0.908257
62	6	0	0.533892	-1.986900	-2.812559
63	1	0	0.727360	-0.973371	-3.173956
64	1	0	1.446232	-2.577290	-2.938066
65	1	0	-0.239350	-2.422174	-3.454359
66	6	0	-1.443404	-2.029085	2.505698
67	1	0	-1.365392	-1.042740	2.972288
68	1	0	-2.485871	-2.355413	2.566073
69	1	0	-0.837465	-2.725247	3.095352
70	1	0	1.077499	-1.368984	1.861572
71	1	0	-1.684052	-0.689706	-2.027785

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SCF Done:  E(RPBE1PBE) =  -6077.60928987     A.U. after    1 cycles
             Convg  =    0.8812D-08             -V/T =  2.0049
Zero-point correction=                           0.599584 (Hartree/Particle)
 Thermal correction to Energy=                    0.631196
 Thermal correction to Enthalpy=                  0.632140
 Thermal correction to Gibbs Free Energy=         0.538037
 Sum of electronic and zero-point Energies=          -6077.009706
 Sum of electronic and thermal Energies=             -6076.978094
 Sum of electronic and thermal Enthalpies=           -6076.977150
 Sum of electronic and thermal Free Energies=        -6077.071252
                    1                      2                      3
Frequencies --  -293.5190               31.3701                38.5936
```
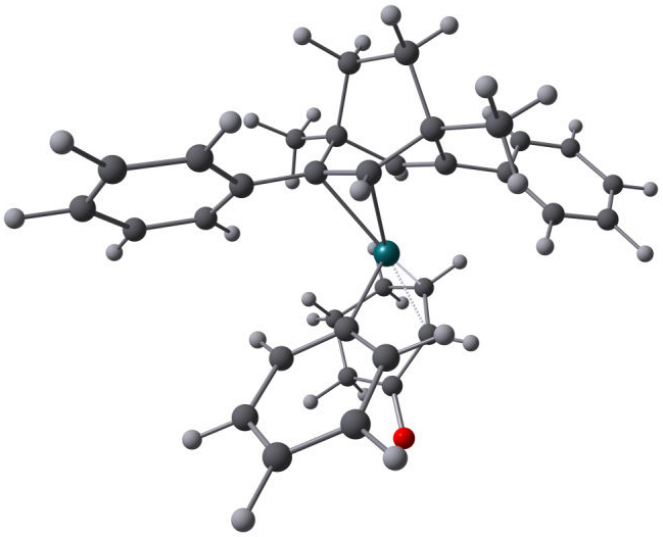

(*S*)- 1,4-Me$_2$BOD -Rh(I)-Ph-CH-re-confU-syn (107a)



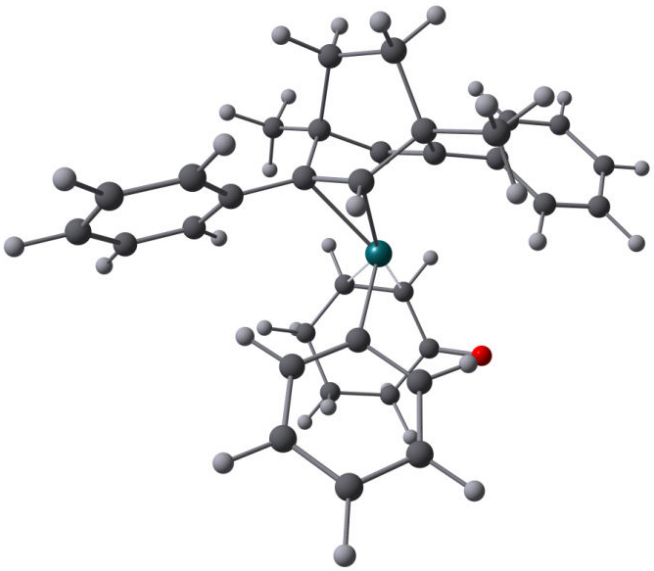
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.167064	0.364010	0.037535
2	6	0	1.958321	-1.069983	-0.140861
3	6	0	0.200969	-2.249186	1.125491
4	6	0	-2.982893	-1.373819	1.331109
5	6	0	3.315634	-0.487756	-0.285603
6	6	0	4.364378	-0.978950	0.504845
7	6	0	1.357764	-1.268650	1.087256
8	6	0	1.276292	-1.878718	-1.253136
9	6	0	4.878124	1.065808	-1.311082
10	6	0	-5.043108	-2.238698	0.408022
11	6	0	0.711358	-3.594275	0.536463
12	6	0	-0.170818	-1.442782	-1.131698
13	6	0	5.652733	-0.457644	0.388742
14	6	0	-0.789521	-1.669982	0.098745
15	6	0	-2.960786	-2.510413	-0.787661
16	6	0	3.593843	0.541588	-1.197513
17	6	0	1.353866	-3.375537	-0.839421
18	6	0	5.914342	0.566410	-0.519862
19	6	0	-2.257839	-1.836374	0.222799
20	6	0	-4.338199	-2.706379	-0.699830
21	6	0	-4.356934	-1.571752	1.424095
22	1	0	-2.471881	-0.830945	2.119610
23	1	0	-6.116455	-2.392705	0.480634
24	1	0	-2.419547	-2.898858	-1.646237
25	1	0	-4.858676	-3.232716	-1.495807
26	1	0	-4.896277	-1.195614	2.289647
27	1	0	4.168135	-1.782356	1.210279
28	1	0	5.070202	1.871078	-2.015314
29	1	0	6.452179	-0.854279	1.009096
30	1	0	2.789961	0.952218	-1.802311
31	1	0	6.917140	0.975232	-0.610213
32	1	0	1.431852	-4.019338	1.243682
33	1	0	-0.131099	-4.292493	0.477298
34	1	0	0.844334	-3.963671	-1.610337
35	1	0	2.404715	-3.685816	-0.842384
36	1	0	-0.755030	-1.262401	-2.031622

37	1	0	1.835680	-0.963922	2.015119
38	6	0	-1.413898	1.271207	-0.941077
39	6	0	-2.680185	1.506510	-0.386143
40	6	0	-1.245620	1.596048	-2.299177
41	6	0	-3.729816	2.035133	-1.144042
42	1	0	-2.870119	1.275989	0.659742
43	6	0	-2.289684	2.119510	-3.066248
44	1	0	-0.279511	1.441110	-2.778754
45	6	0	-3.542298	2.343958	-2.491190
46	1	0	-4.698331	2.205300	-0.676708
47	1	0	-2.122419	2.355431	-4.115795
48	1	0	-4.356766	2.754709	-3.083226
49	6	0	1.346483	1.760619	1.349359
50	1	0	2.372645	1.437621	1.185744
51	6	0	0.738226	2.539052	0.371144
52	1	0	1.252661	2.748295	-0.565752
53	6	0	-0.339173	3.482313	0.714954
54	8	0	-0.662891	4.389520	-0.050849
55	6	0	0.851754	1.770770	2.771062
56	1	0	1.439194	2.524667	3.317731
57	6	0	-0.941437	3.393889	2.100211
58	6	0	-0.631129	2.107417	2.853414
59	1	0	1.062721	0.814449	3.259287
60	1	0	-1.206988	1.278580	2.425645
61	1	0	-0.941072	2.203779	3.898982
62	1	0	-2.017146	3.574045	2.015664
63	1	0	-0.530158	4.252383	2.649601
64	6	0	-0.310407	-2.443274	2.543788
65	1	0	-0.579039	-1.491729	3.012041
66	1	0	-1.181772	-3.103079	2.575996
67	1	0	0.478717	-2.898805	3.151287
68	6	0	1.818008	-1.677248	-2.658657
69	1	0	1.684790	-0.648489	-3.004256
70	1	0	2.881929	-1.925290	-2.717793
71	1	0	1.280588	-2.331880	-3.352661

SCF Done: E(RPBE1PBE) = -6077.62591751 A.U. after 1 cycles
Convg = 0.5135D-08 -V/T = 2.0049
Zero-point correction= 0.599558 (Hartree/Particle)
Thermal correction to Energy= 0.632084
Thermal correction to Enthalpy= 0.633028
Thermal correction to Gibbs Free Energy= 0.536306
Sum of electronic and zero-point Energies= -6077.026359
Sum of electronic and thermal Energies= -6076.993834
Sum of electronic and thermal Enthalpies= -6076.992889
Sum of electronic and thermal Free Energies= -6077.089611

	1	2	3
Frequencies --	24.9877	35.7301	38.1523

(*S*)-1,4-Me$_2$BOD-Rh(I)-Ph-CH-re-confU-close (108a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.125147	0.276924	-0.067614
2	6	0	-1.759757	-1.429477	0.113681
3	6	0	0.182284	-2.434914	-1.001688
4	6	0	3.224744	-1.146421	-1.245219
5	6	0	-3.168288	-0.971001	0.178594
6	6	0	-4.139994	-1.630037	-0.588572
7	6	0	-1.112104	-1.652616	-1.070377
8	6	0	-0.987433	-2.001655	1.317330
9	6	0	-4.900136	0.520091	1.004274
10	6	0	5.356437	-1.742661	-0.272912
11	6	0	-0.135766	-3.780358	-0.281904
12	6	0	0.402468	-1.394335	1.185317
13	6	0	-5.472904	-1.222477	-0.559252
14	6	0	1.062545	-1.633333	-0.026056
15	6	0	3.301436	-2.209460	0.910819
16	6	0	-3.570653	0.108654	0.978055
17	6	0	-0.847339	-3.528380	1.052628
18	6	0	-5.858149	-0.145864	0.238346
19	6	0	2.541713	-1.651079	-0.128086
20	6	0	4.693566	-2.252818	0.841851
21	6	0	4.613697	-1.188786	-1.317415
22	1	0	2.662646	-0.686984	-2.051875
23	1	0	6.441270	-1.774391	-0.328483
24	1	0	2.795289	-2.622696	1.779237
25	1	0	5.259322	-2.690132	1.660501
26	1	0	5.119376	-0.779970	-2.188394
27	1	0	-3.846410	-2.475530	-1.205471
28	1	0	-5.188331	1.367701	1.620449
29	1	0	-6.210604	-1.749190	-1.158977
30	1	0	-2.832238	0.649262	1.563646
31	1	0	-6.896300	0.174519	0.261556
32	1	0	-0.757240	-4.383964	-0.951927
33	1	0	0.803445	-4.325862	-0.137186
34	1	0	-0.287346	-3.963469	1.887542

35	1	0	-1.845649	-3.980271	1.063962
36	1	0	0.952465	-1.119989	2.083502
37	1	0	-1.578246	-1.443144	-2.031600
38	6	0	1.087218	1.550399	0.914981
39	6	0	2.487864	1.576065	0.983598
40	6	0	0.385099	2.436020	1.754239
41	6	0	3.158639	2.449238	1.845386
42	1	0	3.077078	0.919749	0.347310
43	6	0	1.049658	3.301486	2.627223
44	1	0	-0.704779	2.468483	1.724039
45	6	0	2.444955	3.315549	2.674813
46	1	0	4.247025	2.451702	1.866989
47	1	0	0.475358	3.973177	3.262653
48	1	0	2.967082	3.994488	3.344628
49	6	0	0.073283	1.214184	-2.100444
50	1	0	0.024042	0.314407	-2.711993
51	6	0	-1.110609	1.674580	-1.511070
52	1	0	-2.044968	1.127533	-1.629846
53	6	0	-1.286942	3.092876	-1.155694
54	8	0	-2.309448	3.496872	-0.598821
55	6	0	1.209108	2.139521	-2.441448
56	6	0	-0.231094	4.062180	-1.633009
57	6	0	0.754372	-2.704984	-2.384729
58	1	0	0.927142	-1.785756	-2.951245
59	1	0	1.698704	-3.253560	-2.329551
60	1	0	0.045226	-3.313987	-2.955084
61	6	0	-1.597374	-1.746621	2.686728
62	1	0	-1.612041	-0.682895	2.939101
63	1	0	-2.621212	-2.127800	2.746181
64	1	0	-1.002197	-2.258427	3.450024
65	6	0	1.174777	3.480122	-1.716270
66	1	0	2.171042	1.643400	-2.274274
67	1	0	1.146117	2.303325	-3.528844
68	1	0	1.570896	3.356820	-0.706856
69	1	0	1.832610	4.188761	-2.230913
70	1	0	-0.264641	4.956067	-1.003897
71	1	0	-0.568685	4.369929	-2.634018

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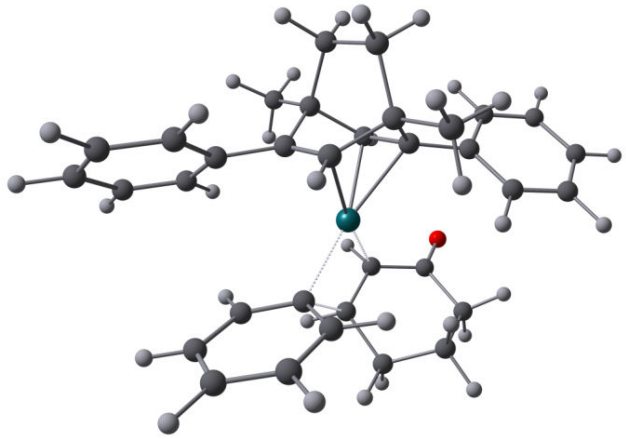
SCF Done:  E(RPBE1PBE) =  -6077.62567624     A.U. after    1 cycles
             Convg  =    0.3813D-08             -V/T =  2.0049
Zero-point correction=                           0.599545 (Hartree/Particle)
 Thermal correction to Energy=                    0.632148
 Thermal correction to Enthalpy=                  0.633092
 Thermal correction to Gibbs Free Energy=         0.536058
 Sum of electronic and zero-point Energies=          -6077.026132
 Sum of electronic and thermal Energies=             -6076.993528
 Sum of electronic and thermal Enthalpies=           -6076.992584
 Sum of electronic and thermal Free Energies=        -6077.089618
                     1                      2                      3
Frequencies --    32.4184                34.4968                36.3337
```

(*S*)-1,4-Me$_2$BOD-Rh(I)-Ph-CH-re-confU-CR-TS (111a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.037246	0.298265	-0.334033
2	6	0	-1.417744	-1.338120	0.262659
3	6	0	0.523638	-2.393459	-0.843557
4	6	0	3.396506	-0.863440	-1.431496
5	6	0	-2.883585	-1.131353	0.369999
6	6	0	-3.748281	-2.001724	-0.310048
7	6	0	-0.796245	-1.651383	-0.945153
8	6	0	-0.567831	-1.765841	1.473012
9	6	0	-4.832401	0.008873	1.272125
10	6	0	5.635478	-1.064839	-0.541402
11	6	0	0.293264	-3.664228	0.022714
12	6	0	0.761937	-1.092966	1.193107
13	6	0	-5.132085	-1.868736	-0.205766
14	6	0	1.382653	-1.430130	-0.003259
15	6	0	3.721590	-1.584460	0.839345
16	6	0	-3.451131	-0.126904	1.165999
17	6	0	-0.361559	-3.301389	1.361460
18	6	0	-5.680825	-0.861714	0.586695
19	6	0	2.843058	-1.275878	-0.210233
20	6	0	5.102253	-1.474962	0.679570
21	6	0	4.774403	-0.760799	-1.597029
22	1	0	2.741197	-0.592961	-2.253297
23	1	0	6.711536	-0.982964	-0.670300
24	1	0	3.317297	-1.925731	1.788799
25	1	0	5.761387	-1.719709	1.508638
26	1	0	5.177929	-0.431273	-2.551136
27	1	0	-3.329713	-2.797428	-0.921090
28	1	0	-5.248691	0.801712	1.888602
29	1	0	-5.781320	-2.555567	-0.742829
30	1	0	-2.805493	0.569881	1.691883
31	1	0	-6.759175	-0.755463	0.670356
32	1	0	-0.338029	-4.352713	-0.549748
33	1	0	1.257030	-4.163939	0.173068
34	1	0	0.260505	-3.622013	2.204407
35	1	0	-1.333840	-3.794439	1.475341
36	1	0	1.302667	-0.601883	1.999877
37	1	0	-1.347384	-1.654322	-1.883928
38	6	0	1.278310	1.924516	0.204649
39	6	0	2.558115	2.097720	-0.345370

40	6	0	1.104796	2.283453	1.555619
41	6	0	3.625224	2.567801	0.418631
42	1	0	2.728739	1.872407	-1.395893
43	6	0	2.169997	2.747142	2.326695
44	1	0	0.128902	2.188096	2.025556
45	6	0	3.439171	2.892244	1.762851
46	1	0	4.604165	2.684970	-0.040797
47	1	0	2.004722	3.000479	3.371676
48	1	0	4.267822	3.264573	2.359798
49	6	0	-0.086960	2.548260	-1.152393
50	1	0	0.729371	2.794253	-1.825770
51	6	0	-1.028067	1.601564	-1.707930
52	1	0	-0.734839	1.086589	-2.626293
53	6	0	-2.471896	1.780769	-1.594427
54	8	0	-3.260474	1.142449	-2.303051
55	6	0	-0.678448	3.758062	-0.454704
56	6	0	-2.997932	2.851193	-0.662851
57	6	0	-1.107213	-1.397288	2.845713
58	1	0	-1.171821	-0.314097	2.982426
59	1	0	-2.098335	-1.826248	3.019700
60	1	0	-0.432532	-1.787151	3.615353
61	6	0	1.056670	-2.778439	-2.214568
62	1	0	1.114356	-1.919123	-2.888392
63	1	0	2.048444	-3.235173	-2.151087
64	1	0	0.379439	-3.508288	-2.670744
65	6	0	-1.958055	3.416391	0.294240
66	1	0	0.055153	4.236373	0.197716
67	1	0	-0.914182	4.481211	-1.249645
68	1	0	-1.742009	2.684586	1.081152
69	1	0	-2.353102	4.307606	0.792742
70	1	0	-3.367834	3.651308	-1.319128
71	1	0	-3.873339	2.455311	-0.140497

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 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6077.60646880     A.U. after    1 cycles
             Convg  =    0.4388D-08             -V/T =  2.0048
Zero-point correction=                           0.600019 (Hartree/Particle)
 Thermal correction to Energy=                   0.631439
 Thermal correction to Enthalpy=                 0.632384
 Thermal correction to Gibbs Free Energy=        0.537821
 Sum of electronic and zero-point Energies=          -6077.006450
 Sum of electronic and thermal Energies=             -6076.975029
 Sum of electronic and thermal Enthalpies=           -6076.974085
 Sum of electronic and thermal Free Energies=        -6077.068648
                    1                    2                    3
Frequencies --  -297.6853                7.0273              33.5901
```
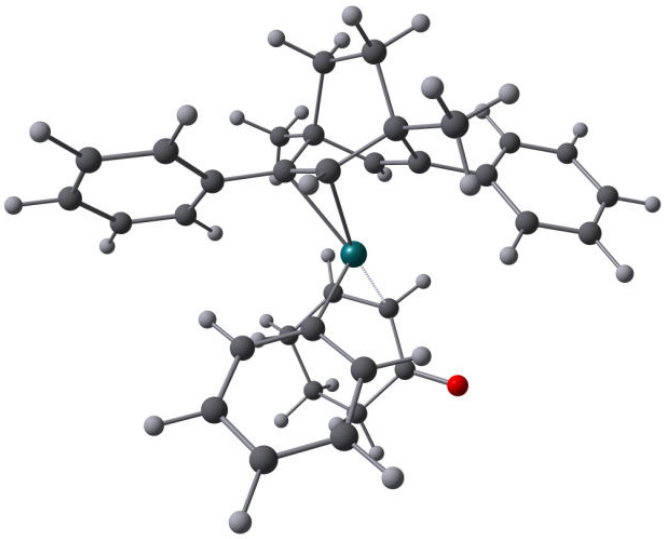

(*S*)-1,4-Me$_2$BOD-Rh(I)-Ph-CH-re-confD-close (108b)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.124450	0.270516	-0.056498
2	6	0	-1.829979	-1.365365	0.087567
3	6	0	0.088284	-2.438759	-1.005594
4	6	0	3.165800	-1.219560	-1.205992
5	6	0	-3.218696	-0.846375	0.138441
6	6	0	-4.215451	-1.487112	-0.611543
7	6	0	-1.176056	-1.608102	-1.088522
8	6	0	-1.099495	-1.976447	1.298677
9	6	0	-4.890212	0.734391	0.920262
10	6	0	5.274440	-1.886738	-0.228952
11	6	0	-0.288898	-3.775249	-0.298064
12	6	0	0.314831	-1.422614	1.193035
13	6	0	-5.531388	-1.026901	-0.594829
14	6	0	0.982537	-1.673140	-0.012858
15	6	0	3.199661	-2.317154	0.934122
16	6	0	-3.577645	0.270735	0.906915
17	6	0	-1.016514	-3.505395	1.024241
18	6	0	-5.873871	0.085461	0.172499
19	6	0	2.462150	-1.725319	-0.102031
20	6	0	4.590728	-2.395327	0.873938
21	6	0	4.553742	-1.297606	-1.269485
22	1	0	2.622567	-0.730892	-2.008637
23	1	0	6.358424	-1.946410	-0.278050
24	1	0	2.676633	-2.730552	1.792477
25	1	0	5.139256	-2.859165	1.689717
26	1	0	5.075876	-0.888372	-2.130560
27	1	0	-3.954876	-2.359302	-1.205665
28	1	0	-5.144864	1.608918	1.513149
29	1	0	-6.289184	-1.540141	-1.181024
30	1	0	-2.821201	0.799665	1.480423
31	1	0	-6.898660	0.446753	0.186241
32	1	0	-0.917361	-4.355376	-0.982155
33	1	0	0.628815	-4.352303	-0.138701
34	1	0	-0.492101	-3.970160	1.866169
35	1	0	-2.032581	-3.915570	1.010744
36	1	0	0.861086	-1.173567	2.100859

37	1	0	-1.620722	-1.375235	-2.054491
38	6	0	1.131881	1.486435	0.948361
39	6	0	2.529399	1.578557	0.909819
40	6	0	0.464039	2.271382	1.908330
41	6	0	3.229704	2.430025	1.771556
42	1	0	3.097715	0.978623	0.201825
43	6	0	1.156645	3.117083	2.777545
44	1	0	-0.624522	2.242158	1.977590
45	6	0	2.549005	3.204965	2.710282
46	1	0	4.315181	2.482443	1.708647
47	1	0	0.606492	3.713342	3.503068
48	1	0	3.093071	3.866844	3.379650
49	6	0	0.140784	1.192931	-2.088427
50	1	0	0.002067	0.309461	-2.707994
51	6	0	-0.997296	1.749004	-1.488103
52	1	0	-1.981988	1.306585	-1.632307
53	6	0	-1.010109	3.145675	-1.024818
54	8	0	-2.015020	3.645825	-0.514225
55	6	0	1.364544	2.024334	-2.397370
56	1	0	1.787643	1.685065	-3.349169
57	1	0	2.140678	1.869199	-1.642509
58	6	0	0.245544	3.961093	-1.239924
59	1	0	0.867171	3.848370	-0.342502
60	1	0	-0.047699	5.013338	-1.300589
61	6	0	1.022401	3.511253	-2.473340
62	1	0	1.937851	4.103057	-2.576533
63	1	0	0.419189	3.698668	-3.370366
64	6	0	0.671177	-2.721579	-2.381505
65	1	0	0.885666	-1.806058	-2.939520
66	1	0	1.594334	-3.303982	-2.315230
67	1	0	-0.050449	-3.301430	-2.966469
68	6	0	-1.724868	-1.703946	2.657423
69	1	0	-1.715339	-0.639701	2.908763
70	1	0	-2.760133	-2.055905	2.697855
71	1	0	-1.158544	-2.232004	3.431564

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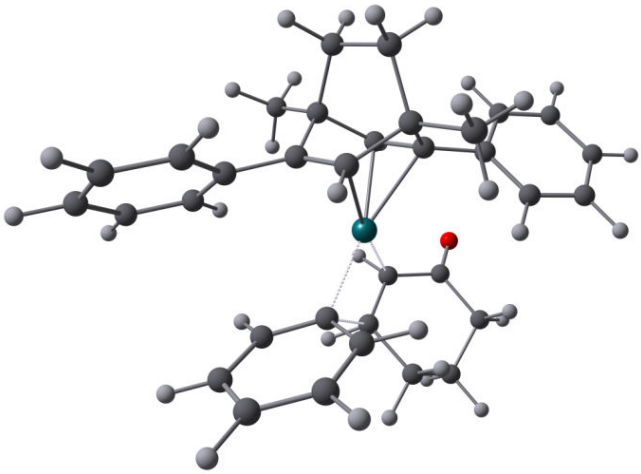
SCF Done:  E(RPBE1PBE) =  -6077.62678712     A.U. after    1 cycles
             Convg  =    0.2188D-08             -V/T =  2.0049
Zero-point correction=                           0.599991 (Hartree/Particle)
 Thermal correction to Energy=                    0.632415
 Thermal correction to Enthalpy=                  0.633360
 Thermal correction to Gibbs Free Energy=         0.537174
 Sum of electronic and zero-point Energies=          -6077.026796
 Sum of electronic and thermal Energies=             -6076.994372
 Sum of electronic and thermal Enthalpies=           -6076.993428
 Sum of electronic and thermal Free Energies=        -6077.089614
                    1                      2                      3
Frequencies --    31.2685               34.2757               36.5220
```

(*S*)-1,4-Me$_2$BOD-Rh(I)-Ph-CH-re-confD-CR-TS (111b)



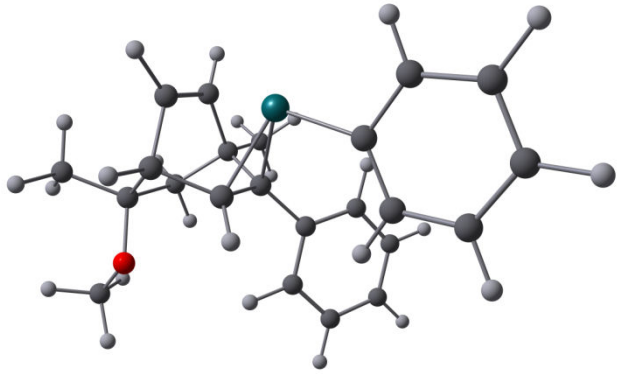
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.038183	0.271320	-0.290167
2	6	0	-1.350731	-1.428331	0.248170
3	6	0	0.598703	-2.370154	-0.940189
4	6	0	3.385057	-0.668186	-1.501627
5	6	0	-2.814769	-1.239957	0.401440
6	6	0	-3.691573	-2.127333	-0.238243
7	6	0	-0.747324	-1.669228	-0.985174
8	6	0	-0.470339	-1.894801	1.421606
9	6	0	-4.740400	-0.103665	1.353730
10	6	0	5.655571	-0.834244	-0.687606
11	6	0	0.428084	-3.688384	-0.135725
12	6	0	0.832168	-1.165551	1.156573
13	6	0	-5.072482	-2.005764	-0.087253
14	6	0	1.439331	-1.419079	-0.067247
15	6	0	3.806588	-1.534752	0.702050
16	6	0	-3.362393	-0.229201	1.203137
17	6	0	-0.220714	-3.415503	1.227718
18	6	0	-5.602819	-0.992889	0.710225
19	6	0	2.886217	-1.191838	-0.299479
20	6	0	5.176398	-1.353845	0.513962
21	6	0	4.751871	-0.493202	-1.695365
22	1	0	2.693871	-0.367864	-2.283019
23	1	0	6.722946	-0.695787	-0.838501
24	1	0	3.444287	-1.958471	1.635161
25	1	0	5.869513	-1.627063	1.305548
26	1	0	5.113037	-0.078120	-2.632947
27	1	0	-3.284846	-2.923856	-0.856403
28	1	0	-5.143893	0.694984	1.971184
29	1	0	-5.733657	-2.704748	-0.593155
30	1	0	-2.701023	0.479744	1.694013
31	1	0	-6.678682	-0.895061	0.828941
32	1	0	-0.185048	-4.372183	-0.733002
33	1	0	1.411819	-4.157975	-0.021900
34	1	0	0.420543	-3.761416	2.045974
35	1	0	-1.176801	-3.942456	1.326009
36	1	0	1.370205	-0.694527	1.976784
37	1	0	-1.315688	-1.643554	-1.913096
38	6	0	1.213978	1.914978	0.360794

39	6	0	2.473652	2.202675	-0.184898
40	6	0	1.033239	2.159440	1.734104
41	6	0	3.520554	2.674386	0.606194
42	1	0	2.642924	2.065868	-1.250829
43	6	0	2.079114	2.619695	2.533415
44	1	0	0.067660	1.968904	2.199439
45	6	0	3.331346	2.881121	1.973255
46	1	0	4.485746	2.884445	0.150621
47	1	0	1.912186	2.779652	3.596434
48	1	0	4.143837	3.254153	2.591610
49	6	0	-0.227062	2.547871	-0.930872
50	1	0	0.568445	2.901422	-1.580895
51	6	0	-1.109020	1.600541	-1.571526
52	1	0	-0.757883	1.160855	-2.509814
53	6	0	-2.565592	1.749071	-1.555238
54	8	0	-3.294969	1.044760	-2.260930
55	6	0	-0.869232	3.641362	-0.087250
56	1	0	-0.173209	4.479382	0.011838
57	1	0	-1.072975	3.282976	0.924396
58	6	0	-3.148757	2.885998	-0.741450
59	1	0	-3.335500	2.524110	0.277874
60	1	0	-4.120382	3.140778	-1.173996
61	6	0	-2.199129	4.079566	-0.692347
62	1	0	-2.632012	4.883444	-0.087428
63	1	0	-2.049718	4.482065	-1.701927
64	6	0	-1.004425	-1.609134	2.815639
65	1	0	-1.108145	-0.536036	2.999899
66	1	0	-1.977379	-2.081484	2.979934
67	1	0	-0.306664	-2.007119	3.560075
68	6	0	1.122965	-2.664045	-2.336719
69	1	0	1.141383	-1.768055	-2.963370
70	1	0	2.130718	-3.088706	-2.310905
71	1	0	0.463909	-3.391508	-2.822407

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6077.60224167     A.U. after    1 cycles
             Convg  =    0.1751D-08             -V/T =  2.0048
Zero-point correction=                           0.599720 (Hartree/Particle)
 Thermal correction to Energy=                    0.631290
 Thermal correction to Enthalpy=                  0.632234
 Thermal correction to Gibbs Free Energy=         0.537601
 Sum of electronic and zero-point Energies=          -6077.002522
 Sum of electronic and thermal Energies=             -6076.970951
 Sum of electronic and thermal Enthalpies=           -6076.970007
 Sum of electronic and thermal Free Energies=        -6077.064640
                    1                      2                      3
Frequencies --  -291.8833               16.8502                30.8823
```

Darses ligand ((1S,4R,8R)-8-methoxy-1,8-dimethyl-2-phenylbicyclo[2.2.2]octa-2,5-diene)-Rh pathway

Darses Ligand-prox-Rh(I)-Ph (114)



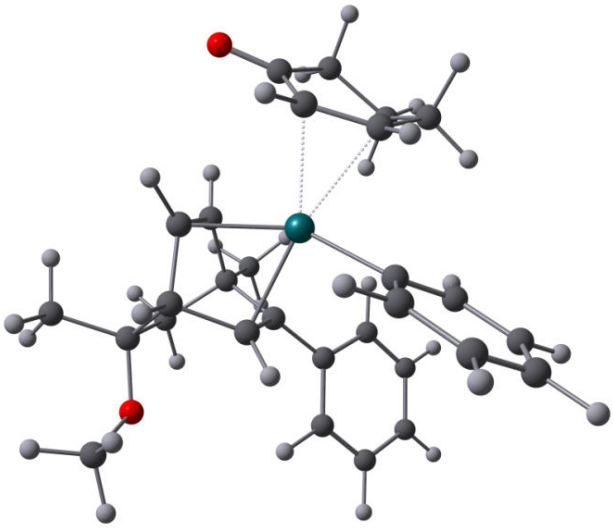
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.650214	-1.437573	0.388299
2	6	0	-1.486489	-2.262227	0.299303
3	6	0	-1.579817	-0.076165	1.360677
4	6	0	1.015053	2.122469	1.290596
5	6	0	-1.364079	-1.576398	1.478570
6	6	0	-1.796492	-1.374395	-0.888177
7	6	0	1.038316	4.347719	0.342012
8	6	0	-2.962870	0.169132	0.703462
9	6	0	-0.627322	-0.407631	-0.880202
10	6	0	-0.496389	0.327734	0.333240
11	6	0	-0.394453	2.639124	-0.591033
12	6	0	-3.108529	-0.583819	-0.641777
13	6	0	0.063464	1.705456	0.350075
14	6	0	0.089335	3.948076	-0.597462
15	6	0	1.498740	3.427864	1.287233
16	1	0	1.399578	1.405235	2.010757
17	1	0	1.419989	5.365439	0.337104
18	1	0	-1.139472	2.330313	-1.320966
19	1	0	-0.275549	4.654818	-1.338813
20	1	0	2.245621	3.727953	2.018090
21	1	0	-3.742255	-0.138032	1.409913
22	1	0	-3.082501	1.245924	0.541006
23	1	0	-0.233199	-0.020118	-1.816744
24	1	0	-1.289303	-2.059778	2.450512
25	6	0	2.442704	-0.832981	-0.316333
26	6	0	2.789444	0.245287	-1.149197
27	6	0	3.483940	-1.702955	0.060272
28	6	0	4.102233	0.442659	-1.583612
29	1	0	2.026049	0.955789	-1.463033
30	6	0	4.802887	-1.513591	-0.364224
31	1	0	3.270075	-2.560918	0.703988
32	6	0	5.116926	-0.434792	-1.192012
33	1	0	4.337863	1.286415	-2.229906
34	1	0	5.582447	-2.205245	-0.050191
35	1	0	6.139348	-0.278511	-1.527768
36	6	0	-1.486946	0.619778	2.708413
37	1	0	-1.606752	1.702662	2.610185
38	1	0	-2.276590	0.250803	3.371956

39	1	0	-0.524427	0.426164	3.192239
40	1	0	-1.866251	-1.933423	-1.823747
41	1	0	-1.511679	-3.347026	0.234401
42	6	0	-4.303316	-1.531420	-0.641380
43	1	0	-5.235393	-1.013450	-0.395680
44	1	0	-4.416565	-2.011178	-1.619287
45	1	0	-4.156730	-2.311075	0.111945
46	8	0	-3.160708	0.326947	-1.749908
47	6	0	-4.347651	1.084109	-1.881108
48	1	0	-4.153749	1.835366	-2.649959
49	1	0	-5.196605	0.468101	-2.202097
50	1	0	-4.620049	1.600782	-0.952116

SCF Done: E(RPBE1PBE) = -5652.88671950 A.U. after 1 cycles
Convg = 0.3677D-08 -V/T = 2.0041
Zero-point correction= 0.420478 (Hartree/Particle)
Thermal correction to Energy= 0.443460
Thermal correction to Enthalpy= 0.444404
Thermal correction to Gibbs Free Energy= 0.367828
Sum of electronic and zero-point Energies= -5652.466242
Sum of electronic and thermal Energies= -5652.443260
Sum of electronic and thermal Enthalpies= -5652.442316
Sum of electronic and thermal Free Energies= -5652.518891

	1	2	3
Frequencies --	20.0555	34.3533	41.3668

(*S*)-DA-prox-Rh(I)-Ph-CH-si-confU-far (117a)



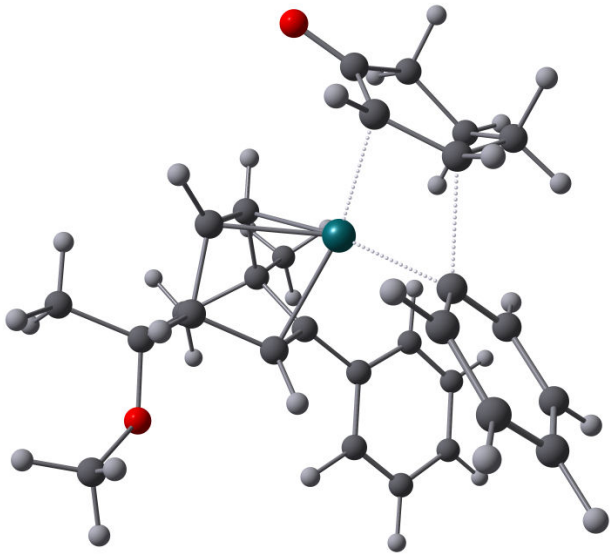
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.729190	-0.574744	-0.440265
2	6	0	-0.819305	-2.192038	-0.646047
3	6	0	-1.472264	-0.955868	1.346368
4	6	0	-0.233712	1.996285	2.229733
5	6	0	-0.617764	-2.033294	0.704036
6	6	0	-1.833021	-1.224189	-1.219953
7	6	0	-1.181470	4.218075	2.334703
8	6	0	-2.955953	-1.267657	1.011516
9	6	0	-1.277850	0.128169	-0.825730
10	6	0	-1.091471	0.308082	0.547344

11	6	0	-1.988359	2.623538	0.707868
12	6	0	-3.206456	-1.404443	-0.502636
13	6	0	-1.083916	1.654426	1.168041
14	6	0	-2.034571	3.893489	1.281151
15	6	0	-0.280638	3.261844	2.806643
16	1	0	0.492277	1.274129	2.590794
17	1	0	-1.217618	5.206436	2.785243
18	1	0	-2.672872	2.370984	-0.097646
19	1	0	-2.744685	4.627132	0.908083
20	1	0	0.394975	3.505978	3.622456
21	1	0	-3.237557	-2.189191	1.531596
22	1	0	-3.591555	-0.464963	1.398747
23	1	0	-1.327426	0.970369	-1.509511
24	1	0	-0.079841	-2.753607	1.313421
25	6	0	1.433755	1.238022	-1.161191
26	6	0	1.871284	2.323956	-0.389350
27	6	0	1.368176	1.434274	-2.553791
28	6	0	2.216433	3.548443	-0.971752
29	1	0	1.944234	2.232134	0.692139
30	6	0	1.707112	2.654596	-3.143200
31	1	0	1.046673	0.618732	-3.201288
32	6	0	2.134668	3.723525	-2.352822
33	1	0	2.550413	4.368602	-0.338522
34	1	0	1.639899	2.768675	-4.223664
35	1	0	2.402206	4.674661	-2.806879
36	6	0	3.015443	-0.828629	-0.683785
37	6	0	2.354408	-2.052244	-0.729227
38	1	0	3.282448	-0.355376	-1.623558
39	1	0	2.071267	-2.489571	-1.686433
40	6	0	2.399858	-2.990488	0.404749
41	8	0	1.942896	-4.130765	0.309362
42	6	0	3.114658	-2.540075	1.659334
43	1	0	2.624322	-3.001869	2.521251
44	6	0	3.781926	-0.395287	0.532636
45	1	0	4.830592	-0.694905	0.382426
46	6	0	-1.272120	-0.902856	2.852282
47	1	0	-0.217296	-0.791474	3.119061
48	1	0	-1.832591	-0.081812	3.307702
49	1	0	-1.625299	-1.839543	3.296446
50	1	0	-1.920328	-1.334409	-2.301962
51	1	0	-0.445246	-3.042100	-1.209221
52	6	0	-3.828547	-2.752759	-0.852283
53	1	0	-4.810469	-2.851827	-0.378181
54	1	0	-3.946910	-2.885255	-1.931797
55	1	0	-3.191979	-3.563490	-0.487028
56	8	0	-4.079027	-0.315848	-0.834432
57	6	0	-4.503456	-0.216807	-2.181501
58	1	0	-5.130714	-1.063908	-2.482764
59	1	0	-5.100578	0.695130	-2.245363
60	1	0	-3.664439	-0.128520	-2.882091
61	6	0	3.236936	-1.027812	1.805564
62	1	0	4.117018	-2.987852	1.598341
63	1	0	2.249164	-0.599418	2.016722
64	1	0	3.880531	-0.787457	2.657874
65	1	0	3.784161	0.696280	0.603905

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5961.24536310     A.U. after    1 cycles
             Convg  =    0.3040D-08             -V/T =  2.0046
Zero-point correction=                           0.551806 (Hartree/Particle)
 Thermal correction to Energy=                    0.581879
 Thermal correction to Enthalpy=                  0.582823
 Thermal correction to Gibbs Free Energy=         0.490951
 Sum of electronic and zero-point Energies=          -5960.693557
```

```
 Sum of electronic and thermal Energies=            -5960.663485
 Sum of electronic and thermal Enthalpies=          -5960.662540
 Sum of electronic and thermal Free Energies=       -5960.754412
                      1                      2                      3
Frequencies --    22.9944                26.4552                38.9849
```

Darses Ligand-prox-Rh(I)-Ph-CH-si-confU-CR-TS (119a)

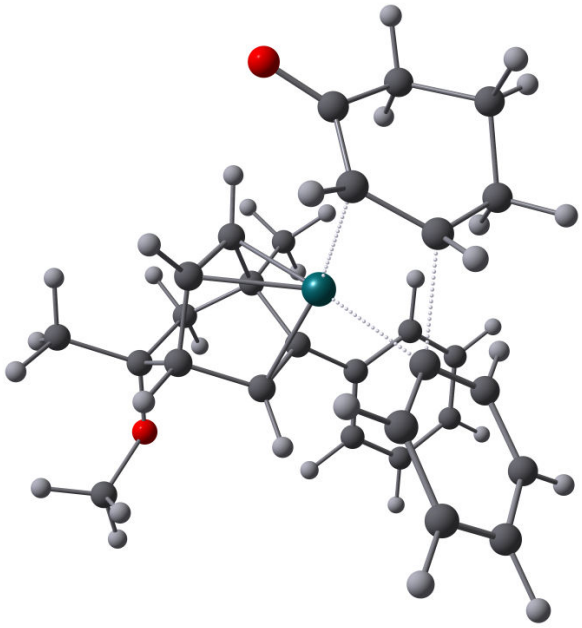


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.646870	-0.746129	0.380716
2	6	0	0.989795	-2.155465	0.560686
3	6	0	1.545201	-0.829254	-1.415799
4	6	0	0.039658	2.049873	-2.165668
5	6	0	0.749946	-1.966763	-0.792376
6	6	0	1.959615	-1.143865	1.137634
7	6	0	0.707464	4.374246	-2.148754
8	6	0	3.047596	-1.074271	-1.110917
9	6	0	1.319016	0.180971	0.780741
10	6	0	1.110674	0.390002	-0.574537
11	6	0	1.738220	2.796488	-0.636178
12	6	0	3.328399	-1.238681	0.395726
13	6	0	0.946529	1.751092	-1.137531
14	6	0	1.617659	4.094067	-1.130614
15	6	0	-0.079453	3.343688	-2.665208
16	1	0	-0.600721	1.269392	-2.564147
17	1	0	0.612311	5.384642	-2.537613
18	1	0	2.465936	2.583039	0.142126
19	1	0	2.242322	4.885322	-0.723893
20	1	0	-0.797223	3.550160	-3.455047
21	1	0	3.368150	-1.966279	-1.659505
22	1	0	3.635617	-0.229802	-1.484478
23	6	0	-1.800071	0.854687	1.230687
24	6	0	-2.061715	2.044244	0.537829
25	6	0	-1.587215	0.937357	2.620559
26	6	0	-2.073226	3.274533	1.197792
27	1	0	-2.238487	2.026154	-0.534311
28	6	0	-1.580006	2.165077	3.278864
29	1	0	-1.432319	0.026782	3.197935

30	6	0	-1.825907	3.343512	2.568838
31	1	0	-2.269991	4.183624	0.633601
32	1	0	-1.398676	2.201438	4.350832
33	1	0	-1.836044	4.301765	3.081871
34	6	0	-2.996186	-0.747336	0.782521
35	6	0	-2.317436	-2.017880	0.708894
36	1	0	-3.462551	-0.542610	1.741629
37	1	0	-2.117788	-2.554458	1.637490
38	6	0	-2.370664	-2.856799	-0.483302
39	8	0	-1.964191	-4.027837	-0.475829
40	6	0	-2.994765	-2.285560	-1.741708
41	1	0	-2.390224	-2.600374	-2.598038
42	6	0	-3.843918	-0.349486	-0.403243
43	1	0	-4.061502	0.720873	-0.389148
44	6	0	1.319257	-0.739202	-2.916219
45	1	0	0.254943	-0.690404	-3.163854
46	1	0	1.815822	0.133305	-3.350341
47	1	0	1.726988	-1.633826	-3.398688
48	1	0	1.275852	0.994393	1.499958
49	1	0	0.274234	-2.720405	-1.416309
50	1	0	0.719107	-3.064026	1.091928
51	1	0	2.071755	-1.270327	2.215831
52	6	0	4.016181	-2.566531	0.698708
53	1	0	4.996341	-2.604650	0.212239
54	1	0	4.152640	-2.725094	1.772629
55	1	0	3.414559	-3.395413	0.315536
56	8	0	4.160723	-0.122976	0.743178
57	6	0	4.595908	-0.037913	2.087279
58	1	0	5.254720	-0.869164	2.364852
59	1	0	5.162933	0.892100	2.165009
60	1	0	3.761786	0.007383	2.797924
61	6	0	-3.205734	-0.776869	-1.715394
62	1	0	-3.963246	-2.793885	-1.846685
63	1	0	-2.235766	-0.270688	-1.821277
64	1	0	-3.824539	-0.467807	-2.564233
65	1	0	-4.808991	-0.862590	-0.280712

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5961.23028340     A.U. after    1 cycles
             Convg  =    0.2138D-08             -V/T =  2.0046
Zero-point correction=                           0.550961 (Hartree/Particle)
 Thermal correction to Energy=                    0.580277
 Thermal correction to Enthalpy=                  0.581221
 Thermal correction to Gibbs Free Energy=         0.491111
 Sum of electronic and zero-point Energies=          -5960.679322
 Sum of electronic and thermal Energies=             -5960.650006
 Sum of electronic and thermal Enthalpies=           -5960.649062
 Sum of electronic and thermal Free Energies=        -5960.739172
                    1                      2                      3
Frequencies --  -296.9667               21.5657                30.6719
```

Darses Ligand-prox-Rh(I)-Ph-CH-si-confD-CR-TS (119b)

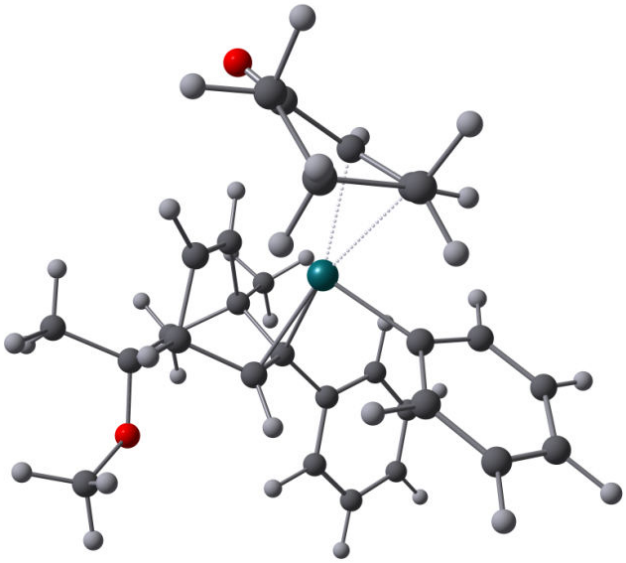


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.651632	-0.662450	0.414254
2	6	0	0.890122	-2.177376	0.614744
3	6	0	1.485398	-0.960814	-1.418142
4	6	0	0.080401	1.948556	-2.222327
5	6	0	0.634011	-2.022486	-0.739211
6	6	0	1.936944	-1.212346	1.135937
7	6	0	0.891957	4.220425	-2.382340
8	6	0	2.975769	-1.288115	-1.134227
9	6	0	1.372769	0.139182	0.746681
10	6	0	1.140562	0.309270	-0.611514
11	6	0	1.910719	2.666882	-0.836172
12	6	0	3.279004	-1.419472	0.371173
13	6	0	1.029127	1.650019	-1.232689
14	6	0	1.841822	3.939663	-1.401259
15	6	0	0.011488	3.217151	-2.790781
16	1	0	-0.630171	1.187570	-2.531410
17	1	0	0.837152	5.211372	-2.825264
18	1	0	2.665830	2.450447	-0.085124
19	1	0	2.536413	4.710807	-1.077875
20	1	0	-0.739074	3.426618	-3.548683
21	1	0	3.228331	-2.216130	-1.658065
22	1	0	3.606974	-0.495581	-1.548844
23	6	0	-1.648707	1.031687	1.278493
24	6	0	-1.790256	2.278808	0.657633
25	6	0	-1.479066	1.007013	2.677268
26	6	0	-1.714061	3.461679	1.396612
27	1	0	-1.943295	2.343057	-0.415783
28	6	0	-1.381728	2.186080	3.412589
29	1	0	-1.425680	0.052959	3.199736
30	6	0	-1.499629	3.423950	2.774208
31	1	0	-1.818647	4.417924	0.888439
32	1	0	-1.229883	2.139274	4.488747

33	1	0	-1.439785	4.345775	3.347041
34	6	0	-2.958065	-0.408313	0.647093
35	6	0	-2.453211	-1.759442	0.710780
36	1	0	-3.508707	-0.102465	1.530917
37	1	0	-2.387418	-2.235064	1.690777
38	6	0	-2.576484	-2.692357	-0.405451
39	8	0	-2.244637	-3.880859	-0.306539
40	6	0	-3.185229	-2.166344	-1.691122
41	1	0	-2.375996	-1.766401	-2.317312
42	1	0	-3.616576	-3.015796	-2.228463
43	6	0	-4.214698	-1.072666	-1.421982
44	1	0	-4.631332	-0.703965	-2.365222
45	1	0	-5.049386	-1.486547	-0.842980
46	6	0	-3.570305	0.080692	-0.659218
47	1	0	-2.807193	0.525764	-1.304733
48	1	0	-4.298018	0.869766	-0.447492
49	6	0	1.235290	-0.905295	-2.916460
50	1	0	0.172297	-0.792868	-3.147530
51	1	0	1.779038	-0.081506	-3.387759
52	1	0	1.574256	-1.839961	-3.375685
53	1	0	1.399274	0.979731	1.435289
54	1	0	0.094940	-2.763611	-1.325111
55	1	0	0.569952	-3.044707	1.185773
56	1	0	2.064656	-1.310183	2.215343
57	6	0	3.888442	-2.777999	0.705522
58	1	0	4.851476	-2.896810	0.198294
59	1	0	4.041747	-2.908827	1.780898
60	1	0	3.225026	-3.578459	0.366514
61	8	0	4.188919	-0.348941	0.661956
62	6	0	4.645996	-0.236000	1.996808
63	1	0	5.237284	-1.104551	2.309824
64	1	0	5.288557	0.646491	2.024386
65	1	0	3.826846	-0.087671	2.710713

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5961.22653876     A.U. after    1 cycles
             Convg  =    0.6145D-08             -V/T =  2.0046
Zero-point correction=                           0.551161 (Hartree/Particle)
 Thermal correction to Energy=                    0.580562
 Thermal correction to Enthalpy=                  0.581506
 Thermal correction to Gibbs Free Energy=         0.491036
 Sum of electronic and zero-point Energies=          -5960.675377
 Sum of electronic and thermal Energies=             -5960.645977
 Sum of electronic and thermal Enthalpies=           -5960.645033
 Sum of electronic and thermal Free Energies=        -5960.735503
                    1                    2                    3
Frequencies --  -298.5238               21.1358              31.9428
```

Darses Ligand-prox-Rh(I)-Ph-CH-re-confU-anti (125a)



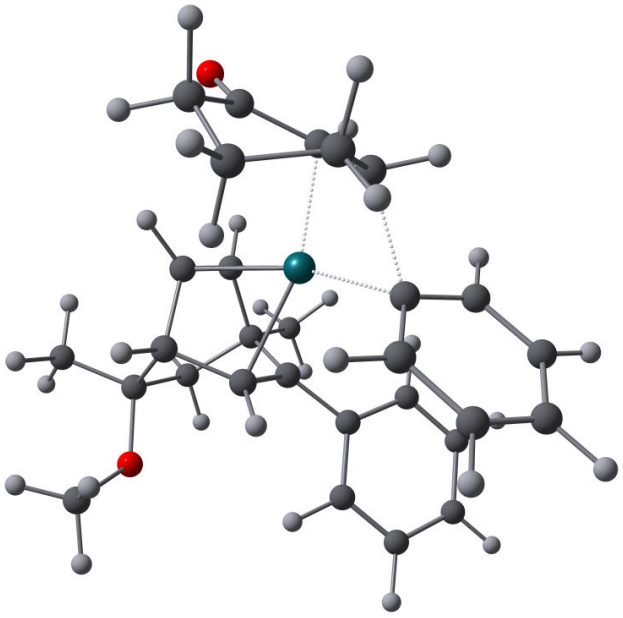
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.835986	-0.354357	-0.312427
2	6	0	1.356164	1.847468	-0.084570
3	6	0	-0.711376	1.767089	-1.362347
4	6	0	-2.696286	-0.896489	-1.632917
5	6	0	0.805044	1.669107	-1.330985
6	6	0	0.332627	2.050945	1.008726
7	6	0	-4.920143	-1.355397	-0.800191
8	6	0	-1.111743	3.124905	-0.724398
9	6	0	-0.545232	0.827959	0.878236
10	6	0	-1.149636	0.666948	-0.371184
11	6	0	-3.439748	0.112348	0.421432
12	6	0	-0.536113	3.307977	0.693841
13	6	0	-2.429705	-0.065211	-0.535722
14	6	0	-4.671534	-0.529038	0.294237
15	6	0	-3.926137	-1.534327	-1.764096
16	1	0	-1.925989	-1.066329	-2.378644
17	1	0	-5.879747	-1.855159	-0.903451
18	1	0	-3.260242	0.775165	1.264026
19	1	0	-5.439255	-0.375545	1.048416
20	1	0	-4.107031	-2.181973	-2.618251
21	1	0	-0.768450	3.927662	-1.385333
22	1	0	-2.203062	3.189351	-0.667408
23	1	0	-0.930137	0.321283	1.758495
24	1	0	1.391799	1.683528	-2.246074
25	6	0	0.021799	-2.115526	0.424330
26	6	0	-0.539396	-3.103738	-0.401864
27	6	0	-0.063994	-2.330309	1.811039
28	6	0	-1.170150	-4.234460	0.122786
29	1	0	-0.482685	-3.001299	-1.484809
30	6	0	-0.689943	-3.460653	2.346234
31	1	0	0.368947	-1.607650	2.501827
32	6	0	-1.252169	-4.420067	1.503984
33	1	0	-1.595947	-4.975183	-0.551844
34	1	0	-0.735592	-3.589848	3.426188
35	1	0	-1.740163	-5.300239	1.915789

36	6	0	2.489717	-1.961057	-0.529539
37	1	0	2.013373	-2.816488	-0.998423
38	6	0	2.760069	-0.846188	-1.314678
39	1	0	2.445886	-0.817732	-2.357897
40	6	0	3.811572	0.117348	-0.944203
41	8	0	4.148262	1.020475	-1.710643
42	6	0	3.229224	-2.216308	0.753132
43	6	0	4.526963	-0.100504	0.370265
44	6	0	-1.252326	1.663499	-2.778839
45	1	0	-0.906413	0.753911	-3.277981
46	1	0	-2.345552	1.674245	-2.797517
47	1	0	-0.896665	2.517555	-3.364902
48	1	0	0.806417	2.118788	1.989422
49	1	0	2.413289	2.026855	0.083014
50	6	0	0.293495	4.583058	0.806283
51	1	0	-0.335137	5.461421	0.627303
52	1	0	0.762971	4.683745	1.789295
53	1	0	1.090402	4.577709	0.057383
54	8	0	-1.681087	3.343601	1.556619
55	6	0	-1.441802	3.533845	2.938961
56	1	0	-1.004230	4.515830	3.154012
57	1	0	-2.417180	3.476359	3.426438
58	1	0	-0.797317	2.756073	3.366338
59	6	0	3.740754	-0.927378	1.381390
60	1	0	2.588744	-2.766099	1.448741
61	1	0	4.074293	-2.881416	0.517711
62	1	0	4.370715	-1.149365	2.248737
63	1	0	2.884310	-0.345931	1.745811
64	1	0	4.824917	0.873508	0.769313
65	1	0	5.457996	-0.624318	0.109655

SCF Done: E(RPBE1PBE) = -5961.24457698 A.U. after 1 cycles
Convg = 0.4838D-08 -V/T = 2.0046
Zero-point correction= 0.551399 (Hartree/Particle)
Thermal correction to Energy= 0.581595
Thermal correction to Enthalpy= 0.582539
Thermal correction to Gibbs Free Energy= 0.489609
Sum of electronic and zero-point Energies= -5960.693178
Sum of electronic and thermal Energies= -5960.662982
Sum of electronic and thermal Enthalpies= -5960.662038
Sum of electronic and thermal Free Energies= -5960.754968

	1	2	3
Frequencies --	13.2860	24.3010	31.1561

Darses Ligand-prox-Rh(I)-Ph-CH-re-confU-CR-TS (126a)

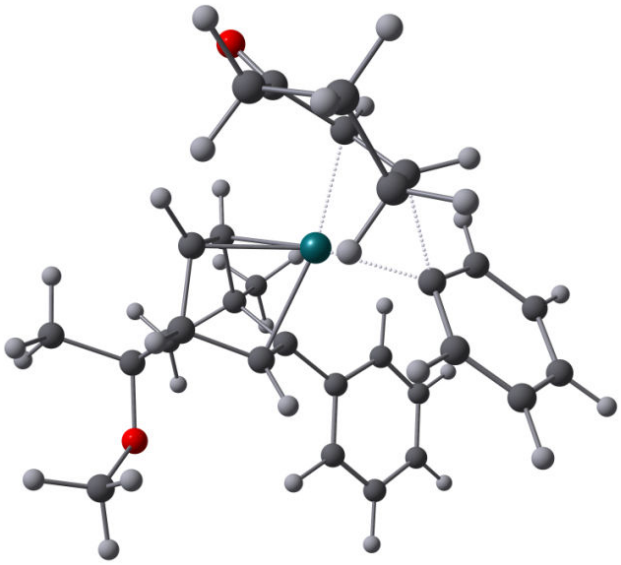


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.858170	-0.300520	-0.444804
2	6	0	1.369749	1.816014	-0.303162
3	6	0	-0.809794	1.761457	-1.399292
4	6	0	-2.759570	-0.935570	-1.432444
5	6	0	0.700312	1.604114	-1.500078
6	6	0	0.443825	2.100658	0.859604
7	6	0	-4.919838	-1.414011	-0.456992
8	6	0	-1.109785	3.156057	-0.787753
9	6	0	-0.479383	0.902354	0.851751
10	6	0	-1.182114	0.710036	-0.329652
11	6	0	-3.402447	0.120040	0.631431
12	6	0	-0.404133	3.375075	0.565164
13	6	0	-2.448416	-0.059857	-0.382096
14	6	0	-4.623844	-0.551916	0.597998
15	6	0	-3.980482	-1.602218	-1.471898
16	1	0	-2.029426	-1.115105	-2.215380
17	1	0	-5.873203	-1.935016	-0.488779
18	1	0	-3.189007	0.810348	1.443586
19	1	0	-5.347904	-0.393287	1.393248
20	1	0	-4.195888	-2.280681	-2.293560
21	1	0	-0.802153	3.921016	-1.508756
22	1	0	-2.189177	3.261301	-0.637067
23	1	0	-0.768683	0.409651	1.775873
24	1	0	1.199628	1.623615	-2.466390
25	6	0	0.354395	-2.236508	0.352137
26	6	0	-0.357825	-3.078722	-0.518806
27	6	0	0.094517	-2.353246	1.728178
28	6	0	-1.318847	-3.969218	-0.043921
29	1	0	-0.145857	-3.051707	-1.586970
30	6	0	-0.863174	-3.245773	2.208123
31	1	0	0.634340	-1.731045	2.438988
32	6	0	-1.577290	-4.058059	1.324642
33	1	0	-1.861355	-4.600684	-0.743881

34	1	0	-1.052081	-3.307052	3.277752
35	1	0	-2.318477	-4.758950	1.700153
36	6	0	2.312267	-2.183236	-0.208996
37	1	0	2.118419	-3.146891	-0.669432
38	6	0	2.678579	-1.147587	-1.144718
39	1	0	2.504284	-1.329597	-2.207510
40	6	0	3.747627	-0.195600	-0.862431
41	8	0	4.210758	0.544157	-1.741412
42	6	0	3.119321	-2.277916	1.066333
43	1	0	2.586679	-2.856160	1.824647
44	6	0	4.336350	-0.162175	0.534008
45	1	0	4.510981	0.882670	0.809477
46	6	0	-1.486006	1.624594	-2.753852
47	1	0	-1.205826	0.694812	-3.256760
48	1	0	-2.575807	1.654475	-2.667267
49	1	0	-1.176053	2.454162	-3.398343
50	1	0	2.433811	2.027327	-0.250085
51	1	0	0.998413	2.190344	1.795575
52	6	0	0.478878	4.619691	0.543473
53	1	0	-0.132244	5.513844	0.383120
54	1	0	1.042437	4.744122	1.473023
55	1	0	1.201660	4.551355	-0.274370
56	8	0	-1.465812	3.502063	1.522209
57	6	0	-1.095326	3.679350	2.876534
58	1	0	-0.515763	4.596268	3.034913
59	1	0	-2.027849	3.759901	3.439016
60	1	0	-0.527927	2.827583	3.271312
61	6	0	3.523350	-0.906752	1.585677
62	1	0	4.023654	-2.851988	0.816468
63	1	0	2.621613	-0.331119	1.833370
64	1	0	4.105741	-1.004785	2.507836
65	1	0	5.330417	-0.621527	0.442206

```
 ----------------------------------------------------------------------SCF Done:
E(RPBE1PBE) =  -5961.22898118     A.U. after    1 cycles
             Convg  =    0.3348D-08             -V/T =  2.0046
Zero-point correction=                           0.550985 (Hartree/Particle)
 Thermal correction to Energy=                    0.580297
 Thermal correction to Enthalpy=                  0.581241
 Thermal correction to Gibbs Free Energy=         0.490691
 Sum of electronic and zero-point Energies=          -5960.677996
 Sum of electronic and thermal Energies=             -5960.648685
 Sum of electronic and thermal Enthalpies=           -5960.647740
 Sum of electronic and thermal Free Energies=        -5960.738290
                    1                    2                    3
Frequencies --  -300.3844               12.6903              26.5820
```

Darses Ligand-prox-Rh(I)-Ph-CH-re-confD-CR-TS (126b)

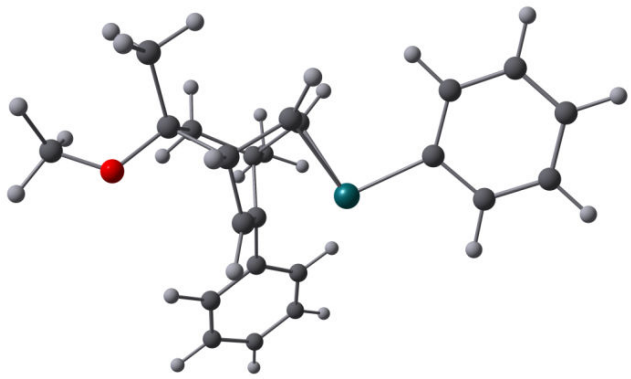


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.847054	-0.273615	-0.418806
2	6	0	1.290825	1.869079	-0.354428
3	6	0	-0.900121	1.696067	-1.414423
4	6	0	-2.784218	-1.057179	-1.306205
5	6	0	0.613501	1.593840	-1.532803
6	6	0	0.371631	2.154675	0.813373
7	6	0	-4.919580	-1.523665	-0.270741
8	6	0	-1.243100	3.098199	-0.844346
9	6	0	-0.501374	0.920212	0.856549
10	6	0	-1.218313	0.667244	-0.307038
11	6	0	-3.411107	0.085729	0.715855
12	6	0	-0.532316	3.384093	0.493002
13	6	0	-2.470286	-0.128217	-0.303773
14	6	0	-4.621865	-0.605649	0.735638
15	6	0	-3.993685	-1.745637	-1.291049
16	1	0	-2.065240	-1.261726	-2.093067
17	1	0	-5.863982	-2.061669	-0.260840
18	1	0	-3.194503	0.819018	1.488622
19	1	0	-5.335779	-0.419886	1.534212
20	1	0	-4.210995	-2.466600	-2.075194
21	1	0	-0.970300	3.850496	-1.592370
22	1	0	-2.323942	3.170238	-0.684825
23	1	0	-0.763387	0.452012	1.801556
24	1	0	1.098496	1.599751	-2.506542
25	6	0	0.364829	-2.216494	0.348525
26	6	0	-0.158172	-3.077036	-0.634494
27	6	0	-0.038375	-2.419452	1.677030
28	6	0	-1.087190	-4.063364	-0.312153
29	1	0	0.177792	-2.984676	-1.666776
30	6	0	-0.960988	-3.413862	2.004120
31	1	0	0.358685	-1.792112	2.471763
32	6	0	-1.494065	-4.238566	1.012058
33	1	0	-1.487185	-4.703979	-1.094966
34	1	0	-1.264137	-3.544819	3.040713

35	1	0	-2.208548	-5.016185	1.269537
36	6	0	2.377178	-1.975236	0.078390
37	1	0	2.323775	-3.016453	-0.221247
38	6	0	2.739990	-1.075401	-0.990197
39	1	0	2.614584	-1.432060	-2.015198
40	6	0	3.793903	-0.074941	-0.837260
41	8	0	4.198801	0.600794	-1.790750
42	6	0	2.998591	-1.764266	1.450517
43	1	0	2.977270	-2.703806	2.010585
44	1	0	2.420403	-1.037937	2.029646
45	6	0	4.426072	0.074699	0.533311
46	1	0	3.860614	0.833988	1.090272
47	1	0	5.436339	0.469281	0.392104
48	6	0	4.423755	-1.235786	1.314023
49	1	0	4.858682	-1.084120	2.307519
50	1	0	5.050669	-1.974480	0.799584
51	6	0	-1.587528	1.483111	-2.753117
52	1	0	-1.282806	0.541025	-3.217621
53	1	0	-2.676654	1.481655	-2.653680
54	1	0	-1.311750	2.293528	-3.436271
55	1	0	2.347186	2.120219	-0.325231
56	1	0	0.935420	2.296773	1.737287
57	6	0	0.297548	4.662970	0.426412
58	1	0	-0.351069	5.525941	0.243881
59	1	0	0.862145	4.838846	1.346993
60	1	0	1.017010	4.599267	-0.394814
61	8	0	-1.588237	3.492779	1.458911
62	6	0	-1.211497	3.725988	2.802932
63	1	0	-0.675579	4.674033	2.928237
64	1	0	-2.140457	3.777429	3.374679
65	1	0	-0.598981	2.914177	3.214181

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5961.22489235     A.U. after    5 cycles
             Convg  =    0.3250D-08             -V/T =  2.0046
Zero-point correction=                           0.551112 (Hartree/Particle)
 Thermal correction to Energy=                   0.580450
 Thermal correction to Enthalpy=                 0.581394
 Thermal correction to Gibbs Free Energy=        0.491663
 Sum of electronic and zero-point Energies=          -5960.673780
 Sum of electronic and thermal Energies=             -5960.644443
 Sum of electronic and thermal Enthalpies=           -5960.643498
 Sum of electronic and thermal Free Energies=        -5960.733229
                    1                    2                    3
Frequencies --  -299.8043               27.7031              36.2030
```

Darses Ligand-dist-Rh(I)-Ph (115)

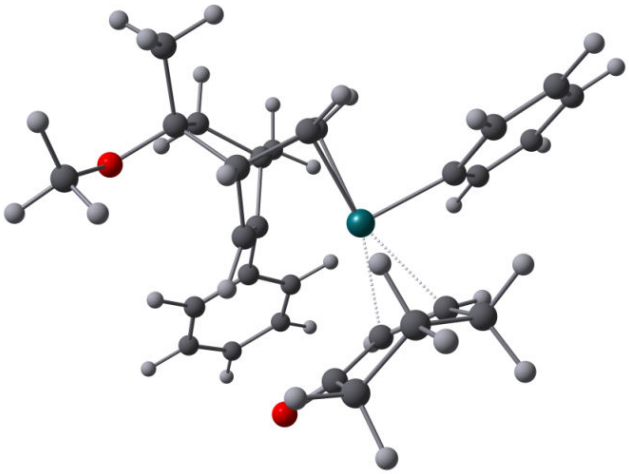


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	1.059364	0.198682	-0.474309
2	6	0	0.498559	-1.777581	-0.136717
3	6	0	-1.018252	-0.436419	1.264761
4	6	0	-1.080274	2.872845	0.571712
5	6	0	0.372196	-1.027254	1.059900
6	6	0	-0.788450	-1.803197	-0.940365
7	6	0	-2.890171	4.364925	-0.016552
8	6	0	-2.062070	-1.583376	1.201218
9	6	0	-1.063959	-0.329743	-1.160094
10	6	0	-1.189770	0.415862	-0.010610
11	6	0	-3.010270	2.019162	-0.588608
12	6	0	-1.940926	-2.412173	-0.100503
13	6	0	-1.756349	1.787421	-0.004769
14	6	0	-3.572608	3.295525	-0.595089
15	6	0	-1.639285	4.148362	0.564082
16	1	0	-0.097489	2.719668	1.011104
17	1	0	-3.326992	5.360042	-0.020372
18	1	0	-3.549526	1.186708	-1.033985
19	1	0	-4.546914	3.452892	-1.050775
20	1	0	-1.094650	4.977624	1.008289
21	1	0	-1.929897	-2.219410	2.083795
22	1	0	-3.063344	-1.143841	1.267076
23	1	0	-1.317702	0.064363	-2.140990
24	1	0	1.020499	-1.183990	1.920781
25	6	0	-1.137511	0.320174	2.577633
26	1	0	-2.109432	0.815199	2.668592
27	1	0	-1.034448	-0.378310	3.414815
28	1	0	-0.357087	1.079414	2.681115
29	1	0	-0.684473	-2.346582	-1.881997
30	1	0	1.254401	-2.548490	-0.268573
31	6	0	-1.662856	-3.885288	0.180996
32	1	0	-2.428111	-4.327948	0.825622
33	1	0	-1.619702	-4.455650	-0.752901
34	1	0	-0.704085	-3.992269	0.696403
35	8	0	-3.096392	-2.249072	-0.936010
36	6	0	-4.286092	-2.865903	-0.483715
37	1	0	-5.090494	-2.498087	-1.124598
38	1	0	-4.242966	-3.958372	-0.570803
39	1	0	-4.523944	-2.606027	0.555635
40	6	0	3.046183	0.029125	-0.158787
41	6	0	3.825745	1.051384	-0.735476
42	6	0	3.738879	-0.964450	0.556003
43	6	0	5.217267	1.086733	-0.607852
44	1	0	3.340715	1.848400	-1.304319
45	6	0	5.129570	-0.940421	0.691099
46	1	0	3.189882	-1.781885	1.023125
47	6	0	5.876397	0.086657	0.109505
48	1	0	5.786969	1.892619	-1.066856
49	1	0	5.634237	-1.725298	1.251623
50	1	0	6.958601	0.106871	0.213574

SCF Done: E(RPBE1PBE) = -5652.88861689 A.U. after 1 cycles
Convg = 0.3503D-08 -V/T = 2.0041
Zero-point correction= 0.420608 (Hartree/Particle)
Thermal correction to Energy= 0.443583
Thermal correction to Enthalpy= 0.444528
Thermal correction to Gibbs Free Energy= 0.367725
Sum of electronic and zero-point Energies= -5652.468009
Sum of electronic and thermal Energies= -5652.445034
Sum of electronic and thermal Enthalpies= -5652.444089

```
 Sum of electronic and thermal Free Energies=         -5652.520892
                      1                      2                      3
Frequencies --     22.7654                33.1316                42.4449
```

(*S*)-DA-dist-Rh(I)-Ph-CH-si-confU-anti (131a)

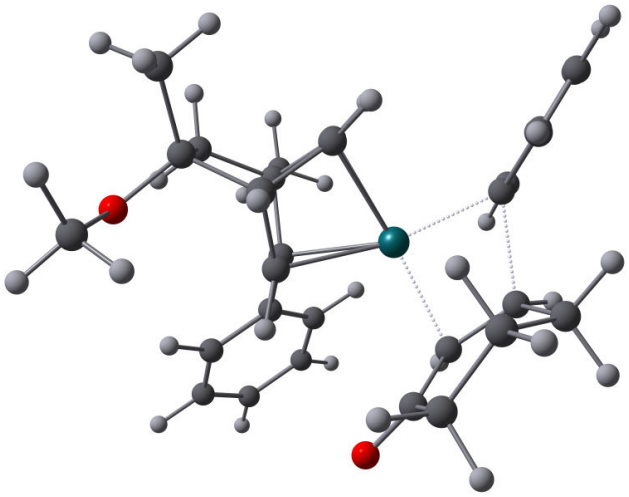


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.804678	-0.166598	0.031856
2	6	0	-1.416896	0.030857	-0.593501
3	6	0	-0.869930	1.917921	0.852303
4	6	0	-1.301818	0.476379	0.705780
5	6	0	-1.080202	1.130925	-1.621367
6	6	0	-1.923310	2.816026	0.132978
7	6	0	0.331107	1.533331	-1.222714
8	6	0	0.441741	1.966601	0.098140
9	6	0	-2.023383	2.326818	-1.325880
10	1	0	1.077155	1.754401	-1.981082
11	1	0	-1.706884	-0.085813	1.541410
12	6	0	2.754447	0.089000	-0.585763
13	6	0	3.653936	1.022343	-0.047813
14	6	0	3.173381	-0.616627	-1.728188
15	6	0	4.908344	1.248392	-0.624976
16	1	0	3.386279	1.589907	0.842412
17	6	0	4.419959	-0.389104	-2.315929
18	1	0	2.518542	-1.365965	-2.173243
19	6	0	5.297898	0.547550	-1.766044
20	1	0	5.581852	1.977492	-0.178207
21	1	0	4.708039	-0.949691	-3.203326
22	1	0	6.271114	0.723963	-2.217545
23	6	0	2.014369	-1.777907	1.140498
24	6	0	0.664007	-2.118184	1.120238
25	1	0	2.665759	-2.226150	0.395432
26	1	0	0.272017	-2.775857	0.345149
27	6	0	-0.160487	-2.011632	2.335060
28	8	0	-1.292927	-2.494226	2.388801
29	6	0	0.466457	-1.388178	3.563860
30	1	0	-0.311477	-0.841328	4.104950
31	6	0	2.676708	-1.252201	2.382708
32	1	0	3.112969	-2.112417	2.913670
33	1	0	1.282719	2.550259	0.460610
34	1	0	-1.775412	3.137106	-2.019706

35	1	0	-3.058529	2.030207	-1.524206
36	1	0	-0.738163	2.204105	1.897248
37	6	0	-2.139153	-1.211595	-0.958580
38	6	0	-1.577818	-2.180728	-1.802367
39	6	0	-3.431552	-1.426741	-0.461820
40	6	0	-2.284622	-3.333847	-2.131942
41	1	0	-0.569058	-2.042048	-2.183022
42	6	0	-4.142613	-2.578917	-0.794816
43	1	0	-3.882922	-0.680077	0.186315
44	6	0	-3.571837	-3.536963	-1.631245
45	1	0	-1.827611	-4.079170	-2.777801
46	1	0	-5.144270	-2.726989	-0.399599
47	1	0	-4.123851	-4.436504	-1.890460
48	6	0	-1.171919	0.726607	-3.083400
49	1	0	-0.450057	-0.055164	-3.334804
50	1	0	-2.172433	0.365179	-3.338588
51	1	0	-0.954341	1.594161	-3.715048
52	6	0	-1.520259	4.286138	0.205312
53	1	0	-2.293426	4.912232	-0.251783
54	1	0	-1.361578	4.622524	1.234252
55	1	0	-0.587370	4.445685	-0.342266
56	8	0	-3.226691	2.599233	0.690649
57	6	0	-3.424543	2.989633	2.036945
58	1	0	-3.308766	4.070562	2.178052
59	1	0	-4.452762	2.717537	2.284029
60	1	0	-2.754314	2.466223	2.729510
61	6	0	1.692390	-0.526234	3.288969
62	1	0	0.745769	-2.236527	4.204958
63	1	0	1.384092	0.406740	2.801221
64	1	0	2.173657	-0.253268	4.233910
65	1	0	3.513278	-0.602419	2.109779

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5961.24730288     A.U. after    1 cycles
             Convg  =    0.3275D-08             -V/T =  2.0046
Zero-point correction=                           0.551297 (Hartree/Particle)
 Thermal correction to Energy=                   0.581459
 Thermal correction to Enthalpy=                 0.582403
 Thermal correction to Gibbs Free Energy=        0.490225
 Sum of electronic and zero-point Energies=          -5960.696005
 Sum of electronic and thermal Energies=             -5960.665844
 Sum of electronic and thermal Enthalpies=           -5960.664899
 Sum of electronic and thermal Free Energies=        -5960.757077
                    1                    2                    3
Frequencies --    24.8949              31.5864              36.8217
```

Darses Ligand-dist-Rh(I)-Ph-CH-si-confU-CR-TS (32a)

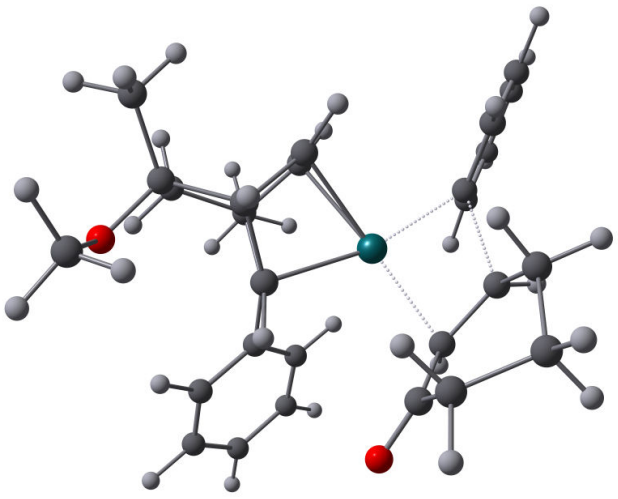


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.731962	-0.157301	0.043914
2	6	0	-1.400128	-0.022321	-0.513582
3	6	0	-0.903513	1.913078	0.897155
4	6	0	-1.238568	0.440124	0.790125
5	6	0	-1.186673	1.095411	-1.559509
6	6	0	-2.049437	2.730568	0.227587
7	6	0	0.215870	1.580923	-1.226105
8	6	0	0.362789	2.028526	0.073078
9	6	0	-2.184612	2.233635	-1.226192
10	6	0	2.806084	-0.094601	-0.448087
11	6	0	3.632609	0.963947	-0.040945
12	6	0	3.021595	-0.642737	-1.726095
13	6	0	4.612533	1.477223	-0.891371
14	1	0	3.503803	1.413405	0.941164
15	6	0	3.986104	-0.118356	-2.584898
16	1	0	2.434057	-1.500669	-2.051220
17	6	0	4.790431	0.945283	-2.169745
18	1	0	5.235153	2.303348	-0.554934
19	1	0	4.121868	-0.552176	-3.573059
20	1	0	5.554441	1.347058	-2.830174
21	6	0	2.437406	-1.573862	0.903061
22	6	0	1.077325	-2.059413	0.955475
23	1	0	3.097155	-2.174820	0.283918
24	1	0	0.772730	-2.823367	0.239625
25	6	0	0.315567	-2.046407	2.199276
26	8	0	-0.742573	-2.678405	2.328488
27	6	0	0.873744	-1.288396	3.390069
28	1	0	0.053402	-0.729703	3.851803
29	6	0	3.067473	-1.131377	2.203976
30	1	0	3.964822	-0.535081	2.022255
31	1	0	0.945555	1.773222	-2.009016
32	1	0	-1.602792	-0.124222	1.644874
33	1	0	1.216710	2.606533	0.413532
34	1	0	-0.734575	2.224695	1.929469
35	1	0	-3.207951	1.874537	-1.376262
36	1	0	-2.018596	3.055569	-1.930878
37	6	0	-2.145768	-1.265362	-0.834828

38	6	0	-1.613766	-2.261227	-1.665505
39	6	0	-3.434420	-1.448336	-0.314658
40	6	0	-2.344527	-3.408457	-1.961829
41	1	0	-0.608530	-2.144167	-2.062719
42	6	0	-4.169041	-2.596288	-0.611751
43	1	0	-3.862470	-0.679696	0.324176
44	6	0	-3.626876	-3.580509	-1.436812
45	1	0	-1.910389	-4.174490	-2.599366
46	1	0	-5.166331	-2.720688	-0.197418
47	1	0	-4.196921	-4.476586	-1.667764
48	6	0	-1.317338	0.667757	-3.011615
49	1	0	-0.576678	-0.092743	-3.275838
50	1	0	-2.312117	0.264672	-3.223522
51	1	0	-1.155593	1.531725	-3.664858
52	6	0	-1.752767	4.226265	0.284714
53	1	0	-2.583785	4.793500	-0.147087
54	1	0	-1.585136	4.576452	1.307767
55	1	0	-0.851902	4.450759	-0.293158
56	8	0	-3.308014	2.421288	0.843792
57	6	0	-3.459638	2.763746	2.208545
58	1	0	-3.382344	3.843984	2.378973
59	1	0	-4.463388	2.441265	2.493064
60	1	0	-2.737499	2.249037	2.853952
61	6	0	2.072744	-0.397034	3.088801
62	1	0	1.160385	-2.061365	4.116148
63	1	0	1.739767	0.515342	2.575745
64	1	0	2.550081	-0.083683	4.023419
65	1	0	3.402278	-2.046999	2.712995

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5961.23187930     A.U. after    1 cycles
             Convg  =    0.3153D-08             -V/T =  2.0046
Zero-point correction=                           0.550733 (Hartree/Particle)
 Thermal correction to Energy=                    0.580089
 Thermal correction to Enthalpy=                  0.581033
 Thermal correction to Gibbs Free Energy=         0.490989
 Sum of electronic and zero-point Energies=          -5960.681146
 Sum of electronic and thermal Energies=             -5960.651790
 Sum of electronic and thermal Enthalpies=           -5960.650846
 Sum of electronic and thermal Free Energies=        -5960.740890
                    1                      2                      3
Frequencies --  -292.6046               27.5638                31.3687
```

Darses Ligand-dist-Rh(I)-Ph-CH-si-confD-CR-TS (132b)

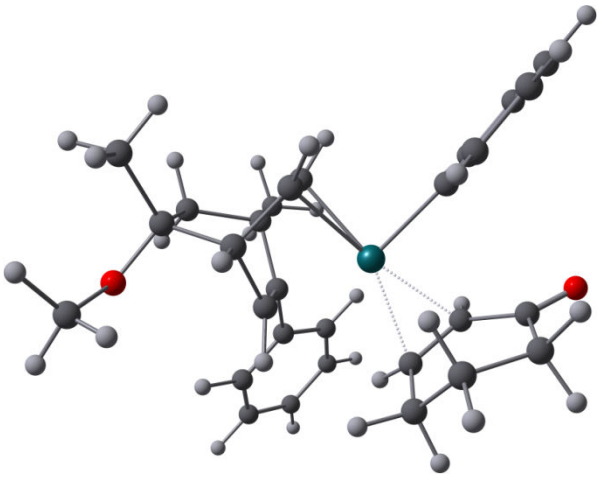


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.745718	-0.090964	0.014529
2	6	0	-1.394769	0.028370	-0.518807
3	6	0	-0.955973	1.809483	1.097987
4	6	0	-1.240530	0.347344	0.827907
5	6	0	-1.223785	1.261338	-1.434610
6	6	0	-2.137126	2.651331	0.525168
7	6	0	0.163201	1.755024	-1.051977
8	6	0	0.301972	2.058512	0.290232
9	6	0	-2.254684	2.324338	-0.977212
10	6	0	2.809699	0.090018	-0.481170
11	6	0	3.637049	1.133890	-0.043151
12	6	0	3.015953	-0.417016	-1.778242
13	6	0	4.605260	1.681655	-0.886207
14	1	0	3.524478	1.540805	0.958857
15	6	0	3.965257	0.146173	-2.629090
16	1	0	2.432004	-1.268493	-2.125421
17	6	0	4.768704	1.199594	-2.185679
18	1	0	5.231433	2.494790	-0.525516
19	1	0	4.090653	-0.249685	-3.634431
20	1	0	5.522156	1.629682	-2.840326
21	6	0	2.472623	-1.391165	0.873432
22	6	0	1.188525	-2.049736	0.765307
23	1	0	3.262183	-1.889788	0.319899
24	1	0	1.053278	-2.761803	-0.050259
25	6	0	0.358426	-2.317209	1.936422
26	8	0	-0.648981	-3.033152	1.880631
27	6	0	0.816093	-1.742080	3.263436
28	1	0	0.415469	-0.724224	3.361210
29	1	0	0.366820	-2.343437	4.058819
30	6	0	2.338376	-1.707377	3.361469
31	1	0	2.647223	-1.293620	4.327280
32	1	0	2.733582	-2.729514	3.310260
33	6	0	2.919405	-0.863769	2.231474
34	1	0	2.587134	0.168631	2.377394
35	1	0	4.012783	-0.848333	2.273666
36	1	0	0.879453	2.062206	-1.810353
37	1	0	-1.581122	-0.320564	1.615237
38	1	0	1.135099	2.628855	0.690612
39	1	0	-0.793386	2.008996	2.158751
40	1	0	-3.267472	1.957715	-1.172984
41	1	0	-2.108804	3.226632	-1.580857
42	6	0	-2.106748	-1.192167	-0.974686
43	6	0	-1.548622	-2.081850	-1.902557
44	6	0	-3.393877	-1.456712	-0.487045
45	6	0	-2.251776	-3.207504	-2.323079
46	1	0	-0.544736	-1.900246	-2.277885
47	6	0	-4.101351	-2.582237	-0.909307
48	1	0	-3.841656	-0.769028	0.226291
49	6	0	-3.532616	-3.462109	-1.828991
50	1	0	-1.797285	-3.892241	-3.034679
51	1	0	-5.097906	-2.771134	-0.518262
52	1	0	-4.080867	-4.341122	-2.157623
53	6	0	-1.348162	0.992259	-2.924757
54	1	0	-0.583144	0.292261	-3.273213
55	1	0	-2.329559	0.579630	-3.176848
56	1	0	-1.221571	1.928410	-3.478801
57	6	0	-1.906440	4.140481	0.762620
58	1	0	-2.760065	4.720371	0.396740
59	1	0	-1.755756	4.370571	1.821595

60	1	0	-1.014952	4.470440	0.222022
61	8	0	-3.379256	2.212803	1.094875
62	6	0	-3.556614	2.407536	2.485608
63	1	0	-3.575184	3.469262	2.758284
64	1	0	-4.526861	1.971282	2.732248
65	1	0	-2.789632	1.900381	3.083474

```
SCF Done:  E(RPBE1PBE) =  -5961.22764061     A.U. after    1 cycles
             Convg  =    0.3722D-08             -V/T =  2.0046
Zero-point correction=                           0.551301 (Hartree/Particle)
 Thermal correction to Energy=                    0.580560
 Thermal correction to Enthalpy=                  0.581504
 Thermal correction to Gibbs Free Energy=         0.492251
 Sum of electronic and zero-point Energies=          -5960.676339
 Sum of electronic and thermal Energies=             -5960.647080
 Sum of electronic and thermal Enthalpies=           -5960.646136
 Sum of electronic and thermal Free Energies=        -5960.735390
                     1                      2                      3
Frequencies --  -296.0367               32.4404                41.2114
```

Darses Ligand-dist-Rh(I)-Ph-CH-re-confU-syn (135a)

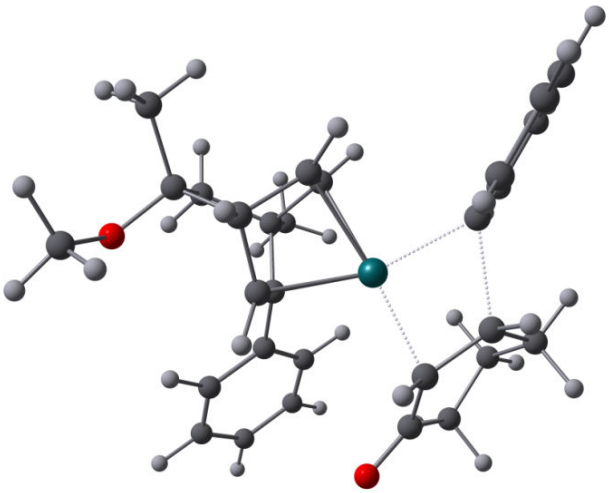


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.624225	0.014755	0.022497
2	6	0	1.658289	0.199037	-0.364032
3	6	0	1.255354	-1.839277	0.921250
4	6	0	1.450770	-0.339080	0.890698
5	6	0	1.621973	-0.872799	-1.470025
6	6	0	2.526209	-2.503694	0.305100
7	6	0	0.263337	-1.519952	-1.261984
8	6	0	0.071359	-2.056615	0.003418
9	6	0	2.708719	-1.921351	-1.110679
10	1	0	-0.365111	-1.774234	-2.111843
11	1	0	1.669300	0.215080	1.798381
12	6	0	-2.487504	-0.612603	-0.606398
13	6	0	-3.279833	-1.475487	0.167603
14	6	0	-2.951242	-0.305134	-1.896525
15	6	0	-4.482892	-1.999839	-0.316492
16	1	0	-2.964940	-1.751684	1.173327
17	6	0	-4.146930	-0.831856	-2.391046
18	1	0	-2.375268	0.363896	-2.534466

19	6	0	-4.923520	-1.682037	-1.601188
20	1	0	-5.074446	-2.661426	0.313886
21	1	0	-4.475103	-0.573770	-3.396370
22	1	0	-5.857204	-2.089535	-1.981398
23	6	0	-0.642237	1.932754	1.184690
24	1	0	0.254165	2.442422	0.837394
25	6	0	-1.768579	1.946573	0.369193
26	1	0	-1.726846	2.385836	-0.626438
27	6	0	-3.119318	1.808082	0.937892
28	8	0	-4.119595	2.120907	0.292735
29	6	0	-0.761898	1.691561	2.666482
30	1	0	-0.858461	2.673276	3.155316
31	6	0	-3.238485	1.395346	2.389038
32	1	0	-3.527600	2.308537	2.927794
33	6	0	2.382055	-4.022094	0.274807
34	1	0	3.298854	-4.481553	-0.108713
35	1	0	2.170911	-4.436618	1.265117
36	1	0	1.558574	-4.306799	-0.385811
37	1	0	-0.712980	-2.770949	0.234794
38	1	0	2.677828	-2.718073	-1.861289
39	1	0	3.695929	-1.452377	-1.170657
40	8	0	3.694918	-2.096812	1.029490
41	6	0	3.822682	-2.562833	2.360280
42	1	0	4.720912	-2.090051	2.762778
43	1	0	2.971892	-2.278545	2.991218
44	1	0	3.952217	-3.650338	2.407742
45	1	0	1.052724	-2.208056	1.928058
46	6	0	1.809139	-0.373354	-2.893080
47	1	0	1.810290	-1.224930	-3.581378
48	1	0	1.000489	0.296939	-3.197075
49	1	0	2.758232	0.157400	-3.011103
50	6	0	2.263308	1.537361	-0.570835
51	6	0	1.717596	2.480562	-1.454750
52	6	0	3.428416	1.878064	0.131055
53	6	0	2.316402	3.725091	-1.628424
54	1	0	0.800654	2.247300	-1.989144
55	6	0	4.030572	3.123770	-0.044284
56	1	0	3.869751	1.153554	0.810673
57	6	0	3.477740	4.051348	-0.925641
58	1	0	1.871627	4.445490	-2.309971
59	1	0	4.934693	3.367307	0.507660
60	1	0	3.945318	5.022690	-1.062783
61	6	0	-1.966462	0.820839	2.999414
62	1	0	0.158145	1.249788	3.059910
63	1	0	-1.789873	-0.188712	2.609281
64	1	0	-2.081945	0.728796	4.084268
65	1	0	-4.085274	0.708335	2.477462

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5961.24562498     A.U. after    1 cycles
             Convg  =    0.5484D-08             -V/T =  2.0046
Zero-point correction=                           0.551096 (Hartree/Particle)
 Thermal correction to Energy=                   0.581429
 Thermal correction to Enthalpy=                 0.582374
 Thermal correction to Gibbs Free Energy=        0.489748
 Sum of electronic and zero-point Energies=          -5960.694529
 Sum of electronic and thermal Energies=             -5960.664196
 Sum of electronic and thermal Enthalpies=           -5960.663251
 Sum of electronic and thermal Free Energies=        -5960.755877
                    1                    2                    3
Frequencies --    26.0570              34.3251              36.1259
```

Darses Ligand-dist-Rh(I)-Ph-CH-re-confU-CR-TS (139a)

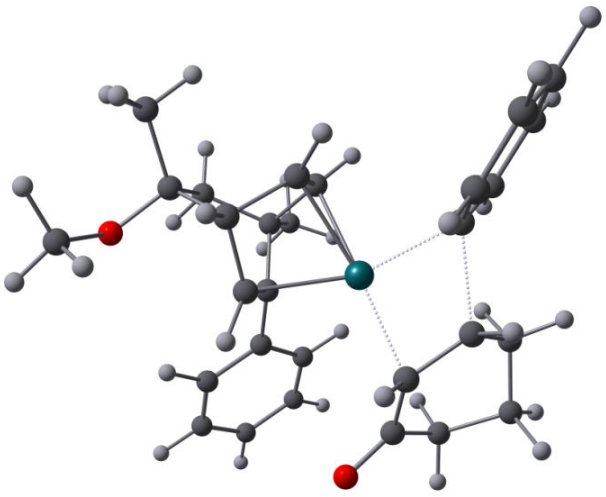


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.745801	-0.029003	-0.317035
2	6	0	-1.411751	-0.112564	0.307127
3	6	0	-0.844580	-2.215602	-0.811819
4	6	0	-1.214976	-0.751472	-0.916088
5	6	0	-1.162275	-1.058978	1.502378
6	6	0	-1.981292	-2.950994	-0.038734
7	6	0	0.252226	-1.549041	1.243580
8	6	0	0.415134	-2.184399	0.029003
9	6	0	-2.126407	-2.263569	1.332679
10	1	0	0.982384	-1.604685	2.047321
11	1	0	-1.590814	-0.332403	-1.846255
12	6	0	2.869947	-0.243309	-0.129205
13	6	0	3.485164	-1.182285	-0.977454
14	6	0	3.393389	-0.098035	1.166684
15	6	0	4.546233	-1.971391	-0.539874
16	1	0	3.130443	-1.294682	-2.001087
17	6	0	4.459148	-0.884383	1.607295
18	1	0	2.957935	0.623999	1.853795
19	6	0	5.039987	-1.827879	0.759253
20	1	0	4.995182	-2.694041	-1.217640
21	1	0	4.835393	-0.757657	2.620060
22	1	0	5.873946	-2.435315	1.101085
23	6	0	2.426512	1.432252	-1.167141
24	1	0	3.106141	1.067331	-1.931925
25	6	0	1.069446	1.617005	-1.637330
26	1	0	0.808867	1.176118	-2.601821
27	6	0	0.305451	2.820159	-1.326462
28	8	0	-0.707766	3.128027	-1.966949
29	6	0	3.009867	2.546576	-0.324008
30	1	0	3.879759	2.201697	0.239184
31	6	0	0.830007	3.753713	-0.255344
32	1	0	-0.014074	4.087022	0.354695
33	1	0	1.283881	-2.787113	-0.218331
34	1	0	-0.660747	-2.667815	-1.788007
35	1	0	-1.932707	-2.975513	2.142055
36	1	0	-3.159607	-1.917640	1.440289
37	6	0	-2.260332	1.097567	0.433271

38	6	0	-1.934026	2.172399	1.271909
39	6	0	-3.469145	1.156204	-0.276335
40	6	0	-2.782609	3.269185	1.393499
41	1	0	-0.995993	2.160286	1.818903
42	6	0	-4.318885	2.255183	-0.159975
43	1	0	-3.750016	0.321935	-0.914015
44	6	0	-3.980317	3.316253	0.678329
45	1	0	-2.504693	4.094578	2.044239
46	1	0	-5.250467	2.277755	-0.719809
47	1	0	-4.642451	4.172732	0.774417
48	6	0	-1.309205	-0.456772	2.890224
49	1	0	-0.571666	0.330016	3.071985
50	1	0	-2.306720	-0.036606	3.046739
51	1	0	-1.150274	-1.237352	3.641917
52	6	0	-1.664165	-4.436346	0.104912
53	1	0	-2.487025	-4.953264	0.609459
54	1	0	-1.491520	-4.915411	-0.863301
55	1	0	-0.760189	-4.568463	0.705947
56	8	0	-3.241147	-2.742419	-0.693218
57	6	0	-3.392494	-3.288221	-1.990568
58	1	0	-3.342661	-4.383485	-1.990386
59	1	0	-4.385396	-2.988499	-2.332311
60	1	0	-2.652406	-2.898976	-2.700384
61	6	0	1.962965	3.176117	0.582309
62	1	0	3.375115	3.307045	-1.029712
63	1	0	1.570111	2.419182	1.274572
64	1	0	2.414308	3.962376	1.196265
65	1	0	1.188107	4.642887	-0.792702

```
 ---------------------------------------------------------------------
SCF Done:  SCF Done:  E(RPBE1PBE) =  -5961.22696678     A.U. after    1 cycles
             Convg  =    0.1634D-08             -V/T =  2.0046
Zero-point correction=                           0.551569 (Hartree/Particle)
 Thermal correction to Energy=                    0.580662
 Thermal correction to Enthalpy=                  0.581606
 Thermal correction to Gibbs Free Energy=         0.492954
 Sum of electronic and zero-point Energies=          -5960.675398
 Sum of electronic and thermal Energies=             -5960.646305
 Sum of electronic and thermal Enthalpies=           -5960.645360
 Sum of electronic and thermal Free Energies=        -5960.734012
                    1                      2                      3
Frequencies --  -294.1035               27.3009                39.8318
```

Darses Ligand-dist-Rh(I)-Ph-CH-re-confD-CR-TS (139b)



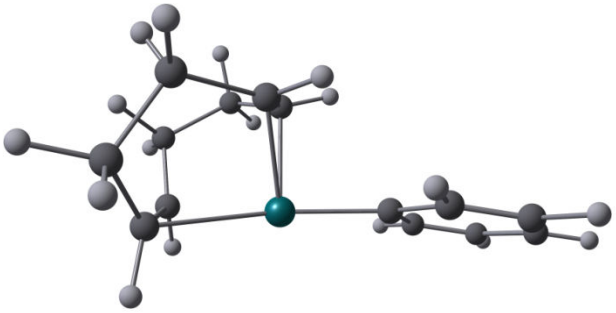
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.746915	-0.049024	-0.259397
2	6	0	-1.426514	-0.129002	0.321385
3	6	0	-0.846966	-2.215314	-0.823472
4	6	0	-1.208374	-0.747643	-0.908274
5	6	0	-1.203997	-1.097355	1.504009
6	6	0	-2.000975	-2.959208	-0.085584
7	6	0	0.213562	-1.587929	1.262925
8	6	0	0.397052	-2.204749	0.041051
9	6	0	-2.168664	-2.295295	1.294844
10	1	0	0.926988	-1.662321	2.079819
11	1	0	-1.562397	-0.310619	-1.838673
12	6	0	2.864795	-0.321016	-0.065454
13	6	0	3.447086	-1.162043	-1.033944
14	6	0	3.434655	-0.314381	1.216716
15	6	0	4.515636	-1.997141	-0.719496
16	1	0	3.059820	-1.158677	-2.051839
17	6	0	4.512916	-1.144469	1.532036
18	1	0	3.029433	0.330056	1.993151
19	6	0	5.056632	-1.994385	0.569680
20	1	0	4.935615	-2.645235	-1.485569
21	1	0	4.927145	-1.124697	2.537743
22	1	0	5.898492	-2.636739	0.814564
23	6	0	2.407132	1.494809	-0.852536
24	1	0	3.210621	1.273894	-1.548869
25	6	0	1.116654	1.663302	-1.484818
26	1	0	0.998340	1.243140	-2.486905
27	6	0	0.312901	2.870454	-1.291653
28	8	0	-0.679565	3.105198	-1.989594
29	6	0	2.791532	2.486363	0.232593
30	1	0	3.873351	2.460241	0.391028
31	1	0	2.324471	2.216701	1.184835
32	6	0	0.794804	3.889644	-0.278422
33	1	0	0.338156	3.650448	0.690001
34	1	0	0.406168	4.866377	-0.580312
35	6	0	2.313663	3.886573	-0.139543
36	1	0	2.624700	4.601090	0.629962
37	1	0	2.777081	4.207064	-1.080905
38	1	0	1.267899	-2.806990	-0.200199
39	1	0	-0.646460	-2.650695	-1.804020
40	1	0	-1.991356	-3.021962	2.094846
41	1	0	-3.202766	-1.948456	1.390353
42	6	0	-2.265791	1.087545	0.447389
43	6	0	-1.956467	2.139087	1.321572
44	6	0	-3.446758	1.179485	-0.304504
45	6	0	-2.790678	3.248026	1.431602
46	1	0	-1.043844	2.097701	1.908557
47	6	0	-4.283095	2.289577	-0.197958
48	1	0	-3.716650	0.362762	-0.968931
49	6	0	-3.958725	3.329478	0.671866
50	1	0	-2.524625	4.055704	2.108877
51	1	0	-5.192766	2.337769	-0.791184
52	1	0	-4.609549	4.195513	0.758994
53	6	0	-1.374866	-0.520987	2.900125
54	1	0	-0.635137	0.255983	3.112703
55	1	0	-2.372357	-0.096485	3.044641
56	1	0	-1.237201	-1.317471	3.639198
57	6	0	-1.692235	-4.448121	0.037761
58	1	0	-2.526324	-4.970213	0.517862
59	1	0	-1.503357	-4.910940	-0.935289

60	1	0	-0.799987	-4.594465	0.652861
61	8	0	-3.247689	-2.733866	-0.759284
62	6	0	-3.374694	-3.248205	-2.072035
63	1	0	-3.315155	-4.342629	-2.098955
64	1	0	-4.365044	-2.948419	-2.420999
65	1	0	-2.627768	-2.834596	-2.760641

```
SCF Done:  E(RPBE1PBE) =  -5961.22233238     A.U. after    1 cycles
             Convg  =    0.2241D-08             -V/T =  2.0046
Zero-point correction=                           0.551241 (Hartree/Particle)
 Thermal correction to Energy=                    0.580580
 Thermal correction to Enthalpy=                  0.581524
 Thermal correction to Gibbs Free Energy=         0.491641
 Sum of electronic and zero-point Energies=          -5960.671092
 Sum of electronic and thermal Energies=             -5960.641753
 Sum of electronic and thermal Enthalpies=           -5960.640808
 Sum of electronic and thermal Free Energies=        -5960.730691
                     1                      2                      3
Frequencies --  -290.0583               23.6179                38.4448
```

COD-Rh pathway

COD-Rh(I)-Ph (142)



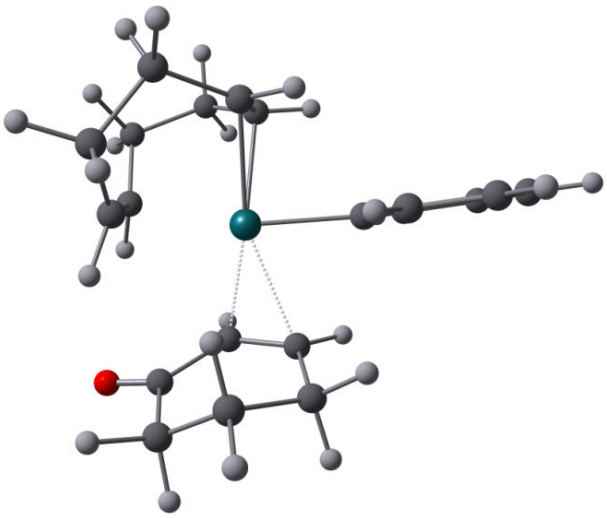
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.228867	-0.056392	-0.562004
2	6	0	0.873465	0.784341	1.245695
3	1	0	0.065163	1.383463	1.665848
4	6	0	2.211603	1.500065	1.122067
5	1	0	2.130952	2.487626	1.587666
6	1	0	2.969918	0.962867	1.700525
7	6	0	2.670029	1.685668	-0.335777
8	1	0	2.227311	2.607496	-0.727210
9	1	0	3.759336	1.833670	-0.372874
10	6	0	2.258322	0.564023	-1.261935
11	1	0	2.094819	0.853474	-2.302345
12	6	0	2.338072	-0.786645	-0.987517
13	1	0	2.206851	-1.475481	-1.823361
14	6	0	2.921385	-1.368168	0.282929
15	1	0	3.424988	-2.311045	0.045345
16	1	0	3.700835	-0.703029	0.664309
17	6	0	1.860030	-1.630631	1.366592
18	1	0	1.412209	-2.616122	1.196923
19	1	0	2.339192	-1.684245	2.356256
20	6	0	0.733479	-0.624163	1.385724
21	1	0	-0.159460	-0.969560	1.908032

22	6	0	-1.728507	0.012821	-0.078316
23	6	0	-2.417875	1.199448	0.226529
24	6	0	-2.498218	-1.155579	-0.228773
25	6	0	-3.810360	1.226085	0.342316
26	1	0	-1.865983	2.128196	0.366609
27	6	0	-3.889762	-1.136933	-0.110386
28	1	0	-2.008166	-2.106454	-0.442013
29	6	0	-4.552895	0.057378	0.174593
30	1	0	-4.316727	2.162718	0.568038
31	1	0	-4.457066	-2.057395	-0.234923
32	1	0	-5.635784	0.075182	0.270937

SCF Done: E(RPBE1PBE) = -5230.34249087 A.U. after 1 cycles
Convg = 0.4220D-08 -V/T = 2.0033
Zero-point correction= 0.274002 (Hartree/Particle)
Thermal correction to Energy= 0.288139
Thermal correction to Enthalpy= 0.289100
Thermal correction to Gibbs Free Energy= 0.231588
Sum of electronic and zero-point Energies= -5230.068489
Sum of electronic and thermal Energies= -5230.054351
Sum of electronic and thermal Enthalpies= -5230.053391
Sum of electronic and thermal Free Energies= -5230.110903

	1	2	3
Frequencies --	25.4414	52.3812	60.8694

COD-Rh(I)-Ph-CH-si-confU-anti (146a)

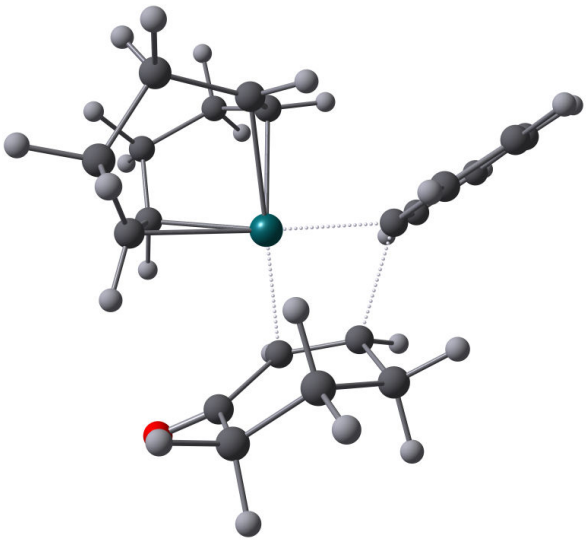


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.151447	-0.224985	-0.163102
2	6	0	-0.223375	-2.079004	0.979447
3	1	0	-1.154987	-1.883183	1.507058
4	6	0	0.941946	-2.503951	1.849898
5	1	0	0.564833	-2.744350	2.849126
6	1	0	1.377000	-3.430708	1.466159
7	6	0	2.007827	-1.411430	1.974068
8	1	0	1.704912	-0.707212	2.756588
9	1	0	2.965082	-1.839048	2.307549
10	6	0	2.219629	-0.620700	0.709759
11	1	0	2.643466	0.368370	0.872235

12	6	0	2.253169	-1.105959	-0.580967
13	1	0	2.665265	-0.440168	-1.336750
14	6	0	2.134076	-2.563742	-0.967640
15	1	0	2.748506	-2.739973	-1.856240
16	1	0	2.560413	-3.191574	-0.181038
17	6	0	0.690476	-2.983619	-1.273583
18	1	0	0.451186	-2.715119	-2.308248
19	1	0	0.590585	-4.078188	-1.215680
20	6	0	-0.341973	-2.334495	-0.388565
21	1	0	-1.352040	-2.351669	-0.794331
22	6	0	-2.574043	0.275321	1.098934
23	6	0	-3.967938	0.350931	1.178587
24	6	0	-1.914815	0.019325	-0.114429
25	6	0	-4.750046	0.165330	0.040046
26	1	0	-4.441459	0.552527	2.137683
27	6	0	-2.725847	-0.164051	-1.247869
28	6	0	-4.118571	-0.094934	-1.176677
29	1	0	-5.834151	0.221323	0.098961
30	1	0	-2.264587	-0.361269	-2.215669
31	1	0	-4.711879	-0.243512	-2.076946
32	6	0	-0.335191	1.984761	-0.811563
33	6	0	0.927406	1.614243	-1.246627
34	1	0	1.061542	1.189459	-2.240291
35	6	0	-0.523359	2.898395	0.365868
36	6	0	0.655900	2.834921	1.326341
37	1	0	0.666241	1.850037	1.812549
38	1	0	0.542668	3.580493	2.120364
39	1	0	-1.168024	1.900852	-1.501549
40	6	0	2.144190	2.180239	-0.636916
41	6	0	1.968931	3.057951	0.585553
42	1	0	2.843868	2.930480	1.229821
43	1	0	2.013027	4.091315	0.212834
44	8	0	3.249380	2.005502	-1.142605
45	1	0	-0.632680	3.920615	-0.028453
46	1	0	-1.464066	2.663889	0.871906
47	1	0	-1.995219	0.419744	2.010816

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5538.69884085     A.U. after    1 cycles
             Convg  =    0.5313D-08             -V/T =  2.0039
Zero-point correction=                           0.405484 (Hartree/Particle)
 Thermal correction to Energy=                    0.426847
 Thermal correction to Enthalpy=                  0.427807
 Thermal correction to Gibbs Free Energy=         0.355615
 Sum of electronic and zero-point Energies=          -5538.293357
 Sum of electronic and thermal Energies=             -5538.271994
 Sum of electronic and thermal Enthalpies=           -5538.271034
 Sum of electronic and thermal Free Energies=        -5538.343226
                    1                      2                      3
Frequencies --    30.4522               60.7545                69.4864
```

COD-Rh(I)-Ph-CH-si-confU-CR-TS (147a)

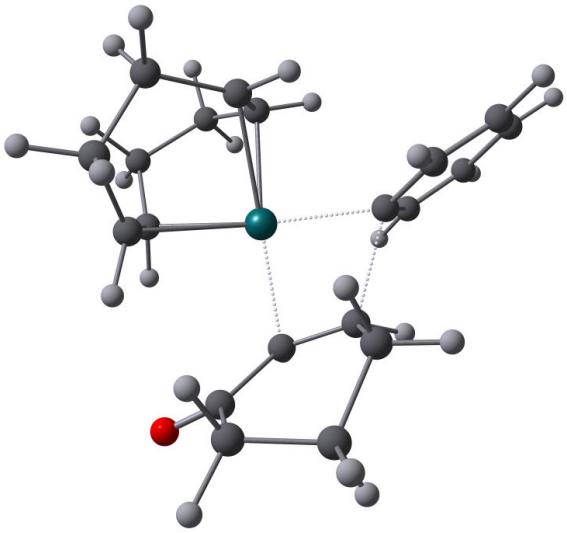


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.267282	-0.220601	-0.225707
2	6	0	-0.081421	-1.877423	1.252942
3	1	0	-0.870291	-1.487646	1.894141
4	6	0	1.199403	-2.287499	1.949162
5	1	0	1.004732	-2.380659	3.022713
6	1	0	1.499788	-3.283896	1.613820
7	6	0	2.335067	-1.280336	1.735325
8	1	0	2.231644	-0.467062	2.462450
9	1	0	3.308965	-1.748737	1.943163
10	6	0	2.346680	-0.655289	0.364171
11	1	0	2.894011	0.282669	0.305567
12	6	0	2.089634	-1.291398	-0.847498
13	1	0	2.417487	-0.761096	-1.741593
14	6	0	1.837273	-2.778414	-1.011888
15	1	0	2.246265	-3.099373	-1.975338
16	1	0	2.397419	-3.332592	-0.253424
17	6	0	0.346660	-3.145065	-0.961474
18	1	0	-0.084628	-3.017136	-1.960235
19	1	0	0.224906	-4.210457	-0.714718
20	6	0	-0.462587	-2.296321	-0.013306
21	1	0	-1.522457	-2.230332	-0.252731
22	6	0	-2.460575	0.487049	1.070508
23	6	0	-3.810755	0.159309	1.202857
24	6	0	-1.803885	0.385155	-0.166056
25	6	0	-4.543807	-0.272956	0.098497
26	1	0	-4.289550	0.239029	2.176441
27	6	0	-2.569475	-0.026498	-1.273703
28	6	0	-3.913593	-0.364910	-1.144610
29	1	0	-5.595928	-0.525204	0.201508
30	1	0	-2.104302	-0.078741	-2.257634
31	1	0	-4.474426	-0.690470	-2.017905
32	6	0	-0.615808	1.961878	-0.716656
33	6	0	0.694011	1.634055	-1.215405
34	1	0	0.787141	1.356598	-2.266927
35	6	0	-0.693903	2.947252	0.427407

36	6	0	0.466924	2.774856	1.394655
37	1	0	0.431638	1.764506	1.825665
38	1	0	0.380675	3.481347	2.227348
39	1	0	-1.362931	2.126506	-1.486690
40	6	0	1.898631	2.250999	-0.660085
41	6	0	1.789211	2.981463	0.666687
42	1	0	2.650609	2.700309	1.280948
43	1	0	1.923389	4.045430	0.429655
44	8	0	2.976086	2.220491	-1.258818
45	1	0	-0.644808	3.949773	-0.023056
46	1	0	-1.660098	2.882746	0.932707
47	1	0	-1.911728	0.812193	1.952321

```
SCF Done:  E(RPBE1PBE) =  -5538.68580296     A.U. after    1 cycles
             Convg  =    0.3430D-08             -V/T =  2.0039
Zero-point correction=                           0.404606 (Hartree/Particle)
 Thermal correction to Energy=                    0.425261
 Thermal correction to Enthalpy=                  0.426221
 Thermal correction to Gibbs Free Energy=         0.355196
 Sum of electronic and zero-point Energies=          -5538.281197
 Sum of electronic and thermal Energies=             -5538.260542
 Sum of electronic and thermal Enthalpies=           -5538.259582
 Sum of electronic and thermal Free Energies=        -5538.330607
                    1                    2                    3
Frequencies --  -286.9705               25.0753              41.4704
```

CHD-Rh(I)-Ph-CH-si-confD-CR-TS (117b)



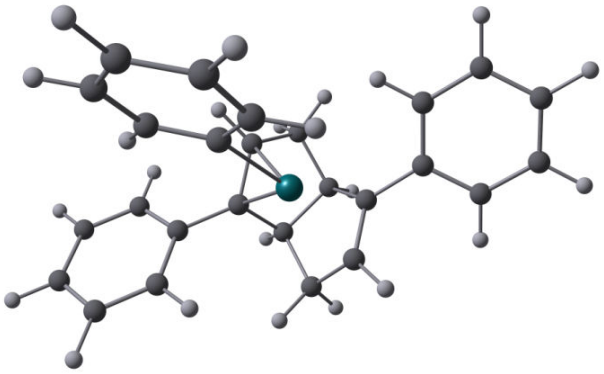
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.208057	-0.286681	-0.186745
2	6	0	-0.333886	-1.910561	1.260442
3	1	0	-1.076719	-1.446252	1.907461
4	6	0	0.887501	-2.480925	1.951485
5	1	0	0.682330	-2.560812	3.024118
6	1	0	1.062939	-3.503337	1.605612
7	6	0	2.139897	-1.618997	1.748550
8	1	0	2.146555	-0.817948	2.496062
9	1	0	3.048074	-2.212002	1.934667
10	6	0	2.220508	-0.968879	0.391236

11	1	0	2.866065	-0.094409	0.350595
12	6	0	1.894835	-1.549438	-0.831666
13	1	0	2.275793	-1.041070	-1.717166
14	6	0	1.474468	-2.995124	-1.015540
15	1	0	1.848509	-3.350694	-1.981074
16	1	0	1.961691	-3.619145	-0.260918
17	6	0	-0.049177	-3.184712	-0.975628
18	1	0	-0.456536	-2.986156	-1.972846
19	1	0	-0.298290	-4.232615	-0.750561
20	6	0	-0.757262	-2.263643	-0.013474
21	1	0	-1.802114	-2.073684	-0.253916
22	6	0	-2.486970	0.695073	1.090516
23	6	0	-3.876963	0.565001	1.128238
24	6	0	-1.776896	0.549694	-0.109615
25	6	0	-4.593032	0.291298	-0.035435
26	1	0	-4.400570	0.677464	2.075178
27	6	0	-2.521169	0.309753	-1.281904
28	6	0	-3.904575	0.162892	-1.244805
29	1	0	-5.674888	0.192097	-0.005346
30	1	0	-2.007049	0.236700	-2.239566
31	1	0	-4.449937	-0.040552	-2.163771
32	6	0	-0.339013	1.986484	-0.435028
33	6	0	0.847717	1.541413	-1.115956
34	1	0	0.769373	1.336976	-2.186049
35	6	0	-0.177984	2.739438	0.875268
36	1	0	-1.107109	2.391607	-1.085475
37	6	0	2.185496	1.983100	-0.713576
38	6	0	2.301884	2.801516	0.559965
39	1	0	3.204646	3.412855	0.476851
40	8	0	3.180607	1.742341	-1.397960
41	1	0	-1.084273	3.316124	1.082274
42	1	0	-1.956781	0.905246	2.016965
43	6	0	1.054310	3.638501	0.822450
44	1	0	2.460965	2.107175	1.396808
45	1	0	1.154883	4.185238	1.766393
46	1	0	0.938073	4.388980	0.030608
47	1	0	-0.051163	2.038852	1.707145

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5538.68203936     A.U. after    1 cycles
             Convg  =    0.1483D-08             -V/T =  2.0039
Zero-point correction=                           0.404825 (Hartree/Particle)
 Thermal correction to Energy=                    0.425519
 Thermal correction to Enthalpy=                  0.426479
 Thermal correction to Gibbs Free Energy=         0.355646
 Sum of electronic and zero-point Energies=          -5538.277214
 Sum of electronic and thermal Energies=             -5538.256520
 Sum of electronic and thermal Enthalpies=           -5538.255560
 Sum of electronic and thermal Free Energies=        -5538.326393
                    1                      2                      3
Frequencies --  -286.8434               36.2889                52.3627
```

(S)-2,6-diphenylbicyclo[3.3.0]octa-2,6-diene-Rh pathway

(*S*)-Ph[3.3.0]BOD-Rh(I)-Ph (150)



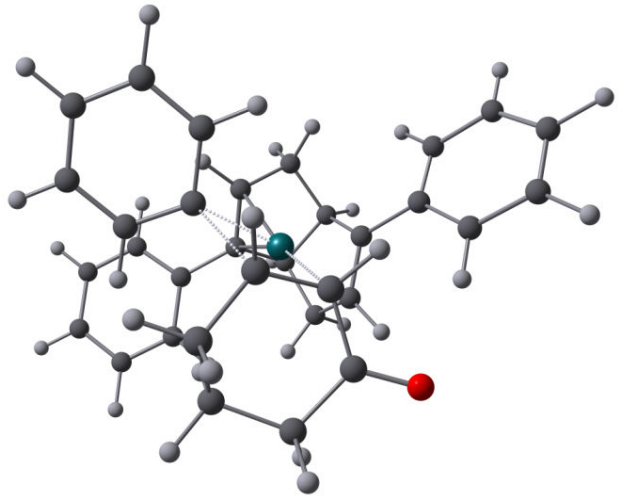
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.199004	0.299031	-0.368096
2	6	0	0.376250	-0.514931	1.506966
3	6	0	0.962646	-1.259912	0.444983
4	6	0	0.936867	1.922474	-0.025529
5	1	0	0.948635	0.182984	2.112685
6	6	0	-0.779133	-1.286154	2.098686
7	6	0	0.087057	-2.493021	0.170578
8	6	0	0.255389	3.035705	-0.543081
9	6	0	2.216329	2.133001	0.506032
10	6	0	-1.228492	-2.096688	0.886339
11	1	0	-1.569982	-0.668183	2.531135
12	1	0	-0.414356	-1.951414	2.896344
13	6	0	-0.274636	-2.576518	-1.310857
14	1	0	0.547456	-3.403547	0.573094
15	6	0	0.824789	4.311639	-0.547940
16	1	0	-0.752597	2.923736	-0.959613
17	6	0	2.794020	3.403808	0.504809
18	1	0	2.786907	1.298652	0.909469
19	6	0	-1.870987	-1.209758	-0.178870
20	1	0	-1.870847	-2.950598	1.135152
21	6	0	-1.266542	-1.442615	-1.402078
22	1	0	0.592138	-2.473761	-1.969509
23	1	0	-0.761549	-3.532817	-1.553597
24	6	0	2.101922	4.497041	-0.020079
25	1	0	0.273301	5.155739	-0.956732
26	1	0	3.794093	3.541964	0.911049
27	1	0	-1.683427	-1.090511	-2.345267
28	1	0	2.555186	5.485309	-0.017182
29	6	0	2.420698	-1.319925	0.158938
30	6	0	2.946697	-1.123426	-1.124194
31	6	0	3.309018	-1.625289	1.199965
32	6	0	4.315105	-1.227584	-1.359890
33	1	0	2.278189	-0.847100	-1.935257
34	6	0	4.679635	-1.728576	0.967506
35	1	0	2.918079	-1.780697	2.203086
36	6	0	5.188096	-1.531954	-0.315317
37	1	0	4.703524	-1.057545	-2.360883
38	1	0	5.350767	-1.960470	1.790816
39	1	0	6.256704	-1.607488	-0.498676

40	6	0	-3.187551	-0.539910	-0.019533
41	6	0	-3.381210	0.550800	0.841426
42	6	0	-4.287501	-1.005951	-0.754851
43	6	0	-4.630941	1.154955	0.959686
44	1	0	-2.538872	0.950666	1.399861
45	6	0	-5.538689	-0.404502	-0.635476
46	1	0	-4.155086	-1.853033	-1.423584
47	6	0	-5.715664	0.678525	0.224435
48	1	0	-4.755247	2.006369	1.623993
49	1	0	-6.376712	-0.782655	-1.215525
50	1	0	-6.690173	1.150599	0.317538

SCF Done: E(RPBE1PBE) = -5690.73365789 A.U. after 1 cycles
Convg = 0.3876D-08 -V/T = 2.0042
Zero-point correction= 0.413483 (Hartree/Particle)
Thermal correction to Energy= 0.436429
Thermal correction to Enthalpy= 0.437389
Thermal correction to Gibbs Free Energy= 0.358203
Sum of electronic and zero-point Energies= -5690.320175
Sum of electronic and thermal Energies= -5690.297229
Sum of electronic and thermal Enthalpies= -5690.296269
Sum of electronic and thermal Free Energies= -5690.375455

	1	2	3
Frequencies --	16.1810	30.9879	33.8380

(*S*)-Ph[3.3.0]BOD-Rh(I)-Ph-CH-si-confU-CR-TS (155a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.227378	0.144418	0.078471
2	6	0	0.530435	-1.902007	0.589637
3	6	0	0.992368	-1.577713	-0.684184
4	6	0	1.069602	0.679971	1.714540
5	1	0	1.155715	-1.847782	1.475465
6	6	0	-0.657079	-2.818956	0.520538
7	6	0	0.030329	-2.153276	-1.725101
8	6	0	0.541200	0.336026	2.973951
9	6	0	2.463798	0.728188	1.587314
10	6	0	-1.215615	-2.448514	-0.853724
11	1	0	-1.360747	-2.674355	1.343505
12	1	0	-0.323746	-3.867822	0.546460

13	6	0	-0.443954	-1.097574	-2.716833
14	1	0	0.457373	-3.047913	-2.194637
15	6	0	1.368934	0.006869	4.043325
16	1	0	-0.538569	0.323867	3.118944
17	6	0	3.298387	0.414115	2.662153
18	1	0	2.917054	0.988452	0.633786
19	6	0	-1.893177	-1.083053	-0.830140
20	1	0	-1.871731	-3.210426	-1.292834
21	6	0	-1.350259	-0.279059	-1.836126
22	1	0	0.361911	-0.534508	-3.190272
23	1	0	-1.034621	-1.553660	-3.526010
24	6	0	2.757944	0.046309	3.892805
25	1	0	0.930684	-0.268748	5.000051
26	1	0	4.377328	0.449310	2.528269
27	1	0	-1.845659	0.610321	-2.212371
28	1	0	3.408384	-0.196935	4.729118
29	6	0	2.417079	-1.305211	-1.001206
30	6	0	2.828609	-0.389248	-1.980919
31	6	0	3.413500	-2.026938	-0.325767
32	6	0	4.177999	-0.192598	-2.262988
33	1	0	2.091408	0.201872	-2.513771
34	6	0	4.764086	-1.833567	-0.604989
35	1	0	3.122191	-2.752760	0.428486
36	6	0	5.154557	-0.913005	-1.575778
37	1	0	4.467594	0.531673	-3.020277
38	1	0	5.512854	-2.406092	-0.063332
39	1	0	6.207573	-0.759003	-1.796337
40	6	0	-3.216056	-0.889448	-0.193945
41	6	0	-3.838299	-1.937965	0.503208
42	6	0	-3.934170	0.311766	-0.337214
43	6	0	-5.106997	-1.786637	1.060791
44	1	0	-3.343161	-2.898518	0.599957
45	6	0	-5.196678	0.463850	0.223350
46	1	0	-3.509769	1.139570	-0.899050
47	6	0	-5.791350	-0.581324	0.933083
48	1	0	-5.561270	-2.619297	1.592087
49	1	0	-5.725273	1.405227	0.095258
50	1	0	-6.780035	-0.460145	1.367975
51	6	0	0.028444	2.378314	1.031233
52	6	0	-1.100234	2.137765	0.189493
53	1	0	-0.204963	2.505135	2.082895
54	1	0	-2.063304	1.969003	0.669594
55	6	0	-1.181344	2.764667	-1.133671
56	8	0	-2.253185	2.868602	-1.737177
57	6	0	0.071947	3.364970	-1.740328
58	1	0	0.134240	3.028420	-2.780198
59	6	0	1.119174	3.287143	0.522511
60	1	0	2.035968	3.158316	1.101441
61	6	0	1.354269	3.091363	-0.965457
62	1	0	-0.117153	4.445626	-1.787051
63	1	0	1.683916	2.059798	-1.136816
64	1	0	2.156612	3.747305	-1.319900
65	1	0	0.771993	4.315119	0.708391

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 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5999.07561066     A.U. after    1 cycles
             Convg  =    0.3505D-08             -V/T =  2.0047
Zero-point correction=                           0.545406 (Hartree/Particle)
 Thermal correction to Energy=                    0.574542
 Thermal correction to Enthalpy=                  0.575502
 Thermal correction to Gibbs Free Energy=         0.485816
 Sum of electronic and zero-point Energies=          -5998.530205
 Sum of electronic and thermal Energies=             -5998.501069
 Sum of electronic and thermal Enthalpies=           -5998.500108
```
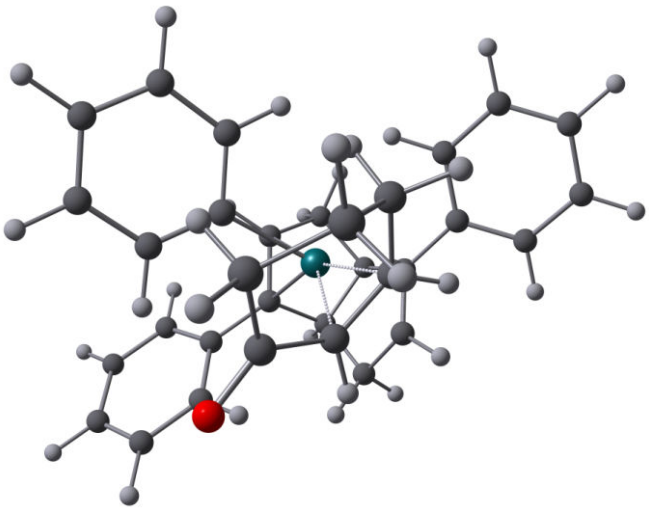

```
 Sum of electronic and thermal Free Energies=         -5998.589794
                      1                      2                      3
Frequencies --   -262.2140              27.5610              32.8179
```

(*S*)-Ph[3.3.0]BOD-Rh(I)-Ph-CH-si-confD-close (152a)

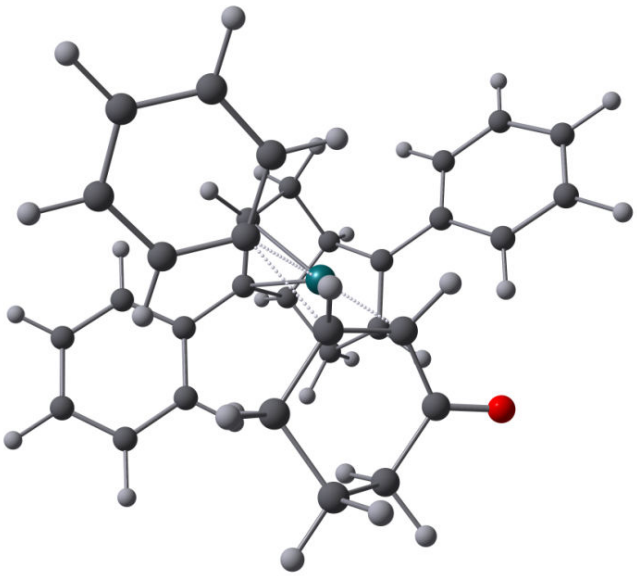


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.239272	-0.048166	-0.023056
2	6	0	0.430306	-1.411257	1.597596
3	6	0	0.976064	-1.873302	0.396677
4	6	0	0.945970	1.263988	0.992632
5	1	0	1.016585	-0.870784	2.335141
6	6	0	-0.770371	-2.240154	1.988968
7	6	0	0.077300	-2.975894	-0.167457
8	6	0	0.309444	1.970726	2.028733
9	6	0	2.316458	1.490951	0.811090
10	6	0	-1.230994	-2.744688	0.625225
11	1	0	-1.542533	-1.701493	2.543117
12	1	0	-0.447224	-3.078374	2.624859
13	6	0	-0.285164	-2.728020	-1.627034
14	1	0	0.528676	-3.958902	0.016133
15	6	0	1.001175	2.882520	2.829590
16	1	0	-0.749101	1.806650	2.233780
17	6	0	3.013585	2.404426	1.606307
18	1	0	2.856411	0.968926	0.025527
19	6	0	-1.890061	-1.656706	-0.223959
20	1	0	-1.874104	-3.632019	0.678545
21	6	0	-1.300981	-1.631157	-1.468448
22	1	0	0.574223	-2.466152	-2.249458
23	1	0	-0.757935	-3.613270	-2.077739
24	6	0	2.361360	3.108685	2.617744
25	1	0	0.475231	3.413914	3.620664
26	1	0	4.074808	2.566287	1.427983
27	1	0	-1.724044	-1.107152	-2.322071
28	1	0	2.904619	3.819917	3.235135
29	6	0	2.416977	-1.827384	0.040117
30	6	0	2.882105	-1.363163	-1.197032
31	6	0	3.353907	-2.316241	0.961520
32	6	0	4.239486	-1.392909	-1.505929

33	1	0	2.184761	-0.914524	-1.898012
34	6	0	4.712395	-2.348477	0.653678
35	1	0	3.010613	-2.675159	1.928836
36	6	0	5.160338	-1.890668	-0.584502
37	1	0	4.578520	-1.004385	-2.462594
38	1	0	5.422002	-2.727896	1.384669
39	1	0	6.220296	-1.908563	-0.824327
40	6	0	-3.216777	-1.062734	0.076673
41	6	0	-3.449074	-0.242369	1.190798
42	6	0	-4.293619	-1.329584	-0.782149
43	6	0	-4.711235	0.293402	1.434237
44	1	0	-2.629568	0.005036	1.859896
45	6	0	-5.557608	-0.795984	-0.539326
46	1	0	-4.135186	-1.971779	-1.645004
47	6	0	-5.771970	0.017335	0.571991
48	1	0	-4.865269	0.934325	2.298539
49	1	0	-6.376544	-1.018986	-1.218392
50	1	0	-6.756796	0.434655	0.764090
51	6	0	-1.295263	1.466489	-1.409598
52	6	0	-0.043015	1.199667	-1.941806
53	1	0	-2.144616	0.861916	-1.716744
54	1	0	0.110809	0.376858	-2.637094
55	6	0	1.015938	2.235052	-1.993223
56	8	0	2.084500	2.005782	-2.548576
57	6	0	0.693190	3.595896	-1.414772
58	1	0	1.053286	3.597821	-0.378836
59	1	0	1.286868	4.334082	-1.961590
60	6	0	-0.798159	3.917422	-1.451358
61	1	0	-0.986049	4.871330	-0.947155
62	1	0	-1.123445	4.037972	-2.492394
63	6	0	-1.621165	2.807246	-0.797701
64	1	0	-1.424974	2.802210	0.279996
65	1	0	-2.692333	3.000087	-0.915083

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5999.08482653     A.U. after    1 cycles
             Convg  =    0.4415D-08             -V/T =  2.0047
Zero-point correction=                           0.544445 (Hartree/Particle)
 Thermal correction to Energy=                    0.574822
 Thermal correction to Enthalpy=                  0.575782
 Thermal correction to Gibbs Free Energy=         0.482146
 Sum of electronic and zero-point Energies=          -5998.540381
 Sum of electronic and thermal Energies=             -5998.510005
 Sum of electronic and thermal Enthalpies=           -5998.509045
 Sum of electronic and thermal Free Energies=        -5998.602680
                    1                      2                      3
Frequencies --    23.0128               32.0735               35.9860
```

(*S*)-Ph[3.3.0]BOD-Rh(I)-Ph-CH-si-confD-CR-TS (155b)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.214246	0.074378	0.121242
2	6	0	0.485674	-2.015237	-0.285026
3	6	0	0.996502	-1.166934	-1.268825
4	6	0	0.976017	-0.222413	1.879905
5	1	0	1.076526	-2.375385	0.551865
6	6	0	-0.703958	-2.780517	-0.791743
7	6	0	0.074680	-1.210484	-2.489744
8	6	0	0.203637	-0.870803	2.863180
9	6	0	2.366703	-0.367237	1.936159
10	6	0	-1.205401	-1.825985	-1.874940
11	1	0	-1.440830	-2.996338	-0.014357
12	1	0	-0.380734	-3.740888	-1.221805
13	6	0	-0.352468	0.182857	-2.935130
14	1	0	0.514885	-1.820586	-3.287985
15	6	0	0.796979	-1.689005	3.820464
16	1	0	-0.877473	-0.738520	2.877678
17	6	0	2.964787	-1.168367	2.911761
18	1	0	3.000480	0.125413	1.203364
19	6	0	-1.859694	-0.591623	-1.263372
20	1	0	-1.855304	-2.293532	-2.625159
21	6	0	-1.285161	0.557190	-1.812915
22	1	0	0.479188	0.873515	-3.087395
23	1	0	-0.912783	0.141136	-3.881578
24	6	0	2.186018	-1.841205	3.851295
25	1	0	0.175510	-2.198266	4.553780
26	1	0	4.047819	-1.270006	2.928676
27	1	0	-1.766173	1.529297	-1.779756
28	1	0	2.653533	-2.466077	4.607868
29	6	0	2.430795	-0.801381	-1.386738
30	6	0	2.868341	0.475954	-1.766813
31	6	0	3.405782	-1.781374	-1.146665
32	6	0	4.224858	0.765146	-1.891709
33	1	0	2.142024	1.264199	-1.938105
34	6	0	4.763765	-1.495789	-1.269172

35	1	0	3.091333	-2.781429	-0.860443
36	6	0	5.180831	-0.219389	-1.642370
37	1	0	4.536757	1.766398	-2.178303
38	1	0	5.497299	-2.273846	-1.073346
39	1	0	6.239495	0.006962	-1.737558
40	6	0	-3.178374	-0.661673	-0.595971
41	6	0	-3.864735	-1.882235	-0.492059
42	6	0	-3.820947	0.491786	-0.111340
43	6	0	-5.127193	-1.955557	0.094580
44	1	0	-3.424508	-2.790951	-0.889979
45	6	0	-5.077563	0.416979	0.477217
46	1	0	-3.343216	1.463723	-0.201903
47	6	0	-5.738301	-0.807910	0.591874
48	1	0	-5.634072	-2.915277	0.157168
49	1	0	-5.548870	1.326330	0.841887
50	1	0	-6.721530	-0.862670	1.051865
51	6	0	0.370852	1.784308	1.669890
52	6	0	-0.878045	1.973053	0.998946
53	1	0	0.285416	1.656918	2.742663
54	1	0	-1.784238	1.736681	1.557342
55	6	0	-1.047425	3.045583	0.014227
56	8	0	-2.161327	3.406927	-0.372447
57	6	0	0.200802	3.758612	-0.464355
58	1	0	0.642871	3.165853	-1.276705
59	1	0	-0.107097	4.717174	-0.890141
60	6	0	1.212639	3.923591	0.665397
61	1	0	2.107086	4.442973	0.304591
62	1	0	0.778508	4.549270	1.455113
63	6	0	1.600849	2.560033	1.230001
64	1	0	2.149109	2.011193	0.459311
65	1	0	2.283207	2.664478	2.078986

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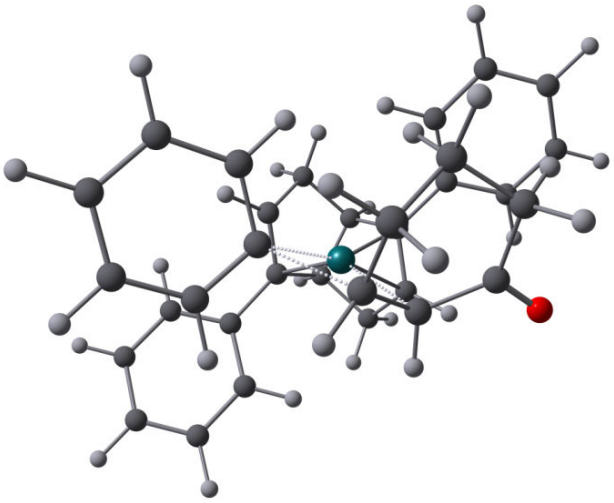
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5999.07352668     A.U. after    1 cycles
             Convg  =    0.4263D-08             -V/T =  2.0047
Zero-point correction=                           0.545179 (Hartree/Particle)
 Thermal correction to Energy=                   0.574365
 Thermal correction to Enthalpy=                 0.575325
 Thermal correction to Gibbs Free Energy=        0.485556
 Sum of electronic and zero-point Energies=          -5998.528348
 Sum of electronic and thermal Energies=             -5998.499162
 Sum of electronic and thermal Enthalpies=           -5998.498202
 Sum of electronic and thermal Free Energies=        -5998.587971
                    1                    2                    3
Frequencies --  -261.9624               27.2505              38.9220
```

(*S*)-Ph[3.3.0]BOD-Rh(I)-Ph-CH-re-confU-CR-TS (162a)

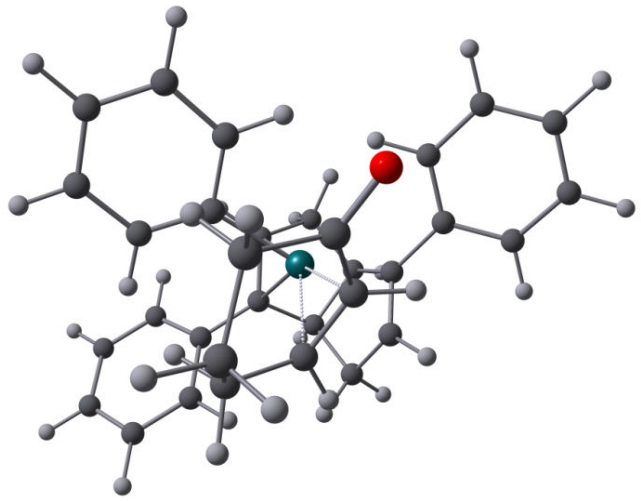


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.013703	-0.038807	0.217137
2	6	0	-0.995410	-0.779062	-1.688050
3	6	0	-1.468513	-1.492680	-0.586272
4	6	0	-1.139191	1.784594	-0.174343
5	1	0	-1.551658	0.032527	-2.148174
6	6	0	0.020025	-1.596953	-2.444381
7	6	0	-0.678175	-2.799149	-0.458376
8	6	0	-0.770517	2.461221	-1.351157
9	6	0	-2.472161	1.912714	0.246911
10	6	0	0.563602	-2.461593	-1.313190
11	1	0	0.781365	-1.017553	-2.969053
12	1	0	-0.487592	-2.217998	-3.198473
13	6	0	-0.131849	-3.000942	0.949176
14	1	0	-1.260872	-3.645027	-0.843790
15	6	0	-1.698290	3.191411	-2.092794
16	1	0	0.253804	2.406316	-1.712436
17	6	0	-3.404686	2.640974	-0.489009
18	1	0	-2.794974	1.436972	1.170852
19	6	0	1.381105	-1.647984	-0.305066
20	1	0	1.121274	-3.344749	-1.648460
21	6	0	0.915452	-1.917704	0.986876
22	1	0	-0.889794	-2.936589	1.732538
23	1	0	0.348733	-3.986507	1.044571
24	6	0	-3.023828	3.283839	-1.667133
25	1	0	-1.381984	3.690907	-3.006077
26	1	0	-4.431331	2.707965	-0.136401
27	1	0	1.498594	-1.698860	1.878354
28	1	0	-3.747231	3.858563	-2.239851
29	6	0	-2.830367	-1.357962	-0.008938
30	6	0	-3.069456	-1.340169	1.373275
31	6	0	-3.934968	-1.284666	-0.868637
32	6	0	-4.364508	-1.251614	1.876345
33	1	0	-2.230486	-1.353009	2.062811
34	6	0	-5.232283	-1.192480	-0.368341
35	1	0	-3.771570	-1.300127	-1.943182
36	6	0	-5.453652	-1.178237	1.007554
37	1	0	-4.523442	-1.230478	2.951693

38	1	0	-6.072049	-1.133146	-1.056198
39	1	0	-6.464696	-1.107752	1.400179
40	6	0	2.751422	-1.164825	-0.616960
41	6	0	3.019887	-0.249078	-1.647061
42	6	0	3.840500	-1.672248	0.107353
43	6	0	4.323819	0.138063	-1.944243
44	1	0	2.200301	0.192811	-2.204921
45	6	0	5.145798	-1.283767	-0.185158
46	1	0	3.658859	-2.379056	0.911560
47	6	0	5.395049	-0.379848	-1.216297
48	1	0	4.503011	0.854901	-2.741853
49	1	0	5.969543	-1.688150	0.397267
50	1	0	6.412965	-0.076398	-1.446817
51	6	0	0.119013	2.067224	1.451897
52	1	0	-0.773130	2.344310	2.005006
53	6	0	0.810931	0.923821	1.966869
54	1	0	0.306074	0.333673	2.733781
55	6	0	2.271766	0.879000	2.073983
56	8	0	2.829743	0.048491	2.794127
57	6	0	0.970170	3.237940	1.012256
58	1	0	0.410918	3.907650	0.355706
59	6	0	3.084303	1.926659	1.343991
60	1	0	3.919800	1.422448	0.848269
61	6	0	2.276282	2.782282	0.377054
62	1	0	1.192911	3.807109	1.927698
63	1	0	2.061591	2.199916	-0.526091
64	1	0	2.865999	3.649159	0.059961
65	1	0	3.526140	2.555875	2.128550

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5999.07199767     A.U. after    1 cycles
             Convg  =    0.6025D-08             -V/T =  2.0047
Zero-point correction=                           0.544987 (Hartree/Particle)
 Thermal correction to Energy=                   0.574077
 Thermal correction to Enthalpy=                 0.575037
 Thermal correction to Gibbs Free Energy=        0.485280
 Sum of electronic and zero-point Energies=          -5998.527011
 Sum of electronic and thermal Energies=             -5998.497921
 Sum of electronic and thermal Enthalpies=           -5998.496961
 Sum of electronic and thermal Free Energies=        -5998.586718
                     1                      2                      3
Frequencies --  -288.2547               22.6675                34.9906
```

(*S*)-Ph[3.3.0]BOD-Rh(I)-Ph-CH-re-confD-close (159b)

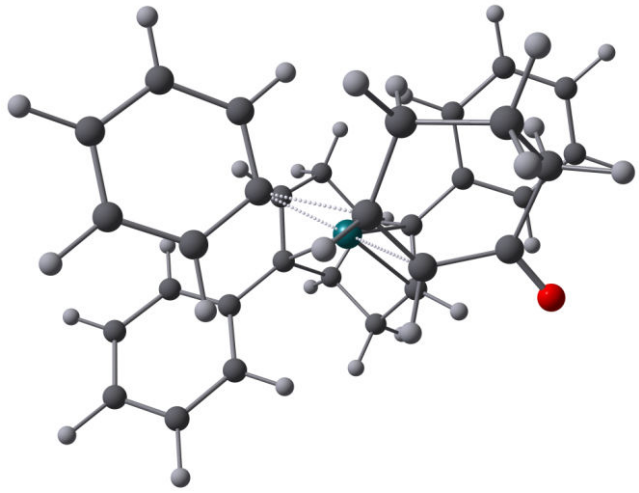


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.198551	-0.063780	-0.044926
2	6	0	0.459406	-1.379761	1.594037
3	6	0	1.036926	-1.840820	0.400799
4	6	0	0.864911	1.327731	0.971967
5	1	0	1.021409	-0.811990	2.330570
6	6	0	-0.703020	-2.254127	1.997773
7	6	0	0.174122	-2.982011	-0.153742
8	6	0	0.068179	2.183461	1.753126
9	6	0	2.253316	1.497360	1.044773
10	6	0	-1.139904	-2.791800	0.641751
11	1	0	-1.498965	-1.742670	2.543896
12	1	0	-0.344383	-3.070085	2.643412
13	6	0	-0.223520	-2.780350	-1.614401
14	1	0	0.659867	-3.946710	0.038612
15	6	0	0.631524	3.180156	2.551961
16	1	0	-1.018624	2.100657	1.723884
17	6	0	2.822999	2.499426	1.836568
18	1	0	2.916071	0.841412	0.483450
19	6	0	-1.845624	-1.743417	-0.216292
20	1	0	-1.748586	-3.702662	0.704020
21	6	0	-1.285756	-1.725648	-1.467369
22	1	0	0.609750	-2.501174	-2.263774
23	1	0	-0.663228	-3.697981	-2.032878
24	6	0	2.016444	3.347669	2.593488
25	1	0	-0.015780	3.833720	3.133226
26	1	0	3.905390	2.610881	1.862897
27	1	0	-1.737172	-1.216024	-2.315246
28	1	0	2.459155	4.127358	3.208396
29	6	0	2.489639	-1.772800	0.099949
30	6	0	2.995060	-1.510218	-1.181626
31	6	0	3.410324	-2.023268	1.128620
32	6	0	4.365706	-1.493454	-1.424363
33	1	0	2.311335	-1.277870	-1.991524
34	6	0	4.782938	-2.005295	0.889656
35	1	0	3.041892	-2.235521	2.128779
36	6	0	5.267924	-1.740883	-0.389600
37	1	0	4.732059	-1.275123	-2.424404
38	1	0	5.474132	-2.197720	1.706280
39	1	0	6.337950	-1.723057	-0.578804
40	6	0	-3.168985	-1.155617	0.107580
41	6	0	-3.376587	-0.298263	1.197797
42	6	0	-4.267470	-1.470822	-0.705827
43	6	0	-4.638193	0.227959	1.461787
44	1	0	-2.540603	-0.009702	1.829511
45	6	0	-5.531270	-0.949553	-0.439396
46	1	0	-4.125912	-2.140464	-1.550609
47	6	0	-5.721433	-0.097945	0.647315
48	1	0	-4.772230	0.904792	2.301339
49	1	0	-6.368249	-1.208971	-1.082557
50	1	0	-6.705262	0.314343	0.854503
51	6	0	0.258618	0.857798	-2.119477
52	1	0	0.202410	-0.060644	-2.698957
53	6	0	-0.923858	1.401230	-1.624671
54	1	0	-1.892697	0.944786	-1.817747
55	6	0	-1.004621	2.825433	-1.223296
56	8	0	-2.055201	3.305659	-0.812457
57	6	0	1.492555	1.698630	-2.337865
58	1	0	2.022619	1.321936	-3.219788
59	1	0	2.184994	1.597621	-1.497104

60	6	0	0.238981	3.670240	-1.397041
61	1	0	0.785537	3.641469	-0.446360
62	1	0	-0.084793	4.703575	-1.551208
63	6	0	1.130438	3.170889	-2.528925
64	1	0	2.041275	3.776350	-2.584338
65	1	0	0.608436	3.292722	-3.486480

```
SCF Done:  E(RPBE1PBE) =  -5999.08451216     A.U. after    1 cycles
             Convg  =    0.2186D-08             -V/T =  2.0047
Zero-point correction=                          0.544514 (Hartree/Particle)
 Thermal correction to Energy=                  0.574789
 Thermal correction to Enthalpy=                0.575749
 Thermal correction to Gibbs Free Energy=       0.482827
 Sum of electronic and zero-point Energies=          -5998.539998
 Sum of electronic and thermal Energies=             -5998.509723
 Sum of electronic and thermal Enthalpies=           -5998.508763
 Sum of electronic and thermal Free Energies=        -5998.601685
                     1                      2                      3
Frequencies --    26.1598                29.9297                40.9864
```

(*S*)-Ph[3.3.0]BOD-Rh(I)-Ph-CH-re-confD-CR-TS (162b)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.020506	-0.030174	-0.185651
2	6	0	1.036017	-0.872077	1.658075
3	6	0	1.505135	-1.514684	0.512231
4	6	0	1.153066	1.777444	0.293537
5	1	0	1.588013	-0.082356	2.159441
6	6	0	0.037594	-1.742932	2.375928
7	6	0	0.727211	-2.819916	0.315156
8	6	0	0.948383	2.377319	1.546174
9	6	0	2.417018	1.943207	-0.298416
10	6	0	-0.508049	-2.546702	1.201321
11	1	0	-0.724760	-1.202820	2.939860
12	1	0	0.559474	-2.400701	3.087903
13	6	0	0.166359	-2.943796	-1.095568
14	1	0	1.322985	-3.680898	0.642857
15	6	0	1.969894	3.068132	2.199399
16	1	0	-0.015875	2.291258	2.042340
17	6	0	3.442353	2.626225	0.350160

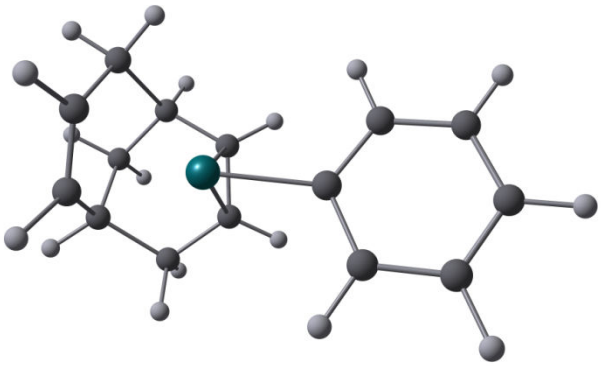
18	1	0	2.610184	1.531711	-1.287111
19	6	0	-1.343985	-1.682166	0.252148
20	1	0	-1.053620	-3.453727	1.489308
21	6	0	-0.890633	-1.869611	-1.059260
22	1	0	0.914653	-2.827781	-1.882235
23	1	0	-0.307043	-3.926425	-1.243045
24	6	0	3.225660	3.193623	1.607162
25	1	0	1.779763	3.509729	3.175389
26	1	0	4.413028	2.718288	-0.131674
27	1	0	-1.480101	-1.599887	-1.932649
28	1	0	4.021157	3.735992	2.111742
29	6	0	2.857751	-1.327538	-0.071091
30	6	0	3.080165	-1.238015	-1.453264
31	6	0	3.970883	-1.277565	0.779155
32	6	0	4.367537	-1.103169	-1.965280
33	1	0	2.233515	-1.231077	-2.133377
34	6	0	5.260652	-1.139763	0.269988
35	1	0	3.820217	-1.349189	1.853300
36	6	0	5.465409	-1.054433	-1.105848
37	1	0	4.513651	-1.026812	-3.039968
38	1	0	6.107389	-1.100335	0.950662
39	1	0	6.470527	-0.948268	-1.505675
40	6	0	-2.712134	-1.231397	0.616295
41	6	0	-2.964357	-0.356079	1.685277
42	6	0	-3.812735	-1.725311	-0.099023
43	6	0	-4.265294	-0.000924	2.032726
44	1	0	-2.134643	0.081256	2.231741
45	6	0	-5.114900	-1.364722	0.241171
46	1	0	-3.642399	-2.397864	-0.934780
47	6	0	-5.348686	-0.506365	1.313732
48	1	0	-4.432876	0.682086	2.861923
49	1	0	-5.948492	-1.757007	-0.335561
50	1	0	-6.364024	-0.226751	1.582371
51	6	0	-0.356892	2.168994	-1.083098
52	1	0	0.434392	2.692635	-1.608749
53	6	0	-0.915618	1.057385	-1.794067
54	1	0	-0.332520	0.659668	-2.628536
55	6	0	-2.362482	0.918846	-2.016556
56	8	0	-2.807021	0.081125	-2.801778
57	6	0	-1.312179	3.067753	-0.319591
58	1	0	-0.826933	4.023437	-0.102454
59	1	0	-1.576369	2.620701	0.643044
60	6	0	-3.281479	1.905108	-1.328293
61	1	0	-3.574712	1.475075	-0.361620
62	1	0	-4.189771	1.984056	-1.931808
63	6	0	-2.605688	3.255597	-1.110476
64	1	0	-3.274398	3.931041	-0.565736
65	1	0	-2.392833	3.728996	-2.077228

SCF Done: E(RPBE1PBE) = -5999.06804751 A.U. after 1 cycles
Convg = 0.3496D-08 -V/T = 2.0047
Zero-point correction= 0.544862 (Hartree/Particle)
Thermal correction to Energy= 0.574020
Thermal correction to Enthalpy= 0.574980
Thermal correction to Gibbs Free Energy= 0.485063
Sum of electronic and zero-point Energies= -5998.523186
Sum of electronic and thermal Energies= -5998.494028
Sum of electronic and thermal Enthalpies= -5998.493068
Sum of electronic and thermal Free Energies= -5998.582984

	1	2	3
Frequencies --	-288.0764	28.0716	35.2935

(R)-BND-Rh pathway

(*R*)-BND-Rh(I)-Ph (165)

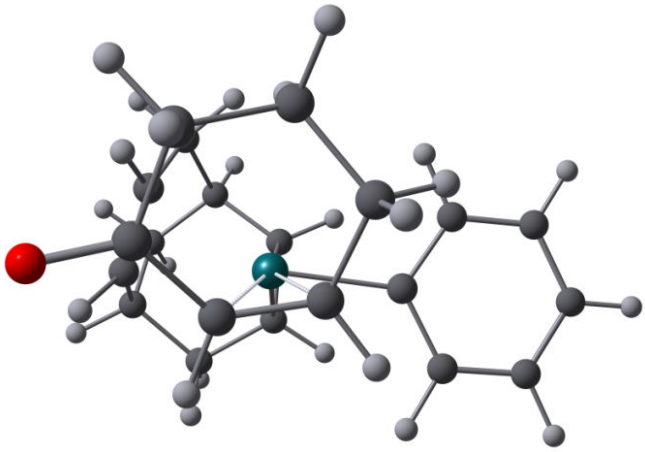


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.053337	0.000737	-0.625157
2	6	0	-0.857648	-0.504145	1.254394
3	1	0	-0.148995	-1.121978	1.806465
4	6	0	-2.255173	-1.098760	1.061851
5	1	0	-2.461737	-1.807995	1.871312
6	6	0	-2.313344	-1.815936	-0.288729
7	1	0	-1.566944	-2.617347	-0.339723
8	1	0	-3.296921	-2.286849	-0.436813
9	6	0	-2.033926	-0.791228	-1.360367
10	1	0	-1.846022	-1.146609	-2.374797
11	6	0	-2.234536	0.557880	-1.153978
12	1	0	-2.162940	1.235628	-2.005017
13	6	0	-2.807870	1.131514	0.132207
14	1	0	-3.624168	1.819956	-0.115755
15	6	0	-1.707250	1.878606	0.888518
16	1	0	-1.310042	2.710067	0.293989
17	1	0	-2.112134	2.316234	1.814321
18	6	0	-0.605748	0.894434	1.192083
19	1	0	0.270094	1.280598	1.711743
20	6	0	1.871878	-0.004015	-0.046202
21	6	0	2.507542	-1.156103	0.449879
22	6	0	2.685010	1.111640	-0.317999
23	6	0	3.892604	-1.206551	0.628085
24	1	0	1.917826	-2.039024	0.693972
25	6	0	4.069442	1.069281	-0.137507
26	1	0	2.234957	2.037365	-0.678053
27	6	0	4.680186	-0.093401	0.334367
28	1	0	4.357534	-2.117046	1.001596
29	1	0	4.672581	1.947378	-0.360587
30	1	0	5.757354	-0.128733	0.478314
31	6	0	-3.312140	0.007200	1.038983
32	1	0	-4.262155	-0.398323	0.671790
33	1	0	-3.492283	0.401021	2.045814

SCF Done: E(RPBE1PBE) = -5268.42428159 A.U. after 1 cycles
Convg = 0.2943D-08 -V/T = 2.0033
Zero-point correction= 0.281347 (Hartree/Particle)
Thermal correction to Energy= 0.295092
Thermal correction to Enthalpy= 0.296052
Thermal correction to Gibbs Free Energy= 0.239310
Sum of electronic and zero-point Energies= -5268.142935

```
 Sum of electronic and thermal Energies=            -5268.129189
 Sum of electronic and thermal Enthalpies=          -5268.128229
 Sum of electronic and thermal Free Energies=       -5268.184972
                      1                      2                      3
Frequencies --    27.4031                50.0441                51.7824
```

(*R*)-BND-Rh(I)-Ph-CH-si-confU-anti (169a)



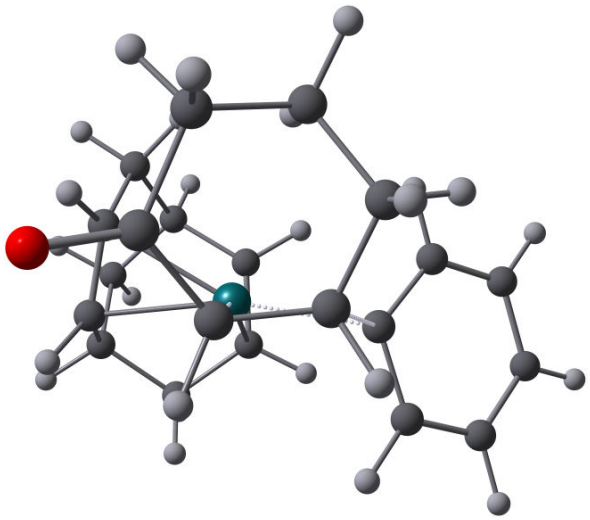
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.108390	-0.080669	-0.189047
2	6	0	0.261030	-2.104350	0.726605
3	1	0	-0.639587	-2.216878	1.327440
4	6	0	1.587501	-2.241661	1.459483
5	1	0	1.464054	-2.941945	2.293199
6	6	0	1.997378	-0.868980	1.984689
7	1	0	1.234535	-0.460061	2.657726
8	1	0	2.932405	-0.926691	2.562374
9	6	0	2.172937	0.036910	0.796814
10	1	0	2.353538	1.089942	0.999765
11	6	0	2.412673	-0.443043	-0.473139
12	1	0	2.714530	0.265245	-1.242503
13	6	0	2.571114	-1.919922	-0.786804
14	1	0	3.467687	-2.052970	-1.402696
15	6	0	1.339398	-2.409247	-1.547711
16	1	0	1.206986	-1.858253	-2.485856
17	1	0	1.446540	-3.471542	-1.815501
18	6	0	0.139966	-2.212617	-0.660908
19	1	0	-0.834341	-2.449657	-1.080755
20	6	0	-2.577779	-0.320068	1.142076
21	6	0	-3.942939	-0.585175	1.285076
22	6	0	-1.944486	-0.356713	-0.111500
23	6	0	-4.719637	-0.901667	0.171803
24	1	0	-4.397569	-0.546346	2.273248
25	6	0	-2.748834	-0.677648	-1.217849
26	6	0	-4.112281	-0.947155	-1.083301
27	1	0	-5.781015	-1.110659	0.279873
28	1	0	-2.309086	-0.715825	-2.214655
29	1	0	-4.701953	-1.192828	-1.964500
30	6	0	-0.876527	1.932564	-0.831736
31	6	0	0.451309	1.887713	-1.232574
32	1	0	0.714777	1.521405	-2.223460
33	6	0	-1.317002	2.768639	0.336986

34	6	0	-0.184740	2.998136	1.328569
35	1	0	0.053508	2.046270	1.821921
36	1	0	-0.499641	3.693031	2.114078
37	1	0	-1.643766	1.656279	-1.547385
38	6	0	1.476919	2.725008	-0.585205
39	6	0	1.053985	3.536725	0.621443
40	1	0	1.913568	3.634799	1.290990
41	1	0	0.849226	4.546494	0.237542
42	8	0	2.609988	2.817287	-1.049833
43	1	0	-1.666794	3.733035	-0.062786
44	1	0	-2.181512	2.305011	0.820890
45	1	0	-1.999631	-0.079823	2.034075
46	6	0	2.680019	-2.728362	0.506344
47	1	0	2.562258	-3.795678	0.286729
48	1	0	3.663792	-2.595074	0.971072

SCF Done: E(RPBE1PBE) = -5576.78272615 A.U. after 1 cycles
Convg = 0.3720D-08 -V/T = 2.0040
Zero-point correction= 0.412525 (Hartree/Particle)
Thermal correction to Energy= 0.433559
Thermal correction to Enthalpy= 0.434520
Thermal correction to Gibbs Free Energy= 0.362776
Sum of electronic and zero-point Energies= -5576.370201
Sum of electronic and thermal Energies= -5576.349167
Sum of electronic and thermal Enthalpies= -5576.348207
Sum of electronic and thermal Free Energies= -5576.419950

	1	2	3
Frequencies --	30.9550	52.0000	66.2234

(*R*)-BND-Rh(I)-Ph-CH-si-confU-CR-TS (170a)



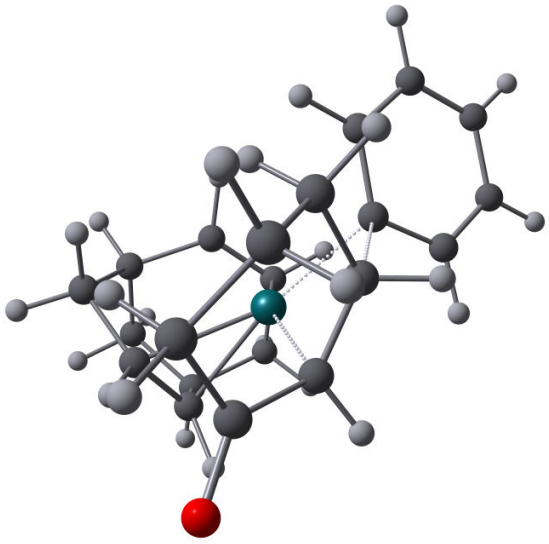
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.231600	-0.028451	-0.274401
2	6	0	0.603951	-1.831033	1.058258
3	1	0	-0.183976	-1.794782	1.809096
4	6	0	2.034810	-1.743164	1.565438
5	1	0	2.101968	-2.256593	2.531578
6	6	0	2.417738	-0.273271	1.723491
7	1	0	1.753516	0.235206	2.432614

8	1	0	3.440140	-0.174990	2.119225
9	6	0	2.308587	0.372432	0.368744
10	1	0	2.484851	1.442901	0.309160
11	6	0	2.360771	-0.367245	-0.810130
12	1	0	2.510659	0.173402	-1.744173
13	6	0	2.612385	-1.869512	-0.837603
14	1	0	3.409936	-2.084238	-1.557939
15	6	0	1.325492	-2.584052	-1.248510
16	1	0	0.989856	-2.257587	-2.240109
17	1	0	1.484337	-3.671411	-1.310007
18	6	0	0.276299	-2.253570	-0.220305
19	1	0	-0.743933	-2.571993	-0.420553
20	6	0	-2.476725	-0.399331	1.122323
21	6	0	-3.604878	-1.199293	1.306682
22	6	0	-1.910002	-0.218784	-0.150145
23	6	0	-4.205616	-1.833946	0.220016
24	1	0	-4.013896	-1.327817	2.306512
25	6	0	-2.548356	-0.846332	-1.236666
26	6	0	-3.669143	-1.652367	-1.056587
27	1	0	-5.087258	-2.453140	0.363149
28	1	0	-2.162327	-0.697285	-2.244613
29	1	0	-4.132351	-2.131853	-1.916055
30	6	0	-1.398267	1.680588	-0.679484
31	6	0	-0.062820	1.881075	-1.184827
32	1	0	0.117653	1.686435	-2.243956
33	6	0	-1.832541	2.548733	0.480745
34	6	0	-0.684001	2.816402	1.440868
35	1	0	-0.326078	1.862385	1.851197
36	1	0	-1.024188	3.423019	2.287068
37	1	0	-2.155410	1.576173	-1.450469
38	6	0	0.821256	2.902834	-0.623201
39	6	0	0.452437	3.522068	0.712644
40	1	0	1.360669	3.585725	1.320501
41	1	0	0.167512	4.558810	0.488679
42	8	0	1.825161	3.290682	-1.224724
43	1	0	-2.169697	3.501334	0.045653
44	1	0	-2.697484	2.116894	0.989210
45	1	0	-2.024721	0.076802	1.990093
46	6	0	2.997136	-2.370182	0.555358
47	1	0	4.027310	-2.090435	0.804082
48	1	0	2.938536	-3.464393	0.583252

SCF Done: E(RPBE1PBE) = -5576.76859710 A.U. after 1 cycles
Convg = 0.2071D-08 -V/T = 2.0040
Zero-point correction= 0.412245 (Hartree/Particle)
Thermal correction to Energy= 0.432396
Thermal correction to Enthalpy= 0.433356
Thermal correction to Gibbs Free Energy= 0.363492
Sum of electronic and zero-point Energies= -5576.356352
Sum of electronic and thermal Energies= -5576.336201
Sum of electronic and thermal Enthalpies= -5576.335241
Sum of electronic and thermal Free Energies= -5576.405105

	1	2	3
Frequencies --	-285.7200	29.3191	40.6889

(*R*)-BND-Rh(I)-Ph-CH-si-confD-CR-TS (170b)

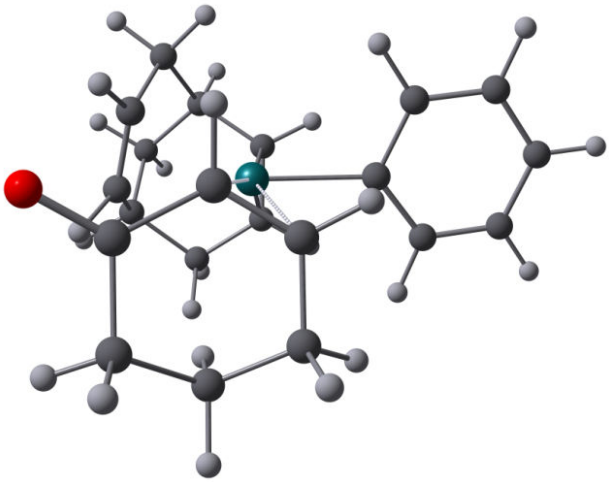


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.224434	-0.067177	-0.230846
2	6	0	0.646967	-1.858324	1.096285
3	1	0	-0.123388	-1.830645	1.865530
4	6	0	2.088438	-1.753020	1.569955
5	1	0	2.183275	-2.260659	2.536810
6	6	0	2.460672	-0.278265	1.711662
7	1	0	1.808582	0.226627	2.434422
8	1	0	3.491467	-0.168235	2.081722
9	6	0	2.311562	0.358769	0.356720
10	1	0	2.475414	1.430662	0.287050
11	6	0	2.343230	-0.386201	-0.819180
12	1	0	2.462943	0.150856	-1.759525
13	6	0	2.611089	-1.885641	-0.845177
14	1	0	3.394331	-2.094646	-1.582700
15	6	0	1.322882	-2.615312	-1.223811
16	1	0	0.960616	-2.295396	-2.208112
17	1	0	1.491221	-3.701231	-1.285463
18	6	0	0.294627	-2.291815	-0.172637
19	1	0	-0.726455	-2.622162	-0.347719
20	6	0	-2.525938	-0.559905	1.143987
21	6	0	-3.668821	-1.357826	1.228291
22	6	0	-1.907939	-0.304386	-0.088514
23	6	0	-4.228211	-1.914893	0.079920
24	1	0	-4.121588	-1.544776	2.199688
25	6	0	-2.509241	-0.845680	-1.242218
26	6	0	-3.639388	-1.653335	-1.160260
27	1	0	-5.118618	-2.534521	0.146364
28	1	0	-2.083416	-0.629099	-2.221337
29	1	0	-4.070023	-2.071867	-2.067294
30	6	0	-1.365908	1.647116	-0.411014
31	6	0	-0.114366	1.862623	-1.090389
32	1	0	-0.087346	1.672244	-2.165804
33	6	0	-1.604508	2.367321	0.905958
34	1	0	-2.231470	1.631463	-1.065199
35	6	0	0.819047	2.915088	-0.676429

36	6	0	0.514656	3.657630	0.611652
37	1	0	0.997586	4.636607	0.550682
38	8	0	1.791683	3.225743	-1.364580
39	1	0	-2.678148	2.412292	1.111340
40	1	0	-2.109905	-0.144270	2.058983
41	6	0	3.033127	-2.375496	0.540619
42	1	0	4.065934	-2.084160	0.763736
43	1	0	2.986312	-3.470062	0.574943
44	6	0	-0.984870	3.761465	0.871109
45	1	0	0.993077	3.113490	1.438007
46	1	0	-1.172213	4.274742	1.820649
47	1	0	-1.456227	4.363946	0.084634
48	1	0	-1.147620	1.816334	1.734123

```
SCF Done:  E(RPBE1PBE) =  -5576.76469624     A.U. after    1 cycles
             Convg  =    0.4514D-08             -V/T =  2.0039
Zero-point correction=                           0.412313 (Hartree/Particle)
 Thermal correction to Energy=                    0.432535
 Thermal correction to Enthalpy=                  0.433495
 Thermal correction to Gibbs Free Energy=         0.363562
 Sum of electronic and zero-point Energies=          -5576.352384
 Sum of electronic and thermal Energies=             -5576.332161
 Sum of electronic and thermal Enthalpies=           -5576.331201
 Sum of electronic and thermal Free Energies=        -5576.401134
                    1                    2                    3
Frequencies --  -284.1199               29.8673              54.3649
```

(*R*)-BND-Rh(I)-Ph-CH-re-confU-anti (176a)

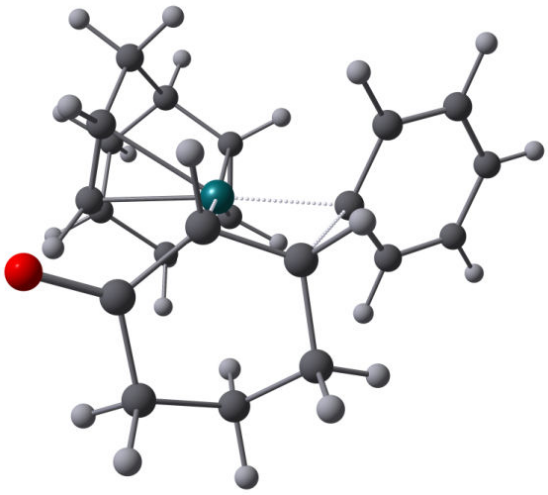


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.042644	-0.067153	-0.195871
2	6	0	0.106012	-2.232848	0.230606
3	1	0	1.100211	-2.528825	-0.097757
4	6	0	-1.066301	-2.943700	-0.437061
5	1	0	-0.747987	-3.950589	-0.729472
6	6	0	-1.499815	-2.156046	-1.673795
7	1	0	-0.674865	-2.060818	-2.389168
8	1	0	-2.315651	-2.672516	-2.201787
9	6	0	-1.951192	-0.792845	-1.220365
10	1	0	-2.168218	-0.039808	-1.975638
11	6	0	-2.355169	-0.556027	0.074155

12	1	0	-2.834401	0.392596	0.304449
13	6	0	-2.440504	-1.630305	1.141438
14	1	0	-3.415408	-1.555119	1.636529
15	6	0	-1.322236	-1.413823	2.159065
16	1	0	-1.403201	-0.429858	2.634786
17	1	0	-1.385498	-2.160354	2.965485
18	6	0	-0.010148	-1.534748	1.435138
19	1	0	0.894172	-1.345056	2.008064
20	6	0	2.692569	-0.415685	-1.265802
21	6	0	4.081109	-0.556626	-1.304425
22	6	0	2.015715	-0.092814	-0.076022
23	6	0	4.841334	-0.370795	-0.149105
24	1	0	4.570080	-0.811409	-2.242740
25	6	0	2.800158	0.091748	1.071708
26	6	0	4.191199	-0.043524	1.039135
27	1	0	5.922834	-0.477361	-0.176235
28	1	0	2.329832	0.355356	2.018165
29	1	0	4.766924	0.109231	1.950080
30	6	0	0.671415	2.138711	-0.385028
31	6	0	-0.457667	1.912289	-1.162717
32	6	0	0.598243	2.865910	0.926453
33	1	0	0.872398	3.914660	0.731403
34	6	0	-1.863623	3.187348	0.542561
35	1	0	-1.764845	4.252342	0.287353
36	6	0	-1.774213	2.449428	-0.777313
37	8	0	-2.743423	2.373597	-1.528419
38	1	0	1.642580	2.114321	-0.867440
39	1	0	-0.351600	1.651765	-2.216243
40	1	0	2.130437	-0.561053	-2.188054
41	6	0	-2.257413	-3.014386	0.518880
42	1	0	-2.084734	-3.755355	1.307880
43	1	0	-3.156289	-3.320351	-0.028777
44	6	0	-0.788589	2.798727	1.551286
45	1	0	1.361625	2.478839	1.608581
46	1	0	-0.968919	1.776281	1.903189
47	1	0	-0.843163	3.454386	2.426945
48	1	0	-2.875245	3.061882	0.939188

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5576.78436289     A.U. after    1 cycles
             Convg  =    0.3276D-08             -V/T =  2.0040
Zero-point correction=                           0.412398 (Hartree/Particle)
 Thermal correction to Energy=                    0.433486
 Thermal correction to Enthalpy=                  0.434446
 Thermal correction to Gibbs Free Energy=         0.362397
 Sum of electronic and zero-point Energies=          -5576.371965
 Sum of electronic and thermal Energies=             -5576.350877
 Sum of electronic and thermal Enthalpies=           -5576.349917
 Sum of electronic and thermal Free Energies=        -5576.421966
                    1                      2                      3
Frequencies --    26.3487               47.4420                61.3759
```

(*R*)-BND-Rh(I)-Ph-CH-re-confU-CR-TS (177a)

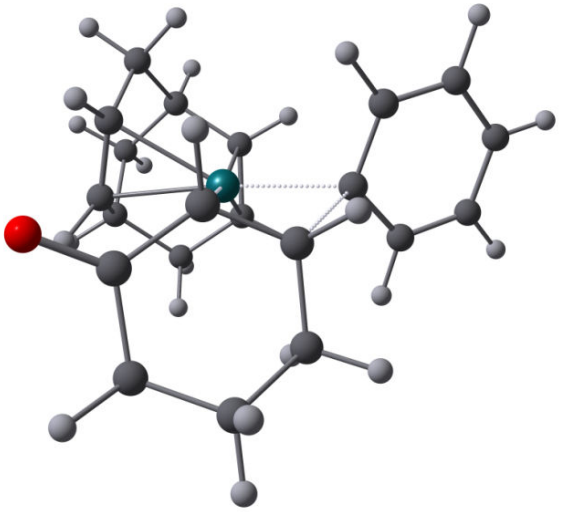


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.207779	0.002306	-0.223048
2	6	0	-0.460022	-2.187440	0.217523
3	1	0	0.447273	-2.646240	-0.172655
4	6	0	-1.773882	-2.621019	-0.418735
5	1	0	-1.702724	-3.678260	-0.699000
6	6	0	-2.037364	-1.768031	-1.661515
7	1	0	-1.234356	-1.884182	-2.398854
8	1	0	-2.969326	-2.082113	-2.155747
9	6	0	-2.125953	-0.330334	-1.219378
10	1	0	-2.208770	0.440936	-1.983812
11	6	0	-2.430657	0.012419	0.095019
12	1	0	-2.708053	1.044606	0.301861
13	6	0	-2.768882	-1.009745	1.169618
14	1	0	-3.691283	-0.701492	1.675003
15	6	0	-1.617367	-1.071286	2.172824
16	1	0	-1.452374	-0.094248	2.642005
17	1	0	-1.843359	-1.779773	2.984360
18	6	0	-0.385520	-1.495901	1.418419
19	1	0	0.565274	-1.474968	1.946296
20	6	0	2.411435	-0.836990	-1.307966
21	6	0	3.528499	-1.665707	-1.251541
22	6	0	1.934109	-0.168364	-0.163697
23	6	0	4.227281	-1.822033	-0.052061
24	1	0	3.864285	-2.179994	-2.149286
25	6	0	2.659367	-0.325775	1.026940
26	6	0	3.789607	-1.142609	1.083692
27	1	0	5.108471	-2.456662	-0.007805
28	1	0	2.334428	0.180303	1.933790
29	1	0	4.326125	-1.251397	2.023756
30	6	0	1.388296	1.739371	-0.628313
31	6	0	0.067001	1.885951	-1.183563
32	6	0	1.736235	2.601416	0.563237
33	1	0	2.618503	2.217146	1.080167
34	6	0	-0.626451	3.390949	0.770023
35	1	0	-1.545482	3.363813	1.363442
36	6	0	-0.924979	2.780931	-0.588436
37	8	0	-1.966435	3.077906	-1.179714

38	1	0	2.181835	1.682440	-1.367592
39	1	0	-0.064024	1.716428	-2.253002
40	1	0	1.902524	-0.699298	-2.261167
41	6	0	-2.931885	-2.399769	0.554144
42	1	0	-3.885359	-2.483788	0.020014
43	1	0	-2.931214	-3.157873	1.345958
44	6	0	0.553592	2.766231	1.505320
45	1	0	2.018777	3.585043	0.159311
46	1	0	0.832036	3.385326	2.365336
47	1	0	0.266573	1.780831	1.897979
48	1	0	-0.423042	4.452806	0.575190

SCF Done: E(RPBE1PBE) = -5576.77119232 A.U. after 1 cycles
Convg = 0.2146D-08 -V/T = 2.0040
Zero-point correction= 0.412201 (Hartree/Particle)
Thermal correction to Energy= 0.432333
Thermal correction to Enthalpy= 0.433293
Thermal correction to Gibbs Free Energy= 0.363488
Sum of electronic and zero-point Energies= -5576.358991
Sum of electronic and thermal Energies= -5576.338860
Sum of electronic and thermal Enthalpies= -5576.337899
Sum of electronic and thermal Free Energies= -5576.407704
Frequencies -- -293.0868 30.1480 43.7414

(*R*)-BND-Rh(I)-Ph-CH-re-confD-CR-TS (177b)

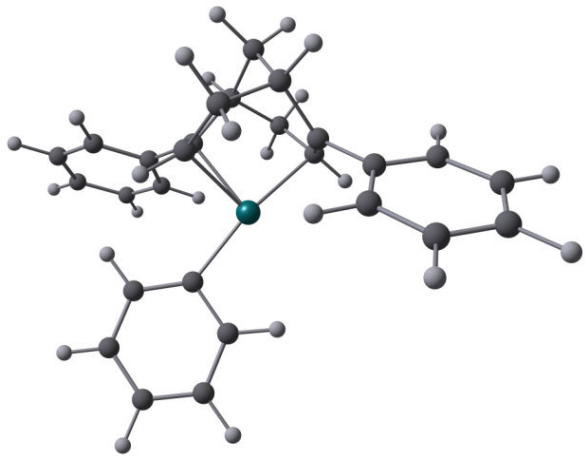


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.198500	-0.046152	-0.187605
2	6	0	-0.437669	-2.231881	0.255876
3	1	0	0.479373	-2.686271	-0.116198
4	6	0	-1.737547	-2.678875	-0.400246
5	1	0	-1.654046	-3.736806	-0.674318
6	6	0	-1.986105	-1.833744	-1.651753
7	1	0	-1.169084	-1.946502	-2.374042
8	1	0	-2.906664	-2.157332	-2.160997
9	6	0	-2.093511	-0.394602	-1.218590
10	1	0	-2.163667	0.374975	-1.986151
11	6	0	-2.423838	-0.049001	0.088866
12	1	0	-2.710761	0.982282	0.286848

13	6	0	-2.772642	-1.067743	1.163071
14	1	0	-3.705890	-0.764536	1.651272
15	6	0	-1.637306	-1.114669	2.185849
16	1	0	-1.488508	-0.134363	2.653704
17	1	0	-1.871388	-1.821928	2.996158
18	6	0	-0.388955	-1.531267	1.454168
19	1	0	0.552149	-1.502312	1.999311
20	6	0	2.414736	-0.782700	-1.312118
21	6	0	3.555320	-1.580361	-1.331214
22	6	0	1.943380	-0.208947	-0.114427
23	6	0	4.286588	-1.791515	-0.159379
24	1	0	3.883635	-2.028259	-2.266562
25	6	0	2.703127	-0.411682	1.046067
26	6	0	3.858762	-1.194796	1.024991
27	1	0	5.185554	-2.402065	-0.174525
28	1	0	2.394852	0.038033	1.987174
29	1	0	4.424480	-1.339878	1.942794
30	6	0	1.323880	1.713912	-0.372270
31	6	0	0.086858	1.862590	-1.098545
32	6	0	1.468833	2.425839	0.966351
33	1	0	1.077132	1.805621	1.779238
34	1	0	2.529116	2.591635	1.180355
35	6	0	0.692955	3.739959	0.962457
36	1	0	0.806680	4.239327	1.930906
37	1	0	1.105720	4.417368	0.204555
38	6	0	-0.780886	3.478782	0.670021
39	1	0	-1.368716	4.400389	0.640241
40	1	0	-1.208276	2.849033	1.462124
41	6	0	-0.976087	2.767954	-0.657488
42	8	0	-1.974963	2.982866	-1.346359
43	1	0	2.212163	1.769963	-0.993713
44	1	0	0.109978	1.703426	-2.178025
45	1	0	1.881599	-0.598296	-2.243710
46	6	0	-2.913948	-2.461903	0.551444
47	1	0	-3.857267	-2.555461	0.001091
48	1	0	-2.921626	-3.216243	1.346788

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5576.76761107     A.U. after    1 cycles
             Convg  =    0.4325D-08             -V/T =  2.0040
Zero-point correction=                           0.412225 (Hartree/Particle)
 Thermal correction to Energy=                    0.432397
 Thermal correction to Enthalpy=                  0.433358
 Thermal correction to Gibbs Free Energy=         0.363606
 Sum of electronic and zero-point Energies=          -5576.355386
 Sum of electronic and thermal Energies=             -5576.335214
 Sum of electronic and thermal Enthalpies=           -5576.334254
 Sum of electronic and thermal Free Energies=        -5576.404005
                     1                      2                      3
Frequencies --  -293.9959               34.0625                48.5668
```

(R)-PhBND-Rh pathway
(*R*)-PhBND-Rh(I)-Ph (180)

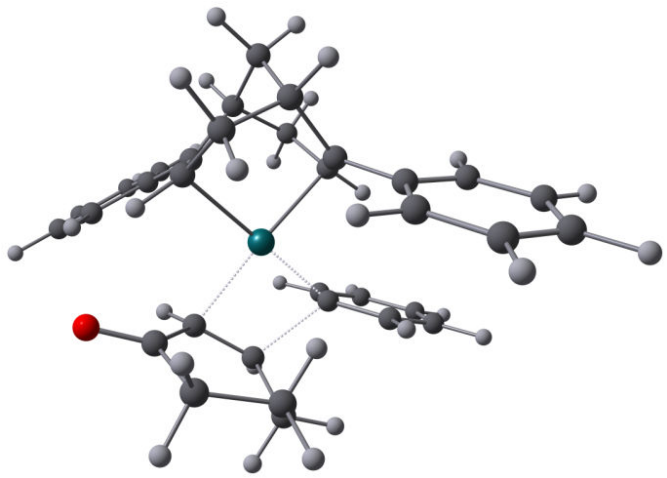


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.193601	0.282310	-0.328323
2	6	0	0.478935	-0.639110	1.426090
3	6	0	1.068602	-1.319450	0.318407
4	6	0	0.935173	1.919854	-0.017015
5	1	0	1.114641	0.032445	2.001743
6	6	0	-0.740588	-1.167700	2.135982
7	6	0	0.452375	-2.635805	-0.216066
8	6	0	0.151189	3.012092	-0.423975
9	6	0	2.233560	2.186960	0.435953
10	6	0	-1.534457	-2.014107	1.140203
11	1	0	-1.330240	-0.338685	2.537162
12	1	0	-0.452133	-1.786909	2.999937
13	6	0	-0.231565	-2.388574	-1.557500
14	1	0	1.252932	-3.373903	-0.332426
15	6	0	0.637607	4.321538	-0.397800
16	1	0	-0.877474	2.858554	-0.773635
17	6	0	2.728904	3.492261	0.466155
18	1	0	2.880803	1.373725	0.757300
19	6	0	-1.922725	-1.179251	-0.087695
20	1	0	-2.448420	-2.393991	1.610829
21	6	0	-1.326862	-1.384138	-1.324599
22	1	0	0.470787	-2.006801	-2.305558
23	1	0	-0.633656	-3.331615	-1.958914
24	6	0	1.935535	4.563268	0.050816
25	1	0	0.006346	5.146856	-0.720589
26	1	0	3.744359	3.675007	0.812291
27	1	0	-1.802808	-0.942061	-2.201939
28	1	0	2.325898	5.577722	0.077280
29	6	0	2.534998	-1.182958	0.067343
30	6	0	3.059859	-0.981100	-1.216679
31	6	0	3.435986	-1.321670	1.132036
32	6	0	4.433511	-0.906388	-1.426281
33	1	0	2.382948	-0.840661	-2.054785
34	6	0	4.813650	-1.245636	0.926009
35	1	0	3.052015	-1.493873	2.134736
36	6	0	5.318806	-1.036690	-0.355107
37	1	0	4.815907	-0.730794	-2.428679

38	1	0	5.491230	-1.350445	1.769811
39	1	0	6.391301	-0.972304	-0.518888
40	6	0	-3.194847	-0.395636	-0.024634
41	6	0	-3.371788	0.690199	0.846609
42	6	0	-4.268699	-0.756167	-0.851976
43	6	0	-4.574960	1.391902	0.882531
44	1	0	-2.553330	1.010877	1.485066
45	6	0	-5.473472	-0.056656	-0.816422
46	1	0	-4.156323	-1.603208	-1.524335
47	6	0	-5.632278	1.021485	0.052655
48	1	0	-4.682938	2.237166	1.557486
49	1	0	-6.290704	-0.357646	-1.467100
50	1	0	-6.570439	1.569306	0.081882
51	6	0	-0.622469	-3.169984	0.731830
52	1	0	-1.187280	-3.961430	0.225392
53	1	0	-0.175267	-3.612501	1.629251

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5730.00166446     A.U. after    1 cycles
             Convg  =    0.3542D-08             -V/T =  2.0043
Zero-point correction=                           0.443916 (Hartree/Particle)
 Thermal correction to Energy=                    0.467671
 Thermal correction to Enthalpy=                  0.468631
 Thermal correction to Gibbs Free Energy=         0.388172
 Sum of electronic and zero-point Energies=          -5729.557748
 Sum of electronic and thermal Energies=             -5729.533993
 Sum of electronic and thermal Enthalpies=           -5729.533033
 Sum of electronic and thermal Free Energies=        -5729.613492
                    1                    2                    3
Frequencies --    21.8351              27.8888              32.2063
```

(*R*)-PhBND-Rh(I)-Ph-CH-si-confU-CR-TS (185a)



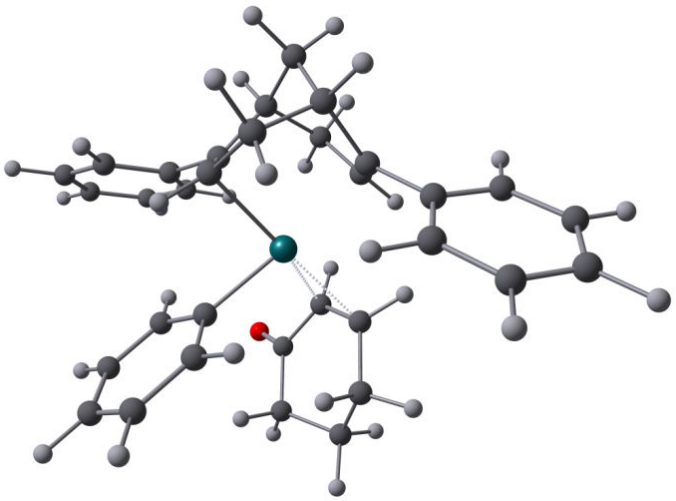
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.224333	0.133914	0.006188
2	6	0	0.643337	-1.661982	0.992918
3	6	0	1.141227	-1.688899	-0.308952
4	6	0	0.984738	1.181620	1.455490
5	1	0	1.299142	-1.306835	1.783807
6	6	0	-0.571360	-2.424120	1.430574
7	6	0	0.453352	-2.524290	-1.403386
8	6	0	0.410059	1.122109	2.740745

9	6	0	2.377462	1.304932	1.375241
10	6	0	-1.436929	-2.675128	0.198530
11	1	0	-1.092337	-1.849364	2.202733
12	1	0	-0.282884	-3.381853	1.891888
13	6	0	-0.311590	-1.641405	-2.382052
14	1	0	1.222302	-3.097971	-1.932233
15	6	0	1.195144	1.131053	3.889904
16	1	0	-0.673697	1.070419	2.842408
17	6	0	3.168141	1.332336	2.526206
18	1	0	2.868173	1.356604	0.406407
19	6	0	-1.904394	-1.345102	-0.413276
20	1	0	-2.319502	-3.266216	0.465214
21	6	0	-1.356992	-0.884279	-1.615272
22	1	0	0.337670	-0.934372	-2.906058
23	1	0	-0.778556	-2.262691	-3.162406
24	6	0	2.584944	1.238982	3.788072
25	1	0	0.721819	1.069742	4.867486
26	1	0	4.248321	1.416222	2.428886
27	1	0	-1.892672	-0.127937	-2.178768
28	1	0	3.201653	1.261412	4.682986
29	6	0	2.569746	-1.342386	-0.565671
30	6	0	2.991547	-0.758367	-1.770545
31	6	0	3.557435	-1.672843	0.373945
32	6	0	4.335047	-0.485180	-2.011085
33	1	0	2.261439	-0.496261	-2.529542
34	6	0	4.903731	-1.405295	0.135831
35	1	0	3.270239	-2.158046	1.302228
36	6	0	5.301055	-0.803833	-1.056490
37	1	0	4.628652	-0.020799	-2.949242
38	1	0	5.644639	-1.674866	0.884378
39	1	0	6.350716	-0.594366	-1.245047
40	6	0	-3.196116	-0.801409	0.108389
41	6	0	-3.695369	-1.199490	1.360949
42	6	0	-3.992492	0.082392	-0.641891
43	6	0	-4.909921	-0.724543	1.850605
44	1	0	-3.137504	-1.894665	1.978545
45	6	0	-5.205340	0.558143	-0.154949
46	1	0	-3.664999	0.428680	-1.615937
47	6	0	-5.675107	0.161480	1.096839
48	1	0	-5.258589	-1.054615	2.826077
49	1	0	-5.789127	1.241968	-0.765945
50	1	0	-6.625086	0.530980	1.474026
51	6	0	-0.576987	-3.466620	-0.785443
52	1	0	-1.190139	-3.904320	-1.581359
53	1	0	-0.090928	-4.293753	-0.255001
54	6	0	-0.130307	2.540900	0.325911
55	6	0	-1.198408	2.017230	-0.470300
56	1	0	-0.436099	2.930988	1.291293
57	1	0	-2.187325	1.941702	-0.020661
58	6	0	-1.207809	2.235549	-1.921942
59	8	0	-2.233626	2.098864	-2.594906
60	6	0	0.058508	2.714968	-2.606652
61	1	0	0.213704	2.092298	-3.493753
62	6	0	0.934320	3.359690	-0.363443
63	1	0	1.811710	3.478069	0.275529
64	6	0	1.292973	2.770478	-1.717230
65	1	0	-0.179966	3.717769	-2.984725
66	1	0	1.693968	1.760328	-1.570343
67	1	0	2.080196	3.359878	-2.199781
68	1	0	0.507189	4.364700	-0.501732

SCF Done: E(RPBE1PBE) = -5576.76859710 A.U. after 1 cycles
Convg = 0.2071D-08 -V/T = 2.0040

```
Zero-point correction=                           0.575856 (Hartree/Particle)
 Thermal correction to Energy=                    0.605794
 Thermal correction to Enthalpy=                  0.606754
 Thermal correction to Gibbs Free Energy=         0.515850
 Sum of electronic and zero-point Energies=           -6037.764842
 Sum of electronic and thermal Energies=              -6037.734904
 Sum of electronic and thermal Enthalpies=            -6037.733944
 Sum of electronic and thermal Free Energies=         -6037.824848
                     1                      2                      3
Frequencies --  -267.2570               30.6621                35.9779
```

(*R*)-PhBND-Rh(I)-Ph-CH-si-confD-close (182b)



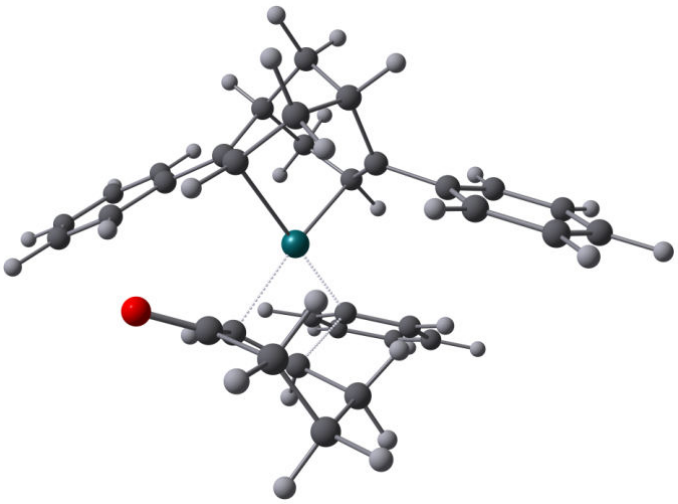
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.231768	-0.002888	-0.011619
2	6	0	0.514223	-1.482798	1.445397
3	6	0	1.048615	-1.928909	0.236464
4	6	0	1.091871	1.230157	0.915948
5	1	0	1.173685	-0.954642	2.130469
6	6	0	-0.763378	-2.022800	2.031687
7	6	0	0.336136	-3.015316	-0.585807
8	6	0	0.593205	1.854434	2.073579
9	6	0	2.431090	1.467671	0.584389
10	6	0	-1.608105	-2.622893	0.910640
11	1	0	-1.291709	-1.235561	2.578119
12	1	0	-0.534379	-2.799653	2.778116
13	6	0	-0.351592	-2.437558	-1.817124
14	1	0	1.087915	-3.749037	-0.895052
15	6	0	1.390752	2.693640	2.855630
16	1	0	-0.436765	1.682914	2.390841
17	6	0	3.232071	2.310154	1.359298
18	1	0	2.862387	1.010902	-0.302289
19	6	0	-2.026011	-1.564172	-0.120000
20	1	0	-2.518277	-3.066800	1.329105
21	6	0	-1.438065	-1.509084	-1.364343
22	1	0	0.346125	-1.906158	-2.469632
23	1	0	-0.778798	-3.252121	-2.422485
24	6	0	2.718207	2.930166	2.497785
25	1	0	0.972418	3.161339	3.745033
26	1	0	4.265482	2.482073	1.064977

27	1	0	-1.920237	-0.911350	-2.136675
28	1	0	3.342686	3.586288	3.099273
29	6	0	2.500429	-1.752087	-0.050489
30	6	0	2.981531	-1.477192	-1.339617
31	6	0	3.439954	-1.931997	0.974303
32	6	0	4.345932	-1.370702	-1.589852
33	1	0	2.285339	-1.296557	-2.152163
34	6	0	4.807205	-1.827603	0.726419
35	1	0	3.097437	-2.168792	1.977887
36	6	0	5.267903	-1.545716	-0.557558
37	1	0	4.688666	-1.133111	-2.593490
38	1	0	5.513172	-1.970351	1.540627
39	1	0	6.333546	-1.459909	-0.753088
40	6	0	-3.317929	-0.854471	0.114534
41	6	0	-3.558977	-0.084234	1.261992
42	6	0	-4.353452	-0.974631	-0.823810
43	6	0	-4.781867	0.551873	1.456622
44	1	0	-2.772974	0.046734	1.999139
45	6	0	-5.578955	-0.338422	-0.631873
46	1	0	-4.199885	-1.587846	-1.708091
47	6	0	-5.799010	0.428617	0.510120
48	1	0	-4.938371	1.153252	2.348510
49	1	0	-6.365451	-0.450128	-1.373831
50	1	0	-6.753712	0.924587	0.663293
51	6	0	-0.750036	-3.698670	0.246161
52	1	0	-0.308989	-4.339343	1.018259
53	1	0	-1.355659	-4.339780	-0.404832
54	6	0	-1.367374	1.587743	-1.169920
55	6	0	-0.189670	1.308739	-1.857416
56	1	0	-2.270255	1.040422	-1.427033
57	1	0	-0.150571	0.530386	-2.616766
58	6	0	0.883129	2.322325	-1.996861
59	8	0	1.878191	2.091997	-2.675029
60	6	0	0.660070	3.673081	-1.349642
61	1	0	1.136340	3.638878	-0.362473
62	1	0	1.205358	4.413206	-1.942549
63	6	0	-0.816947	4.027249	-1.203518
64	1	0	-0.921170	4.972076	-0.659142
65	1	0	-1.259793	4.180396	-2.195857
66	6	0	-1.579350	2.916341	-0.481366
67	1	0	-1.247761	2.877030	0.561971
68	1	0	-2.651398	3.137031	-0.457706

SCF Done: E(RPBE1PBE) = -6038.35237963 A.U. after 1 cycles
Convg = 0.4255D-08 -V/T = 2.0048
Zero-point correction= 0.574917 (Hartree/Particle)
Thermal correction to Energy= 0.606060
Thermal correction to Enthalpy= 0.607020
Thermal correction to Gibbs Free Energy= 0.512432
Sum of electronic and zero-point Energies= -6037.777463
Sum of electronic and thermal Energies= -6037.746320
Sum of electronic and thermal Enthalpies= -6037.745359
Sum of electronic and thermal Free Energies= -6037.839947

	1	2	3
Frequencies --	25.6641	33.8994	37.0476

(*R*)-PhBND-Rh(I)-Ph-CH-si-confD-CR-TS (185b)

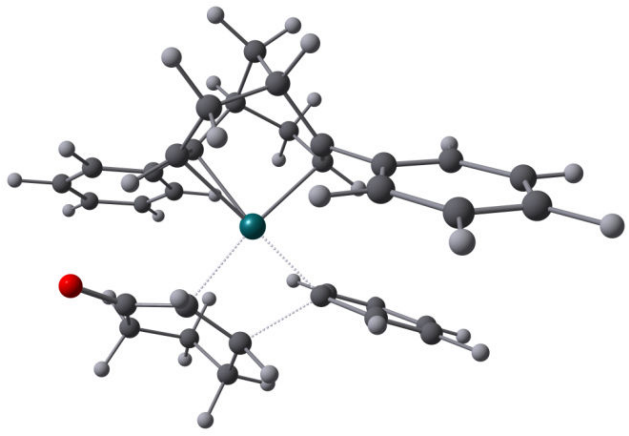


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.210161	0.079456	0.076898
2	6	0	0.583735	-1.938773	-0.376225
3	6	0	1.135955	-1.075741	-1.328016
4	6	0	0.887265	-0.201684	1.901784
5	1	0	1.209042	-2.242151	0.460183
6	6	0	-0.643254	-2.767068	-0.620463
7	6	0	0.506547	-0.931130	-2.726755
8	6	0	0.055067	-0.900558	2.798979
9	6	0	2.271282	-0.302984	2.078301
10	6	0	-1.445986	-2.085750	-1.724829
11	1	0	-1.206324	-2.853934	0.314304
12	1	0	-0.369593	-3.790286	-0.922166
13	6	0	-0.230895	0.393817	-2.878041
14	1	0	1.304567	-1.008351	-3.473163
15	6	0	0.590301	-1.728623	3.781589
16	1	0	-1.027068	-0.797746	2.727223
17	6	0	2.809181	-1.114513	3.080364
18	1	0	2.950787	0.235805	1.423816
19	6	0	-1.883629	-0.685832	-1.268233
20	1	0	-2.338915	-2.669522	-1.971631
21	6	0	-1.306869	0.456066	-1.832284
22	1	0	0.432936	1.256130	-2.769173
23	1	0	-0.663437	0.468725	-3.887932
24	6	0	1.975783	-1.839915	3.928990
25	1	0	-0.075320	-2.276074	4.445422
26	1	0	3.889605	-1.181684	3.189027
27	1	0	-1.828808	1.403215	-1.751496
28	1	0	2.396786	-2.472174	4.706475
29	6	0	2.573084	-0.687847	-1.227201
30	6	0	3.035126	0.577292	-1.621934
31	6	0	3.526357	-1.621076	-0.794111
32	6	0	4.386329	0.906017	-1.557897
33	1	0	2.328263	1.325329	-1.967886
34	6	0	4.880282	-1.297137	-0.730302
35	1	0	3.204520	-2.619070	-0.510649
36	6	0	5.318278	-0.029273	-1.106984
37	1	0	4.712868	1.898141	-1.859664

38	1	0	5.594962	-2.042059	-0.389335
39	1	0	6.373520	0.225941	-1.058058
40	6	0	-3.160505	-0.613470	-0.492482
41	6	0	-3.750015	-1.772810	0.041744
42	6	0	-3.847181	0.598427	-0.294415
43	6	0	-4.949273	-1.726184	0.749813
44	1	0	-3.279817	-2.740979	-0.089139
45	6	0	-5.044362	0.646346	0.410511
46	1	0	-3.446427	1.532211	-0.674660
47	6	0	-5.606762	-0.514614	0.942047
48	1	0	-5.369846	-2.646204	1.148194
49	1	0	-5.542639	1.603733	0.541328
50	1	0	-6.543977	-0.474526	1.490964
51	6	0	-0.537300	-2.020438	-2.951472
52	1	0	-0.066824	-2.998988	-3.101295
53	1	0	-1.111394	-1.791698	-3.856519
54	6	0	0.246064	1.777448	1.668732
55	6	0	-0.957509	1.968131	0.916180
56	1	0	0.084244	1.643268	2.732352
57	1	0	-1.901902	1.734150	1.407585
58	6	0	-1.053572	3.041425	-0.079642
59	8	0	-2.131033	3.392413	-0.567785
60	6	0	0.218724	3.781451	-0.442212
61	1	0	0.741056	3.210357	-1.221809
62	1	0	-0.071653	4.739774	-0.880590
63	6	0	1.130652	3.945304	0.768614
64	1	0	2.041878	4.486901	0.492107
65	1	0	0.621869	4.545815	1.532972
66	6	0	1.494794	2.574683	1.328196
67	1	0	2.096102	2.050964	0.579450
68	1	0	2.120269	2.664251	2.221578

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6038.33765384     A.U. after    1 cycles
             Convg  =    0.3950D-08             -V/T =  2.0048
Zero-point correction=                           0.575712 (Hartree/Particle)
 Thermal correction to Energy=                   0.605693
 Thermal correction to Enthalpy=                 0.606653
 Thermal correction to Gibbs Free Energy=        0.515709
 Sum of electronic and zero-point Energies=          -6037.761942
 Sum of electronic and thermal Energies=             -6037.731961
 Sum of electronic and thermal Enthalpies=           -6037.731001
 Sum of electronic and thermal Free Energies=        -6037.821945
                    1                    2                    3
Frequencies --  -269.0237               29.8149              38.3445
```

(*R*)-PhBND-Rh(I)-Ph-CH-re-confU-CR-TS (192a)

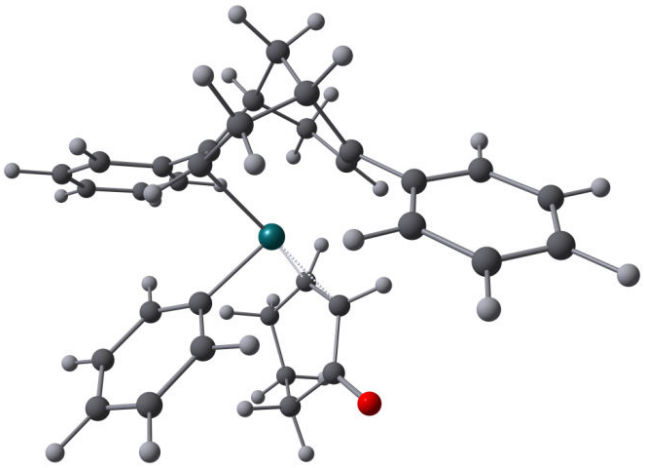


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.004090	-0.010680	-0.219228
2	6	0	1.069068	-0.912303	1.527064
3	6	0	1.546844	-1.556630	0.384067
4	6	0	1.166379	1.772281	0.237289
5	1	0	1.685712	-0.133114	1.969755
6	6	0	-0.031889	-1.474105	2.378725
7	6	0	0.969081	-2.911408	-0.072486
8	6	0	0.800212	2.346853	1.469023
9	6	0	2.488334	1.964570	-0.190954
10	6	0	-0.875759	-2.388917	1.496681
11	1	0	-0.613102	-0.658656	2.817316
12	1	0	0.380216	-2.045587	3.225289
13	6	0	0.112109	-2.751969	-1.324766
14	1	0	1.805662	-3.590269	-0.270578
15	6	0	1.723023	3.037619	2.253270
16	1	0	-0.217743	2.242783	1.838368
17	6	0	3.413833	2.661093	0.583507
18	1	0	2.807257	1.560787	-1.149797
19	6	0	-1.472319	-1.610321	0.308027
20	1	0	-1.701239	-2.817749	2.075222
21	6	0	-1.007660	-1.807111	-0.997561
22	1	0	0.681120	-2.369899	-2.176469
23	1	0	-0.283031	-3.731702	-1.635552
24	6	0	3.037847	3.199228	1.814391
25	1	0	1.410828	3.454902	3.208339
26	1	0	4.432452	2.781394	0.222172
27	1	0	-1.647445	-1.495838	-1.821567
28	1	0	3.756470	3.746674	2.419070
29	6	0	2.912916	-1.242330	-0.130968
30	6	0	3.209396	-1.204837	-1.502253
31	6	0	3.969149	-1.047261	0.769347
32	6	0	4.503375	-0.961994	-1.953695
33	1	0	2.415432	-1.335064	-2.230821
34	6	0	5.266265	-0.804236	0.321665
35	1	0	3.773633	-1.094234	1.837104
36	6	0	5.540898	-0.757918	-1.043265
37	1	0	4.701522	-0.926246	-3.022146
38	1	0	6.065078	-0.655777	1.044018
39	1	0	6.551771	-0.569776	-1.395485
40	6	0	-2.843484	-1.058701	0.534187
41	6	0	-3.147786	-0.230412	1.627127
42	6	0	-3.901893	-1.440479	-0.303113
43	6	0	-4.448188	0.203475	1.867335
44	1	0	-2.357608	0.097433	2.294599
45	6	0	-5.204519	-1.004790	-0.068586
46	1	0	-3.705830	-2.092944	-1.148103
47	6	0	-5.486942	-0.182095	1.019507
48	1	0	-4.649822	0.850421	2.717638
49	1	0	-6.000646	-1.313970	-0.740769
50	1	0	-6.503000	0.156129	1.205299
51	6	0	0.056564	-3.494515	1.004345
52	6	0	-0.104210	2.154127	-1.351713
53	1	0	0.786190	2.414580	-1.915587
54	6	0	-0.856110	1.062689	-1.893243
55	1	0	-0.385855	0.477175	-2.685869
56	6	0	-2.315208	1.102193	-2.004060
57	8	0	-2.912904	0.338035	-2.765108
58	6	0	-0.895368	3.343302	-0.850131
59	1	0	-0.300189	3.953148	-0.167396

60	6	0	-3.072655	2.156348	-1.227691
61	1	0	-3.932332	1.674173	-0.752168
62	6	0	-2.219541	2.923990	-0.226610
63	1	0	-1.095711	3.965576	-1.735773
64	1	0	-2.032759	2.289893	0.647403
65	1	0	-2.762984	3.804164	0.133517
66	1	0	-3.482975	2.841707	-1.981820
67	1	0	0.636809	-3.882330	1.849566
68	1	0	-0.509281	-4.334119	0.584597

```
SCF Done:  E(RPBE1PBE) =  -6038.33641537     A.U. after    1 cycles
            Convg  =    0.2519D-08             -V/T =  2.0048
Zero-point correction=                           0.575096 (Hartree/Particle)
 Thermal correction to Energy=                    0.605133
 Thermal correction to Enthalpy=                  0.606093
 Thermal correction to Gibbs Free Energy=         0.514749
 Sum of electronic and zero-point Energies=          -6037.761319
 Sum of electronic and thermal Energies=             -6037.731283
 Sum of electronic and thermal Enthalpies=           -6037.730323
 Sum of electronic and thermal Free Energies=        -6037.821666
                    1                      2                      3
Frequencies --  -293.1241               19.4420                40.5735
```

(*R*)-PhBND-Rh(I)-Ph-CH-re-confD-close (189a)



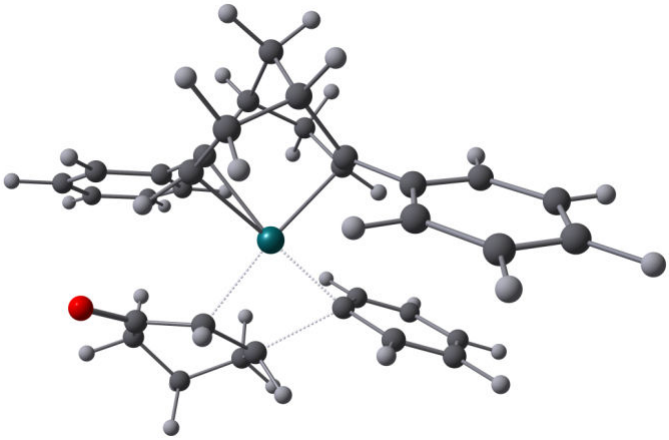
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.152983	-0.032512	0.037234
2	6	0	-0.640015	-1.394714	-1.487349
3	6	0	-1.188095	-1.880184	-0.297473
4	6	0	-1.020160	1.343825	-0.868636
5	1	0	-1.278357	-0.803671	-2.140889
6	6	0	0.610799	-1.952795	-2.111884
7	6	0	-0.522897	-3.048752	0.451305
8	6	0	-0.329812	2.099475	-1.833473
9	6	0	-2.391220	1.586485	-0.723081
10	6	0	1.429248	-2.664586	-1.036513
11	1	0	1.175196	-1.155480	-2.605191
12	1	0	0.347177	-2.666949	-2.907640
13	6	0	0.206678	-2.586706	1.707351
14	1	0	-1.307338	-3.762592	0.724553
15	6	0	-0.975499	3.069990	-2.601523

16	1	0	0.741806	1.957066	-1.977402
17	6	0	-3.042537	2.561464	-1.484842
18	1	0	-2.977562	1.010118	-0.010356
19	6	0	1.907623	-1.697464	0.052425
20	1	0	2.313500	-3.126166	-1.489771
21	6	0	1.340790	-1.693639	1.301989
22	1	0	-0.458172	-2.059466	2.396901
23	1	0	0.590230	-3.459386	2.258282
24	6	0	-2.339249	3.310183	-2.426959
25	1	0	-0.407595	3.646928	-3.328657
26	1	0	-4.108176	2.729766	-1.340902
27	1	0	1.858186	-1.154669	2.094307
28	1	0	-2.844747	4.070290	-3.017560
29	6	0	-2.631789	-1.658904	0.000478
30	6	0	-3.103153	-1.478113	1.310204
31	6	0	-3.578388	-1.690865	-1.033477
32	6	0	-4.459550	-1.311314	1.571978
33	1	0	-2.399769	-1.435258	2.135990
34	6	0	-4.937805	-1.524545	-0.775104
35	1	0	-3.248730	-1.857000	-2.055072
36	6	0	-5.386622	-1.330665	0.529087
37	1	0	-4.794376	-1.157830	2.594858
38	1	0	-5.647338	-1.550493	-1.598203
39	1	0	-6.445941	-1.199161	0.732980
40	6	0	3.220519	-1.018285	-0.152595
41	6	0	3.469030	-0.145769	-1.221173
42	6	0	4.268841	-1.278300	0.742264
43	6	0	4.714951	0.453538	-1.381564
44	1	0	2.674873	0.100969	-1.919155
45	6	0	5.518589	-0.683720	0.580492
46	1	0	4.104541	-1.967886	1.566585
47	6	0	5.747062	0.185838	-0.483718
48	1	0	4.874677	1.145054	-2.204358
49	1	0	6.315096	-0.904184	1.286615
50	1	0	6.718702	0.655717	-0.609720
51	6	0	0.520068	-3.734292	-0.432806
52	1	0	0.041396	-4.301863	-1.238986
53	1	0	1.095176	-4.445651	0.171102
54	6	0	0.028097	0.973005	2.081705
55	1	0	0.157758	0.095937	2.710763
56	6	0	1.142301	1.457943	1.391220
57	1	0	2.121564	0.991330	1.483467
58	6	0	1.198832	2.860979	0.919668
59	8	0	2.189398	3.293601	0.340326
60	6	0	-1.131904	1.865823	2.453074
61	1	0	-1.522661	1.545241	3.425392
62	1	0	-1.954362	1.756464	1.741631
63	6	0	0.018498	3.753480	1.239976
64	1	0	-0.667920	3.708978	0.385810
65	1	0	0.391533	4.780076	1.299429
66	6	0	-0.703554	3.331709	2.515705
67	1	0	-1.577818	3.970600	2.680283
68	1	0	-0.038020	3.476662	3.376256

SCF Done: E(RPBE1PBE) = -6038.35211057 A.U. after 1 cycles
Convg = 0.5541D-08 -V/T = 2.0048
Zero-point correction= 0.574790 (Hartree/Particle)
Thermal correction to Energy= 0.605972
Thermal correction to Enthalpy= 0.606932
Thermal correction to Gibbs Free Energy= 0.511775
Sum of electronic and zero-point Energies= -6037.777320
Sum of electronic and thermal Energies= -6037.746139
Sum of electronic and thermal Enthalpies= -6037.745179

```
 Sum of electronic and thermal Free Energies=         -6037.840335
                      1                      2                      3
Frequencies --    13.3072                35.2586                37.8827
```

(*R*)-PhBND-Rh(I)-Ph-CH-re-confD-CR-TS (192b)



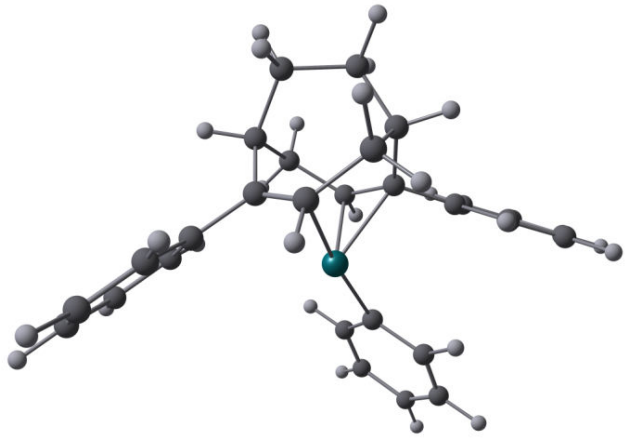
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.002504	0.009814	-0.196728
2	6	0	1.076936	-0.994465	1.484687
3	6	0	1.568116	-1.564146	0.309293
4	6	0	1.218473	1.750216	0.315671
5	1	0	1.683033	-0.235249	1.973476
6	6	0	-0.010570	-1.624053	2.303711
7	6	0	0.996080	-2.886884	-0.239186
8	6	0	1.088617	2.252931	1.620444
9	6	0	2.442098	1.974675	-0.338573
10	6	0	-0.847900	-2.488370	1.367857
11	1	0	-0.599730	-0.849625	2.801598
12	1	0	0.416958	-2.245188	3.106540
13	6	0	0.130538	-2.647854	-1.473828
14	1	0	1.834833	-3.545846	-0.488242
15	6	0	2.143539	2.906629	2.259219
16	1	0	0.155775	2.122320	2.165561
17	6	0	3.497881	2.626726	0.291533
18	1	0	2.575787	1.637138	-1.364575
19	6	0	-1.456784	-1.635314	0.238275
20	1	0	-1.666873	-2.962908	1.919386
21	6	0	-0.996489	-1.737261	-1.080138
22	1	0	0.691338	-2.203479	-2.300411
23	1	0	-0.257287	-3.607908	-1.848913
24	6	0	3.356129	3.096913	1.598623
25	1	0	2.011428	3.272281	3.275427
26	1	0	4.434811	2.769213	-0.241833
27	1	0	-1.638441	-1.372893	-1.880633
28	1	0	4.176022	3.614428	2.090205
29	6	0	2.938579	-1.216517	-0.169652
30	6	0	3.262378	-1.151503	-1.533631
31	6	0	3.975447	-1.028725	0.754780
32	6	0	4.562620	-0.889232	-1.954742
33	1	0	2.484786	-1.279458	-2.280051
34	6	0	5.278344	-0.764684	0.337737
35	1	0	3.761950	-1.101846	1.817515

36	6	0	5.579771	-0.691599	-1.020280
37	1	0	4.781855	-0.834046	-3.018249
38	1	0	6.061145	-0.622662	1.078645
39	1	0	6.595870	-0.488782	-1.348578
40	6	0	-2.831371	-1.118354	0.517977
41	6	0	-3.129456	-0.358611	1.661625
42	6	0	-3.897722	-1.473101	-0.320530
43	6	0	-4.434462	0.028201	1.953809
44	1	0	-2.331091	-0.045247	2.326356
45	6	0	-5.204188	-1.079586	-0.036144
46	1	0	-3.703938	-2.070942	-1.205670
47	6	0	-5.482110	-0.331263	1.105203
48	1	0	-4.632520	0.619747	2.844343
49	1	0	-6.007227	-1.365767	-0.710349
50	1	0	-6.501231	-0.028362	1.330620
51	6	0	0.091843	-3.549578	0.798966
52	1	0	0.678566	-3.988635	1.614037
53	1	0	-0.468838	-4.363349	0.324995
54	6	0	-0.355135	2.268552	-0.934691
55	1	0	0.419688	2.813015	-1.463330
56	6	0	-0.980841	1.225559	-1.690470
57	1	0	-0.438521	0.858615	-2.566027
58	6	0	-2.435205	1.180652	-1.896441
59	8	0	-2.931457	0.432655	-2.739180
60	6	0	-1.247168	3.130376	-0.061930
61	1	0	-0.714927	4.039418	0.231283
62	1	0	-1.507431	2.600614	0.859413
63	6	0	-3.292799	2.154893	-1.118302
64	1	0	-3.598427	1.661511	-0.186705
65	1	0	-4.202088	2.329332	-1.699870
66	6	0	-2.547334	3.447198	-0.798605
67	1	0	-3.171141	4.101048	-0.179231
68	1	0	-2.332291	3.996126	-1.724147

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6038.33231964     A.U. after    1 cycles
             Convg  =    0.2338D-08             -V/T =  2.0048
Zero-point correction=                           0.574827 (Hartree/Particle)
 Thermal correction to Energy=                    0.605054
 Thermal correction to Enthalpy=                  0.606014
 Thermal correction to Gibbs Free Energy=         0.513303
 Sum of electronic and zero-point Energies=          -6037.757493
 Sum of electronic and thermal Energies=             -6037.727266
 Sum of electronic and thermal Enthalpies=           -6037.726306
 Sum of electronic and thermal Free Energies=        -6037.819017
                    1                      2                      3
Frequencies --  -290.3372               12.9139                35.0402
```

(S)-PhBDD-Rh pathway

(*S*)-PhBDD-Rh(I)-Ph (195)

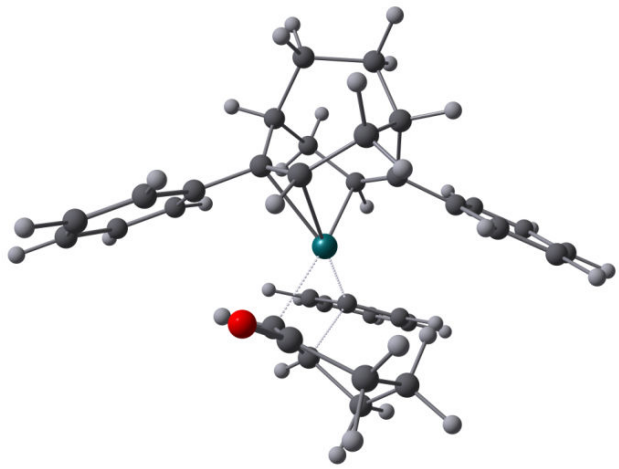


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.230108	0.329371	-0.323925
2	6	0	0.338161	-0.679414	1.402453
3	6	0	0.968272	-1.337476	0.301621
4	6	0	1.115208	1.797456	0.017082
5	1	0	0.973402	-0.029807	2.004294
6	6	0	-0.903923	-1.133664	2.127603
7	6	0	0.430117	-2.658272	-0.304489
8	6	0	0.979560	2.691108	1.093369
9	6	0	2.073953	2.107598	-0.961685
10	6	0	-1.971739	-1.727616	1.195889
11	1	0	-1.306930	-0.264231	2.658166
12	1	0	-0.653301	-1.863274	2.914120
13	6	0	-0.473371	-2.402440	-1.513612
14	1	0	1.307518	-3.205597	-0.662780
15	6	0	1.746240	3.856899	1.174074
16	1	0	0.261296	2.484428	1.886691
17	6	0	2.838818	3.272971	-0.889587
18	1	0	2.243102	1.424870	-1.793678
19	6	0	-2.095016	-0.934507	-0.115210
20	1	0	-2.941618	-1.636074	1.697813
21	6	0	-1.442111	-1.272122	-1.293289
22	1	0	0.142814	-2.135728	-2.379564
23	1	0	-0.999213	-3.328178	-1.795563
24	6	0	2.678171	4.154536	0.180172
25	1	0	1.615846	4.532940	2.017181
26	1	0	3.571734	3.487584	-1.665072
27	1	0	-1.796863	-0.794932	-2.208565
28	1	0	3.279258	5.058507	0.242891
29	6	0	2.433779	-1.135755	0.076085
30	6	0	2.980070	-1.282684	-1.209409
31	6	0	3.317559	-0.851136	1.125509
32	6	0	4.342513	-1.127987	-1.441546
33	1	0	2.322386	-1.500047	-2.047920
34	6	0	4.683307	-0.692616	0.897155
35	1	0	2.941225	-0.761568	2.140452
36	6	0	5.205456	-0.827346	-0.386944
37	1	0	4.732338	-1.236654	-2.450805
38	1	0	5.343071	-0.470277	1.732199

39	1	0	6.270553	-0.704358	-0.564434
40	6	0	-3.200710	0.067777	-0.185264
41	6	0	-3.426145	0.972659	0.866034
42	6	0	-4.062941	0.129696	-1.292115
43	6	0	-4.450196	1.913902	0.802026
44	1	0	-2.782701	0.951401	1.740828
45	6	0	-5.088726	1.069258	-1.357319
46	1	0	-3.946340	-0.584021	-2.103078
47	6	0	-5.286080	1.970426	-0.312248
48	1	0	-4.592881	2.608522	1.625860
49	1	0	-5.744332	1.088773	-2.224306
50	1	0	-6.086927	2.703232	-0.362005
51	6	0	-1.721214	-3.224950	0.978132
52	6	0	-0.258580	-3.572767	0.717042
53	1	0	-2.350244	-3.578869	0.153337
54	1	0	-2.057831	-3.766331	1.870845
55	1	0	0.311967	-3.558763	1.652610
56	1	0	-0.205070	-4.604446	0.347937

```
SCF Done:  E(RPBE1PBE) =  -5769.25932365     A.U. after    1 cycles
             Convg  =    0.4280D-08             -V/T =  2.0044
Zero-point correction=                           0.473117 (Hartree/Particle)
 Thermal correction to Energy=                    0.498073
 Thermal correction to Enthalpy=                  0.499033
 Thermal correction to Gibbs Free Energy=         0.414642
 Sum of electronic and zero-point Energies=          -5768.786207
 Sum of electronic and thermal Energies=             -5768.761251
 Sum of electronic and thermal Enthalpies=           -5768.760291
 Sum of electronic and thermal Free Energies=        -5768.844681
                    1                    2                    3
Frequencies --     4.6487              21.0459              27.4508
```

(*S*)-PhBDD-Rh(I)-Ph-CH-si-confU-CR-TS (200a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.198674	-0.158626	-0.030781
2	6	0	-0.688073	1.294271	1.385216
3	6	0	-1.189411	1.653292	0.133667
4	6	0	-1.005419	-1.615449	1.034909
5	1	0	-1.347254	0.710587	2.024866
6	6	0	0.469419	1.918330	2.112205

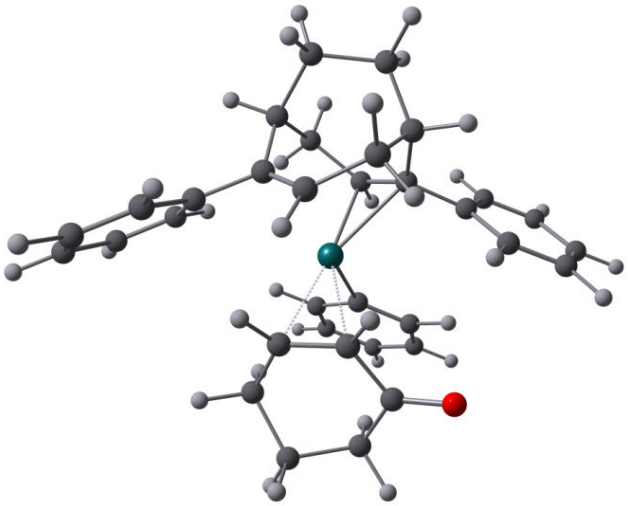
7	6	0	-0.624515	2.806056	-0.722901
8	6	0	-0.444960	-1.914442	2.293428
9	6	0	-2.392913	-1.751096	0.900394
10	6	0	1.605549	2.348618	1.183150
11	1	0	0.833422	1.183329	2.838368
12	1	0	0.128989	2.778460	2.711018
13	6	0	0.401027	2.318301	-1.746922
14	1	0	-1.477465	3.208728	-1.278456
15	6	0	-1.238368	-2.276985	3.377794
16	1	0	0.636165	-1.873009	2.424459
17	6	0	-3.191973	-2.132472	1.980624
18	1	0	-2.874149	-1.538285	-0.051163
19	6	0	1.899064	1.285697	0.105588
20	1	0	2.516477	2.421371	1.786229
21	6	0	1.369827	1.314805	-1.189070
22	1	0	-0.111292	1.840457	-2.589517
23	1	0	0.937873	3.178204	-2.178794
24	6	0	-2.623093	-2.390358	3.225711
25	1	0	-0.775029	-2.489581	4.338896
26	1	0	-4.267863	-2.216803	1.843927
27	1	0	1.905284	0.746412	-1.945552
28	1	0	-3.246050	-2.688442	4.065255
29	6	0	-2.597758	1.296463	-0.215243
30	6	0	-2.967916	1.044652	-1.546059
31	6	0	-3.610429	1.290301	0.753243
32	6	0	-4.285392	0.759446	-1.889688
33	1	0	-2.208141	1.057979	-2.323362
34	6	0	-4.933262	1.012473	0.412943
35	1	0	-3.365635	1.515441	1.787225
36	6	0	-5.278144	0.738102	-0.908542
37	1	0	-4.538870	0.553514	-2.926700
38	1	0	-5.697771	1.016755	1.185906
39	1	0	-6.309217	0.520837	-1.174868
40	6	0	3.139298	0.489212	0.367335
41	6	0	3.366235	-0.083710	1.630190
42	6	0	4.127503	0.320139	-0.611287
43	6	0	4.517568	-0.817354	1.895656
44	1	0	2.619513	0.026956	2.412063
45	6	0	5.283403	-0.412901	-0.347989
46	1	0	3.994614	0.760753	-1.593976
47	6	0	5.484847	-0.988850	0.904008
48	1	0	4.660329	-1.258961	2.878945
49	1	0	6.029979	-0.530889	-1.129107
50	1	0	6.385739	-1.561521	1.108096
51	6	0	1.355606	3.746250	0.604307
52	6	0	-0.071241	3.965339	0.115027
53	1	0	2.069344	3.928634	-0.207152
54	1	0	1.581777	4.488249	1.380112
55	1	0	-0.742398	4.145100	0.962742
56	1	0	-0.100593	4.877539	-0.493613
57	6	0	0.153819	-2.564627	-0.423155
58	6	0	1.222956	-1.812464	-1.005836
59	1	0	0.452299	-3.218688	0.389891
60	1	0	2.203053	-1.856892	-0.534451
61	6	0	1.260691	-1.577372	-2.454161
62	8	0	2.292404	-1.218940	-3.027374
63	6	0	0.016335	-1.852826	-3.278950
64	1	0	-0.143275	-0.994429	-3.939829
65	6	0	-0.879052	-3.158898	-1.349829
66	1	0	-1.764353	-3.479675	-0.796903
67	6	0	-1.229682	-2.198953	-2.474358
68	1	0	0.285472	-2.689837	-3.936593
69	1	0	-1.661610	-1.288610	-2.041768

70	1	0	-1.993253	-2.633266	-3.129020
71	1	0	-0.424932	-4.068673	-1.771471

SCF Done: E(RPBE1PBE) = -6077.59717589 A.U. after 2 cycles
Convg = 0.5727D-08 -V/T = 2.0049
Zero-point correction= 0.604935 (Hartree/Particle)
Thermal correction to Energy= 0.636055
Thermal correction to Enthalpy= 0.637015
Thermal correction to Gibbs Free Energy= 0.543770
Sum of electronic and zero-point Energies= -6076.992241
Sum of electronic and thermal Energies= -6076.961121
Sum of electronic and thermal Enthalpies= -6076.960161
Sum of electronic and thermal Free Energies= -6077.053406

	1	2	3
Frequencies --	-274.4342	25.8680	39.3173

(*S*)-PhBDD-Rh(I)-Ph-CH-si-confD-close (197b)



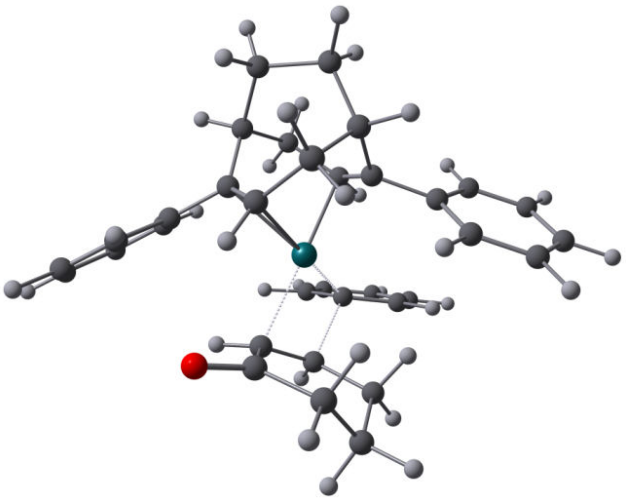
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.246508	0.034626	-0.014352
2	6	0	0.458275	-1.501114	1.361694
3	6	0	1.063143	-1.836450	0.143297
4	6	0	1.005283	1.269020	1.006181
5	1	0	1.093363	-0.995446	2.087930
6	6	0	-0.775930	-2.118366	1.969601
7	6	0	0.528921	-2.937633	-0.797017
8	6	0	0.371041	1.871766	2.107675
9	6	0	2.364505	1.545360	0.819436
10	6	0	-1.844415	-2.524536	0.948947
11	1	0	-1.192553	-1.398460	2.683339
12	1	0	-0.499299	-2.995126	2.577579
13	6	0	-0.416999	-2.404504	-1.872946
14	1	0	1.407523	-3.332229	-1.316323
15	6	0	1.058532	2.721158	2.978178
16	1	0	-0.684838	1.678918	2.305994
17	6	0	3.056540	2.398879	1.683047
18	1	0	2.901218	1.110713	-0.019571
19	6	0	-2.071423	-1.451423	-0.128214
20	1	0	-2.795156	-2.608775	1.486855
21	6	0	-1.452812	-1.447563	-1.359686

22	1	0	0.163630	-1.886866	-2.644762
23	1	0	-0.901472	-3.249145	-2.388437
24	6	0	2.410530	2.992236	2.766738
25	1	0	0.534889	3.170579	3.819929
26	1	0	4.110487	2.599814	1.501085
27	1	0	-1.892415	-0.813698	-2.128773
28	1	0	2.951440	3.655529	3.437322
29	6	0	2.518188	-1.562278	-0.046782
30	6	0	3.026135	-1.189689	-1.300325
31	6	0	3.426887	-1.750463	1.002281
32	6	0	4.389133	-0.993007	-1.493067
33	1	0	2.341010	-0.997306	-2.120998
34	6	0	4.794777	-1.559259	0.811225
35	1	0	3.062973	-2.060506	1.978088
36	6	0	5.282894	-1.179168	-0.436762
37	1	0	4.751824	-0.675265	-2.466928
38	1	0	5.479567	-1.711379	1.641785
39	1	0	6.348451	-1.025373	-0.586192
40	6	0	-3.276205	-0.591889	0.075950
41	6	0	-3.480709	0.086873	1.287451
42	6	0	-4.251760	-0.459510	-0.922403
43	6	0	-4.598679	0.892416	1.481567
44	1	0	-2.745595	-0.000414	2.083122
45	6	0	-5.374282	0.344450	-0.729580
46	1	0	-4.140598	-1.007501	-1.854408
47	6	0	-5.550941	1.029049	0.471278
48	1	0	-4.725346	1.418817	2.424165
49	1	0	-6.118006	0.426653	-1.518101
50	1	0	-6.425347	1.656225	0.622447
51	6	0	-1.548774	-3.908979	0.358737
52	6	0	-0.090422	-4.118295	-0.036159
53	1	0	-2.204455	-4.075612	-0.503655
54	1	0	-1.825471	-4.667320	1.101467
55	1	0	0.518394	-4.328786	0.850703
56	1	0	-0.022269	-5.012379	-0.668109
57	6	0	-1.234361	1.680009	-1.293170
58	6	0	-0.052164	1.288834	-1.909559
59	1	0	-2.158876	1.174777	-1.558035
60	1	0	-0.031369	0.474470	-2.630390
61	6	0	1.093079	2.220504	-2.043638
62	8	0	2.097871	1.891723	-2.664788
63	6	0	0.933999	3.613632	-1.472148
64	1	0	1.356097	3.596904	-0.460247
65	1	0	1.558162	4.284819	-2.069332
66	6	0	-0.520543	4.071841	-1.418845
67	1	0	-0.585049	5.049124	-0.928380
68	1	0	-0.905469	4.200360	-2.438522
69	6	0	-1.386580	3.052132	-0.679469
70	1	0	-1.103128	3.045510	0.378980
71	1	0	-2.441594	3.342188	-0.716589

SCF Done: E(RPBE1PBE) = -6077.60896250 A.U. after 1 cycles
Convg = 0.3732D-08 -V/T = 2.0049
Zero-point correction= 0.604471 (Hartree/Particle)
Thermal correction to Energy= 0.636647
Thermal correction to Enthalpy= 0.637607
Thermal correction to Gibbs Free Energy= 0.541686
Sum of electronic and zero-point Energies= -6077.004491
Sum of electronic and thermal Energies= -6076.972315
Sum of electronic and thermal Enthalpies= -6076.971355
Sum of electronic and thermal Free Energies= -6077.067276

	1	2	3
Frequencies --	26.2668	37.3361	40.7703

(*S*)-PhBDD-Rh(I)-Ph-CH-si-confD-CR-TS (200b)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.164909	-0.135151	0.000381
2	6	0	-0.713621	1.475458	1.235872
3	6	0	-1.215403	1.657808	-0.054403
4	6	0	-0.982928	-1.432482	1.297463
5	1	0	-1.370522	0.978875	1.947402
6	6	0	0.446720	2.189182	1.869589
7	6	0	-0.675513	2.706173	-1.050361
8	6	0	-0.242957	-1.636235	2.479566
9	6	0	-2.372356	-1.574685	1.367156
10	6	0	1.570425	2.504081	0.879646
11	1	0	0.821235	1.546930	2.674054
12	1	0	0.110244	3.115259	2.362665
13	6	0	0.351807	2.113057	-2.014882
14	1	0	-1.539349	3.025148	-1.642919
15	6	0	-0.874162	-1.894471	3.692817
16	1	0	0.844790	-1.594105	2.446761
17	6	0	-3.007094	-1.857024	2.579772
18	1	0	-2.983080	-1.446987	0.477756
19	6	0	1.858576	1.313323	-0.057150
20	1	0	2.488239	2.657591	1.456654
21	6	0	1.323951	1.183255	-1.344135
22	1	0	-0.158977	1.545890	-2.801331
23	1	0	0.884657	2.922147	-2.539446
24	6	0	-2.266424	-2.006875	3.749861
25	1	0	-0.278493	-2.025316	4.593800
26	1	0	-4.090605	-1.952268	2.604698
27	1	0	1.859892	0.531463	-2.029256
28	1	0	-2.762526	-2.223929	4.692385
29	6	0	-2.614504	1.224875	-0.352863
30	6	0	-2.957460	0.705069	-1.611320
31	6	0	-3.641363	1.393127	0.585300
32	6	0	-4.265648	0.335237	-1.907677
33	1	0	-2.183758	0.573476	-2.363939
34	6	0	-4.954911	1.029780	0.290351
35	1	0	-3.412789	1.820650	1.557537
36	6	0	-5.273756	0.492284	-0.954517
37	1	0	-4.500462	-0.077601	-2.885735

38	1	0	-5.731662	1.171693	1.037655
39	1	0	-6.296602	0.206358	-1.185103
40	6	0	3.090860	0.541509	0.299757
41	6	0	3.333253	0.156960	1.629778
42	6	0	4.064043	0.222074	-0.656485
43	6	0	4.483804	-0.539182	1.984555
44	1	0	2.602310	0.390294	2.399225
45	6	0	5.219015	-0.473266	-0.303735
46	1	0	3.924450	0.518216	-1.690664
47	6	0	5.435728	-0.861251	1.016066
48	1	0	4.638056	-0.832002	3.020260
49	1	0	5.953807	-0.709228	-1.069101
50	1	0	6.337044	-1.403374	1.289931
51	6	0	1.304536	3.816879	0.133192
52	6	0	-0.128601	3.964384	-0.364995
53	1	0	2.009718	3.902020	-0.701563
54	1	0	1.532292	4.650801	0.808543
55	1	0	-0.793918	4.242991	0.460208
56	1	0	-0.170433	4.794221	-1.081374
57	6	0	-0.116227	-2.475982	-0.303678
58	6	0	1.091218	-1.931039	-0.846905
59	1	0	0.040480	-3.193119	0.494244
60	1	0	2.015957	-2.086528	-0.291823
61	6	0	1.283806	-1.826978	-2.298673
62	8	0	2.386038	-1.597019	-2.798461
63	6	0	0.083150	-2.096017	-3.185277
64	1	0	-0.504883	-1.171402	-3.264179
65	1	0	0.457172	-2.332191	-4.184881
66	6	0	-0.787302	-3.208199	-2.609879
67	1	0	-1.642949	-3.404636	-3.265189
68	1	0	-0.206589	-4.137477	-2.555312
69	6	0	-1.280314	-2.809857	-1.223092
70	1	0	-1.943203	-1.947065	-1.335429
71	1	0	-1.880813	-3.604688	-0.770257

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SCF Done:  E(RPBE1PBE) =  -6077.59416936     A.U. after    1 cycles
             Convg  =    0.2304D-08             -V/T =  2.0049
Zero-point correction=                           0.604587 (Hartree/Particle)
 Thermal correction to Energy=                    0.635799
 Thermal correction to Enthalpy=                  0.636759
 Thermal correction to Gibbs Free Energy=         0.543405
 Sum of electronic and zero-point Energies=          -6076.989583
 Sum of electronic and thermal Energies=             -6076.958370
 Sum of electronic and thermal Enthalpies=           -6076.957410
 Sum of electronic and thermal Free Energies=        -6077.050764
                    1                      2                      3
Frequencies --  -270.6979               30.6289                38.8512
```
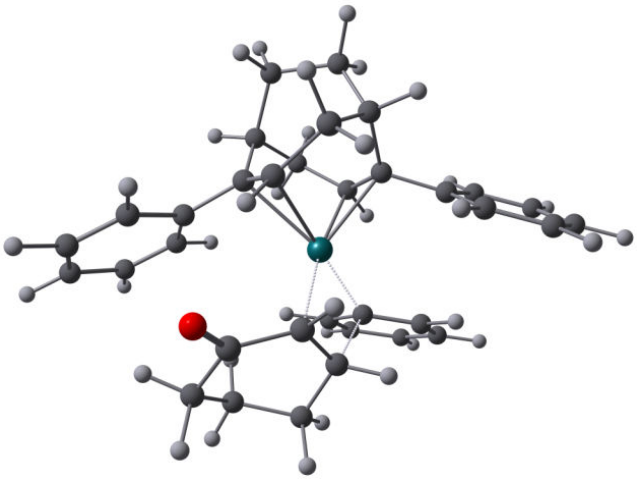

(*S*)-PhBDD-Rh(I)-Ph-CH-re-confU-CR-TS (207a)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.011729	-0.000735	-0.209201
2	6	0	-1.113933	1.012253	1.420108
3	6	0	-1.620216	1.487999	0.203935
4	6	0	-1.036547	-1.816821	0.433228
5	1	0	-1.696214	0.240865	1.921875
6	6	0	-0.091378	1.686199	2.291246
7	6	0	-1.239711	2.847823	-0.426555
8	6	0	-0.472524	-2.250630	1.649109
9	6	0	-2.373737	-2.161767	0.190622
10	6	0	0.979065	2.424190	1.484553
11	1	0	0.373309	0.913162	2.913217
12	1	0	-0.572983	2.381091	2.997957
13	6	0	-0.129514	2.709401	-1.470572
14	1	0	-2.138769	3.193249	-0.947271
15	6	0	-1.222888	-2.953038	2.590823
16	1	0	0.565750	-2.025670	1.882123
17	6	0	-3.125838	-2.875475	1.122271
18	1	0	-2.846593	-1.869970	-0.745305
19	6	0	1.446317	1.599647	0.263969
20	1	0	1.861716	2.530087	2.123897
21	6	0	0.969942	1.778507	-1.040928
22	1	0	-0.543699	2.316779	-2.405576
23	1	0	0.274699	3.702876	-1.722721
24	6	0	-2.556599	-3.272214	2.331800
25	1	0	-0.760823	-3.256807	3.527823
26	1	0	-4.162453	-3.118429	0.900068
27	1	0	1.607972	1.423276	-1.849547
28	1	0	-3.140409	-3.830807	3.059084
29	6	0	-2.933203	0.970300	-0.290802
30	6	0	-3.164335	0.786835	-1.663653
31	6	0	-3.996731	0.735105	0.588662
32	6	0	-4.400291	0.357146	-2.135569
33	1	0	-2.356793	0.962247	-2.369958
34	6	0	-5.238763	0.308515	0.119496
35	1	0	-3.854697	0.894494	1.653958
36	6	0	-5.446641	0.112629	-1.243803
37	1	0	-4.548381	0.210838	-3.202729
38	1	0	-6.047859	0.134083	0.824430

39	1	0	-6.414270	-0.219469	-1.610778
40	6	0	2.786451	0.962615	0.466723
41	6	0	3.038833	0.159290	1.591917
42	6	0	3.856177	1.225098	-0.399455
43	6	0	4.300959	-0.373784	1.831801
44	1	0	2.231559	-0.056116	2.287111
45	6	0	5.123627	0.695650	-0.160103
46	1	0	3.700764	1.856048	-1.268682
47	6	0	5.353915	-0.106905	0.954680
48	1	0	4.464422	-0.999484	2.705925
49	1	0	5.933277	0.915037	-0.851188
50	1	0	6.342191	-0.518971	1.141419
51	6	0	0.531065	3.845061	1.126348
52	6	0	-0.900366	3.923894	0.610924
53	1	0	1.226249	4.263386	0.389460
54	1	0	0.622376	4.473761	2.020753
55	1	0	-1.610925	3.856227	1.442702
56	1	0	-1.060641	4.908428	0.154322
57	6	0	0.029236	-2.195223	-1.307774
58	1	0	-0.919591	-2.405013	-1.793235
59	6	0	0.781096	-1.132407	-1.901409
60	1	0	0.279871	-0.524717	-2.657129
61	6	0	2.226521	-1.213342	-2.105154
62	8	0	2.801989	-0.443056	-2.878138
63	6	0	0.803034	-3.428097	-0.889399
64	1	0	0.239087	-4.022977	-0.167858
65	6	0	2.994749	-2.322013	-1.419952
66	1	0	3.911297	-1.892853	-1.004201
67	6	0	2.193280	-3.083687	-0.372701
68	1	0	0.899571	-4.041236	-1.798702
69	1	0	2.112325	-2.473915	0.532809
70	1	0	2.723713	-3.998342	-0.086624
71	1	0	3.310515	-3.000150	-2.224607

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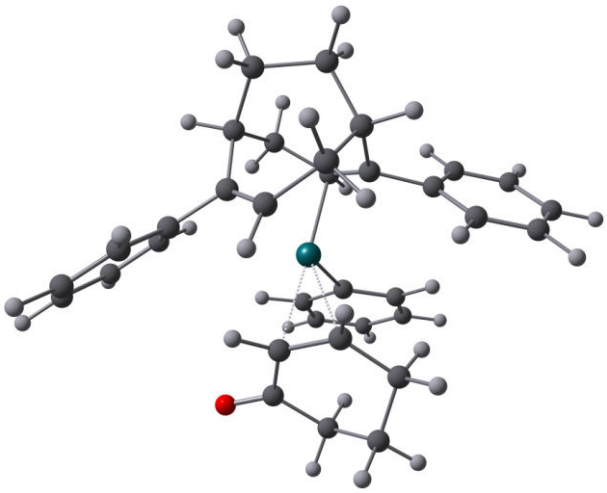
SCF Done:  E(RPBE1PBE) =  -6077.59260620     A.U. after    1 cycles
             Convg  =    0.3957D-08             -V/T =  2.0049
Zero-point correction=                           0.604603 (Hartree/Particle)
 Thermal correction to Energy=                    0.635656
 Thermal correction to Enthalpy=                  0.636616
 Thermal correction to Gibbs Free Energy=         0.544066
 Sum of electronic and zero-point Energies=          -6076.988003
 Sum of electronic and thermal Energies=             -6076.956950
 Sum of electronic and thermal Enthalpies=           -6076.955990
 Sum of electronic and thermal Free Energies=        -6077.048540
                  1                      2                      3
Frequencies --  -294.9982               27.5404                42.0634
```

(*S*)-PhBDD-Rh(I)-Ph-CH-re-confD-close (204b)



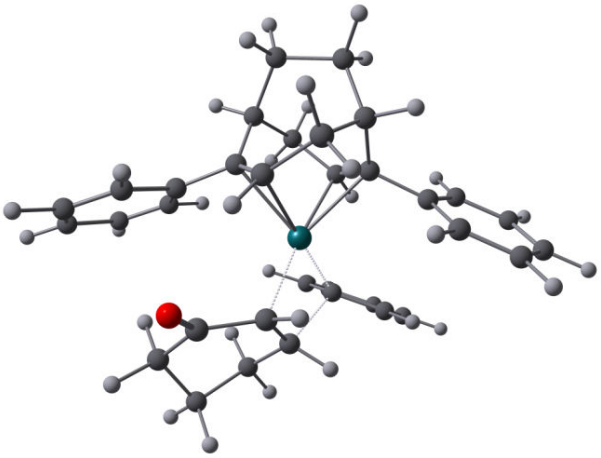
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.163166	-0.016717	-0.041546
2	6	0	0.657069	-1.415788	1.399892
3	6	0	1.271150	-1.767638	0.189867
4	6	0	0.903758	1.398206	0.946074
5	1	0	1.256106	-0.821515	2.089110
6	6	0	-0.524064	-2.085186	2.054823
7	6	0	0.822972	-2.969862	-0.668264
8	6	0	0.089496	2.089665	1.861805
9	6	0	2.260341	1.739362	0.911233
10	6	0	-1.564207	-2.635517	1.072258
11	1	0	-0.990460	-1.354046	2.724661
12	1	0	-0.181186	-2.899090	2.713939
13	6	0	-0.169282	-2.588278	-1.766277
14	1	0	1.727594	-3.328248	-1.169424
15	6	0	0.602622	3.087014	2.692715
16	1	0	-0.979072	1.877434	1.914107
17	6	0	2.779957	2.742274	1.736234
18	1	0	2.940248	1.225856	0.235346
19	6	0	-1.883273	-1.658645	-0.071163
20	1	0	-2.502156	-2.756769	1.624934
21	6	0	-1.275233	-1.684274	-1.304346
22	1	0	0.364688	-2.080716	-2.577856
23	1	0	-0.587714	-3.500847	-2.219844
24	6	0	1.956121	3.422064	2.631271
25	1	0	-0.060395	3.610987	3.378176
26	1	0	3.838624	2.988112	1.676739
27	1	0	-1.764370	-1.123749	-2.100092
28	1	0	2.360513	4.203491	3.269956
29	6	0	2.695436	-1.384282	-0.040360
30	6	0	3.156422	-1.067243	-1.327412
31	6	0	3.630125	-1.404600	1.002707
32	6	0	4.491710	-0.755627	-1.558892
33	1	0	2.448475	-1.036125	-2.151645
34	6	0	4.970963	-1.096070	0.774461
35	1	0	3.308774	-1.671014	2.005711
36	6	0	5.408796	-0.766242	-0.505699
37	1	0	4.818593	-0.496275	-2.562852

38	1	0	5.674644	-1.116907	1.602784
39	1	0	6.452749	-0.522817	-0.684465
40	6	0	-3.141086	-0.870393	0.089221
41	6	0	-3.388181	-0.131148	1.255687
42	6	0	-4.121264	-0.865238	-0.913053
43	6	0	-4.552830	0.615824	1.398708
44	1	0	-2.648548	-0.117506	2.051685
45	6	0	-5.294278	-0.127277	-0.766385
46	1	0	-3.974352	-1.462607	-1.809080
47	6	0	-5.512537	0.622235	0.387305
48	1	0	-4.708256	1.202333	2.300231
49	1	0	-6.041301	-0.142874	-1.555867
50	1	0	-6.421941	1.206272	0.498491
51	6	0	-1.163974	-4.027747	0.568335
52	6	0	0.304577	-4.144176	0.173421
53	1	0	-1.808172	-4.301303	-0.275235
54	1	0	-1.375130	-4.756333	1.360614
55	1	0	0.933409	-4.246273	1.065231
56	1	0	0.442114	-5.068601	-0.400851
57	6	0	0.043615	1.003128	-2.084083
58	1	0	-0.043778	0.119681	-2.712461
59	6	0	-1.107112	1.484629	-1.459268
60	1	0	-2.075098	1.007204	-1.596102
61	6	0	-1.200414	2.887795	-0.995323
62	8	0	-2.229926	3.317270	-0.485819
63	6	0	1.222633	1.898629	-2.381402
64	1	0	1.673534	1.581671	-3.328589
65	1	0	1.999238	1.785425	-1.620641
66	6	0	-0.003286	3.782327	-1.236738
67	1	0	0.628169	3.733042	-0.341271
68	1	0	-0.371518	4.809266	-1.315854
69	6	0	0.797041	3.364163	-2.466130
70	1	0	1.679280	4.004101	-2.574837
71	1	0	0.185890	3.510345	-3.365936

SCF Done: E(RPBE1PBE) = -6077.60897976 A.U. after 1 cycles
Convg = 0.5419D-08 -V/T = 2.0049
Zero-point correction= 0.604697 (Hartree/Particle)
Thermal correction to Energy= 0.636698
Thermal correction to Enthalpy= 0.637658
Thermal correction to Gibbs Free Energy= 0.542835
Sum of electronic and zero-point Energies= -6077.004283
Sum of electronic and thermal Energies= -6076.972282
Sum of electronic and thermal Enthalpies= -6076.971322
Sum of electronic and thermal Free Energies= -6077.066144

	1	2	3
Frequencies --	30.2249	41.2043	46.1278

(*S*)-PhBND-Rh(I)-Ph-CH-re-confD-CR-TS (207b)

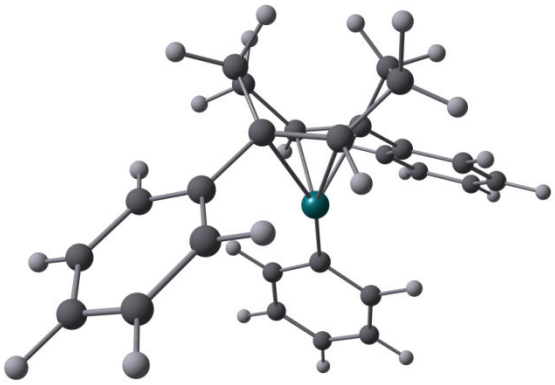


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.020020	-0.004579	-0.190734
2	6	0	-1.169742	1.052821	1.382368
3	6	0	-1.658120	1.479424	0.142683
4	6	0	-1.039849	-1.812912	0.523881
5	1	0	-1.750216	0.290387	1.898709
6	6	0	-0.170054	1.765800	2.248212
7	6	0	-1.285033	2.823215	-0.524809
8	6	0	-0.606563	-2.164385	1.814280
9	6	0	-2.334797	-2.206136	0.155547
10	6	0	0.905499	2.489513	1.435995
11	1	0	0.291868	1.017886	2.902042
12	1	0	-0.671655	2.477222	2.923858
13	6	0	-0.153847	2.667407	-1.543449
14	1	0	-2.179447	3.139473	-1.071427
15	6	0	-1.442797	-2.829488	2.710156
16	1	0	0.397268	-1.900462	2.143693
17	6	0	-3.172226	-2.883406	1.040043
18	1	0	-2.706658	-1.980395	-0.842519
19	6	0	1.402843	1.629456	0.252132
20	1	0	1.775563	2.627639	2.086338
21	6	0	0.945728	1.759743	-1.066542
22	1	0	-0.545390	2.245737	-2.475454
23	1	0	0.245753	3.657564	-1.814961
24	6	0	-2.733693	-3.195410	2.326680
25	1	0	-1.080494	-3.068345	3.707871
26	1	0	-4.172377	-3.165982	0.719598
27	1	0	1.600059	1.387419	-1.853810
28	1	0	-3.383517	-3.726920	3.017343
29	6	0	-2.950489	0.920983	-0.362250
30	6	0	-3.155117	0.706415	-1.734958
31	6	0	-4.022956	0.677730	0.504158
32	6	0	-4.372905	0.239119	-2.218063
33	1	0	-2.342005	0.888989	-2.432980
34	6	0	-5.247161	0.214675	0.023492
35	1	0	-3.903006	0.860476	1.568379
36	6	0	-5.428169	-0.011934	-1.338867
37	1	0	-4.499862	0.069406	-3.284496
38	1	0	-6.063605	0.035539	0.718695
39	1	0	-6.382109	-0.372407	-1.714893

40	6	0	2.746955	1.018134	0.502377
41	6	0	2.983851	0.249308	1.655147
42	6	0	3.833075	1.272896	-0.345220
43	6	0	4.248375	-0.254811	1.941631
44	1	0	2.162528	0.039107	2.334888
45	6	0	5.101912	0.768390	-0.061424
46	1	0	3.688732	1.877385	-1.234995
47	6	0	5.318037	0.003714	1.082154
48	1	0	4.400572	-0.851070	2.838073
49	1	0	5.924547	0.979833	-0.739546
50	1	0	6.307726	-0.386849	1.304019
51	6	0	0.446506	3.892314	1.024031
52	6	0	-0.977171	3.936095	0.483099
53	1	0	1.148989	4.295786	0.285762
54	1	0	0.515098	4.550270	1.899239
55	1	0	-1.700777	3.886104	1.304840
56	1	0	-1.141713	4.903273	-0.007803
57	6	0	0.268983	-2.266702	-1.031701
58	1	0	-0.602063	-2.686516	-1.524769
59	6	0	0.901132	-1.204220	-1.753129
60	1	0	0.327955	-0.750812	-2.565846
61	6	0	2.341626	-1.192687	-2.031156
62	8	0	2.825471	-0.398585	-2.839188
63	6	0	1.166468	-3.281687	-0.344483
64	1	0	0.599567	-4.194481	-0.141022
65	1	0	1.505945	-2.901805	0.622045
66	6	0	3.192454	-2.258575	-1.376999
67	1	0	3.522813	-1.878309	-0.401309
68	1	0	4.086881	-2.392004	-1.991265
69	6	0	2.410143	-3.555099	-1.186978
70	1	0	3.032812	-4.305285	-0.687160
71	1	0	2.129963	-3.971313	-2.162843

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6077.58854961     A.U. after    1 cycles
             Convg  =    0.2395D-08             -V/T =  2.0049
Zero-point correction=                           0.604459 (Hartree/Particle)
 Thermal correction to Energy=                    0.635632
 Thermal correction to Enthalpy=                  0.636592
 Thermal correction to Gibbs Free Energy=         0.543323
 Sum of electronic and zero-point Energies=          -6076.984091
 Sum of electronic and thermal Energies=             -6076.952918
 Sum of electronic and thermal Enthalpies=           -6076.951958
 Sum of electronic and thermal Free Energies=        -6077.045227
                    1                    2                    3
Frequencies --  -295.9850               22.3546              40.8202
```

Ligand XV-XX-Rh pathways
$PhCOD_{2,6}$-Rh(I)-Ph (210)



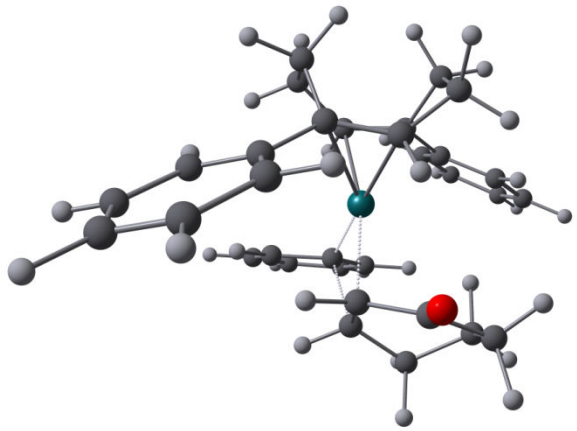
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.343138	-0.033546	-0.260845
2	6	0	0.306870	-0.846651	1.536068
3	6	0	1.042333	-1.484169	0.491558
4	6	0	0.828802	1.602066	-0.036675
5	1	0	0.819463	-0.076019	2.111084
6	6	0	-0.845760	-1.488882	2.279541
7	6	0	0.645210	-2.905749	0.068632
8	6	0	0.636733	2.540496	0.990675
9	6	0	1.715386	1.946839	-1.070363
10	6	0	-1.955701	-2.072752	1.379171
11	1	0	-1.275547	-0.721105	2.931334
12	1	0	-0.469622	-2.273035	2.955021
13	6	0	-0.389958	-2.976494	-1.063746
14	1	0	1.540348	-3.452938	-0.239851
15	6	0	1.282872	3.779846	0.974110
16	1	0	-0.033024	2.313460	1.819660
17	6	0	2.359723	3.184887	-1.094897
18	1	0	1.926924	1.234144	-1.867613
19	6	0	-2.092211	-1.381717	0.029519
20	1	0	-2.911940	-2.020261	1.909381
21	6	0	-1.372899	-1.830638	-1.070355
22	1	0	0.135643	-2.954080	-2.024075
23	1	0	-0.914774	-3.943093	-1.030862
24	6	0	2.146414	4.108248	-0.070468
25	1	0	1.110982	4.490185	1.780838
26	1	0	3.040855	3.424161	-1.909332
27	1	0	-1.678068	-1.493663	-2.061395
28	1	0	2.653815	5.069923	-0.082556
29	6	0	2.464312	-1.125632	0.213487
30	6	0	3.024260	-1.422368	-1.039849
31	6	0	3.296332	-0.531562	1.171817
32	6	0	4.349924	-1.118956	-1.332568
33	1	0	2.404438	-1.882576	-1.806588
34	6	0	4.624259	-0.225748	0.882543
35	1	0	2.909470	-0.308571	2.161754
36	6	0	5.160052	-0.514457	-0.370896
37	1	0	4.751574	-1.351858	-2.315832
38	1	0	5.244993	0.237244	1.645561
39	1	0	6.196216	-0.275286	-0.595105
40	6	0	-3.155924	-0.354078	-0.132427

41	6	0	-3.508315	0.469416	0.952725
42	6	0	-3.831567	-0.149631	-1.348751
43	6	0	-4.473488	1.463821	0.823207
44	1	0	-3.012461	0.337212	1.910307
45	6	0	-4.797468	0.843836	-1.478037
46	1	0	-3.621657	-0.791369	-2.199606
47	6	0	-5.122198	1.659984	-0.394709
48	1	0	-4.717545	2.089435	1.677904
49	1	0	-5.308216	0.973426	-2.428803
50	1	0	-5.877386	2.434498	-0.497085
51	1	0	-1.779429	-3.137326	1.202515
52	1	0	0.278219	-3.432676	0.955464

SCF Done: E(RPBE1PBE) = -5691.92218549 A.U. after 1 cycles
Convg = 0.2009D-08 -V/T = 2.0042
Zero-point correction= 0.436445 (Hartree/Particle)
Thermal correction to Energy= 0.460337
Thermal correction to Enthalpy= 0.461297
Thermal correction to Gibbs Free Energy= 0.381397
Sum of electronic and zero-point Energies= -5691.485741
Sum of electronic and thermal Energies= -5691.461849
Sum of electronic and thermal Enthalpies= -5691.460889
Sum of electronic and thermal Free Energies= -5691.540789

	1	2	3
Frequencies --	24.1984	30.8442	35.6122

PhCOD$_{2,6}$-Rh(I)-Ph-CH-si-confU-CR-TS (212a)



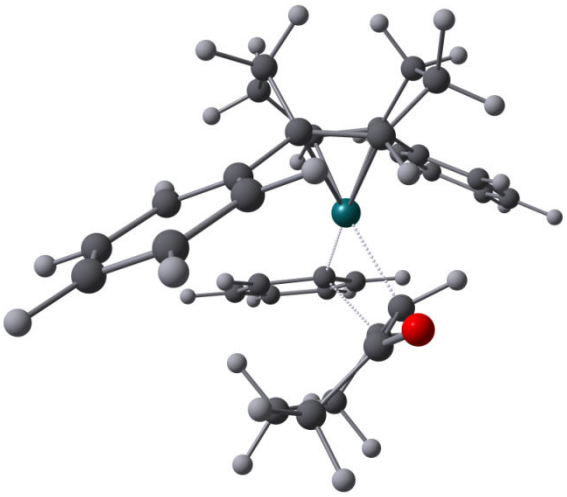
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.225501	-0.045246	-0.065388
2	6	0	-0.695998	0.659625	-1.946684
3	6	0	-1.248196	-0.599822	-1.712778
4	6	0	-0.900364	1.563654	0.863382
5	1	0	-1.293787	1.524314	-1.665155
6	6	0	0.412215	0.965325	-2.921098
7	6	0	-0.744691	-1.837287	-2.459216
8	6	0	-0.292570	2.805776	0.590340
9	6	0	-2.279499	1.560850	1.104102
10	6	0	1.599302	-0.002183	-2.858237
11	1	0	0.762532	1.980733	-2.706116
12	1	0	0.012084	0.998775	-3.946589
13	6	0	0.389267	-2.591703	-1.759287
14	1	0	-1.584195	-2.522489	-2.606836

15	6	0	-1.036978	3.978535	0.505108
16	1	0	0.786616	2.854909	0.449125
17	6	0	-3.028498	2.738407	1.040455
18	1	0	-2.794478	0.629965	1.328324
19	6	0	1.906201	-0.526236	-1.456311
20	1	0	2.488061	0.500984	-3.249884
21	6	0	1.341376	-1.716417	-0.987359
22	1	0	-0.041616	-3.306086	-1.049298
23	1	0	0.941955	-3.199225	-2.492993
24	6	0	-2.415896	3.950846	0.732767
25	1	0	-0.539377	4.919189	0.278922
26	1	0	-4.099999	2.699543	1.224384
27	1	0	1.852092	-2.221293	-0.171172
28	1	0	-2.999772	4.866504	0.683556
29	6	0	-2.631915	-0.740743	-1.175058
30	6	0	-2.986354	-1.868113	-0.416498
31	6	0	-3.639809	0.182287	-1.482024
32	6	0	-4.283740	-2.044855	0.052795
33	1	0	-2.229111	-2.612826	-0.181672
34	6	0	-4.943523	0.004427	-1.022037
35	1	0	-3.407572	1.046006	-2.098122
36	6	0	-5.271762	-1.104722	-0.245339
37	1	0	-4.526142	-2.919746	0.651016
38	1	0	-5.706604	0.735269	-1.278003
39	1	0	-6.287900	-1.243280	0.114513
40	6	0	3.151828	0.024999	-0.845519
41	6	0	3.406615	1.405692	-0.897495
42	6	0	4.116354	-0.796981	-0.248327
43	6	0	4.563907	1.948113	-0.349161
44	1	0	2.676473	2.067278	-1.357765
45	6	0	5.278191	-0.256324	0.299452
46	1	0	3.958797	-1.869423	-0.201714
47	6	0	5.508186	1.117132	0.256153
48	1	0	4.730361	3.021655	-0.393247
49	1	0	6.008169	-0.916747	0.760286
50	1	0	6.414945	1.536608	0.683980
51	6	0	0.266533	0.571194	2.305810
52	6	0	1.294600	-0.295811	1.822451
53	1	0	0.598292	1.572935	2.559098
54	1	0	2.281623	0.125436	1.643457
55	6	0	1.301279	-1.716529	2.191418
56	8	0	2.308349	-2.416702	2.061837
57	6	0	0.058449	-2.319755	2.819822
58	1	0	-0.142548	-3.271025	2.316692
59	6	0	-0.761053	-0.002184	3.249543
60	1	0	-1.625111	0.659254	3.338781
61	6	0	-1.161899	-1.408893	2.839964
62	1	0	0.351222	-2.579969	3.845637
63	1	0	-1.617354	-1.370270	1.843512
64	1	0	-1.920776	-1.808718	3.521409
65	1	0	-0.282270	-0.029023	4.240479
66	1	0	-0.445314	-1.530712	-3.465544
67	1	0	1.437003	-0.858664	-3.518123

SCF Done: E(RPBE1PBE) = -6000.25740654 A.U. after 1 cycles
Convg = 0.4422D-08 -V/T = 2.0047
Zero-point correction= 0.567665 (Hartree/Particle)
Thermal correction to Energy= 0.598061
Thermal correction to Enthalpy= 0.599021
Thermal correction to Gibbs Free Energy= 0.506828
Sum of electronic and zero-point Energies= -5999.689742
Sum of electronic and thermal Energies= -5999.659345
Sum of electronic and thermal Enthalpies= -5999.658385

```
 Sum of electronic and thermal Free Energies=         -5999.750579
                      1                      2                      3
Frequencies --   -269.5337               28.3745                36.4029
```

PhCOD$_{2,6}$-Rh(I)-Ph-CH-re-confU-CR-TS (214a)



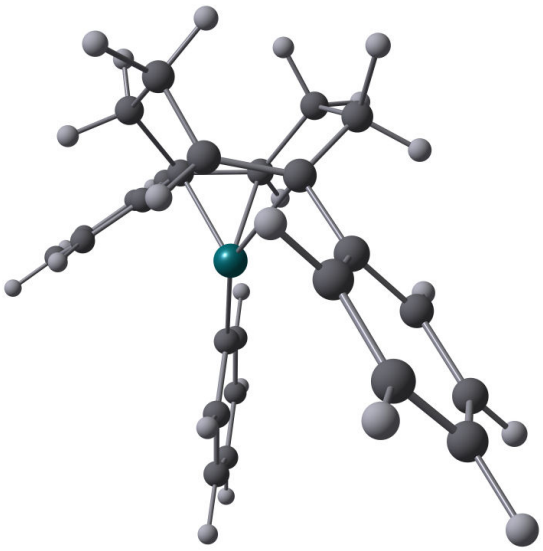
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.020677	-0.279468	0.102527
2	6	0	-1.111692	-1.067252	-1.639864
3	6	0	-1.649248	-1.654124	-0.485850
4	6	0	-1.009070	1.622287	-0.297031
5	1	0	-1.654657	-0.225561	-2.067137
6	6	0	-0.138597	-1.730983	-2.580392
7	6	0	-1.296509	-3.089544	-0.079134
8	6	0	-0.348001	2.193070	-1.402240
9	6	0	-2.344480	1.992277	-0.088480
10	6	0	1.019375	-2.444050	-1.873107
11	1	0	0.265374	-0.950947	-3.234846
12	1	0	-0.662371	-2.436437	-3.244541
13	6	0	-0.096436	-3.211429	0.869046
14	1	0	-2.170243	-3.539818	0.400912
15	6	0	-1.004623	3.056490	-2.277561
16	1	0	0.691350	1.944652	-1.602614
17	6	0	-3.001961	2.868989	-0.950467
18	1	0	-2.889579	1.595519	0.766034
19	6	0	1.470358	-1.765757	-0.577973
20	1	0	1.873884	-2.501183	-2.554080
21	6	0	0.964231	-2.159969	0.665431
22	1	0	-0.447596	-3.123226	1.902716
23	1	0	0.342247	-4.218306	0.788984
24	6	0	-2.337831	3.403733	-2.053902
25	1	0	-0.469966	3.463444	-3.133270
26	1	0	-4.039540	3.132121	-0.757362
27	1	0	1.559420	-1.927422	1.547612
28	1	0	-2.848690	4.088352	-2.726272
29	6	0	-2.940462	-1.169807	0.085008
30	6	0	-3.148165	-1.176065	1.473578
31	6	0	-3.999516	-0.769604	-0.737590
32	6	0	-4.358715	-0.764133	2.021025
33	1	0	-2.339184	-1.487905	2.130881

34	6	0	-5.217383	-0.363372	-0.192808
35	1	0	-3.872387	-0.780782	-1.816561
36	6	0	-5.401592	-0.352187	1.188000
37	1	0	-4.490974	-0.763277	3.100200
38	1	0	-6.025634	-0.057374	-0.852390
39	1	0	-6.349611	-0.033411	1.613351
40	6	0	2.772891	-1.043197	-0.677349
41	6	0	3.001641	-0.143344	-1.733092
42	6	0	3.830857	-1.300012	0.204450
43	6	0	4.227486	0.495575	-1.884557
44	1	0	2.203583	0.060679	-2.443308
45	6	0	5.062581	-0.665060	0.051507
46	1	0	3.696484	-2.007049	1.016343
47	6	0	5.267999	0.237032	-0.989904
48	1	0	4.374463	1.193140	-2.705535
49	1	0	5.865270	-0.882733	0.751214
50	1	0	6.229699	0.729236	-1.109262
51	6	0	-0.079498	1.700162	1.558422
52	1	0	-1.062874	1.767175	2.015702
53	6	0	0.702656	0.584351	1.989656
54	1	0	0.206807	-0.168517	2.604362
55	6	0	2.133827	0.686995	2.265014
56	8	0	2.722496	-0.195183	2.895886
57	6	0	0.637649	3.027044	1.414867
58	1	0	0.074156	3.713912	0.779646
59	6	0	2.864735	1.946389	1.852616
60	1	0	3.825374	1.655993	1.417074
61	6	0	2.070964	2.860718	0.928340
62	1	0	0.650737	3.466225	2.424391
63	1	0	2.074965	2.447692	-0.085172
64	1	0	2.557151	3.840162	0.864058
65	1	0	3.098166	2.466682	2.791718
66	1	0	-1.134559	-3.673371	-0.989788
67	1	0	0.758378	-3.481492	-1.647859

SCF Done: E(RPBE1PBE) = -6000.25302657 A.U. after 1 cycles
Convg = 0.3565D-08 -V/T = 2.0047
Zero-point correction= 0.567415 (Hartree/Particle)
Thermal correction to Energy= 0.597716
Thermal correction to Enthalpy= 0.598676
Thermal correction to Gibbs Free Energy= 0.506788
Sum of electronic and zero-point Energies= -5999.685611
Sum of electronic and thermal Energies= -5999.655311
Sum of electronic and thermal Enthalpies= -5999.654351
Sum of electronic and thermal Free Energies= -5999.746238

	1	2	3
Frequencies --	-292.0518	21.7608	39.9799

PhCOD$_{3,7}$-Rh(I)-Ph (215)

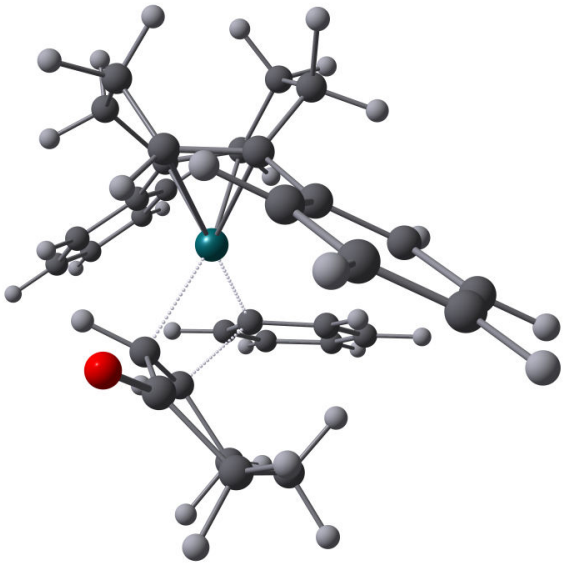


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.346889	-0.082481	-0.149822
2	6	0	-0.580233	-1.275308	1.286744
3	1	0	-1.103195	-0.640464	2.001323
4	6	0	0.372139	-2.282646	1.918643
5	1	0	0.284091	-2.207626	3.007257
6	1	0	0.047549	-3.297664	1.667334
7	6	0	1.850256	-2.072035	1.539222
8	1	0	2.319043	-1.434752	2.292589
9	1	0	2.393914	-3.026795	1.580786
10	6	0	2.068530	-1.430721	0.178432
11	6	0	1.438719	-1.893618	-0.967461
12	1	0	1.784181	-1.525706	-1.933725
13	6	0	0.518096	-3.088280	-0.990999
14	1	0	0.648940	-3.626187	-1.936089
15	1	0	0.799270	-3.795360	-0.206247
16	6	0	-0.956759	-2.680813	-0.863787
17	1	0	-1.339118	-2.431803	-1.859222
18	1	0	-1.563764	-3.534095	-0.523185
19	6	0	-1.240766	-1.482372	0.036811
20	6	0	-0.705122	1.619204	0.135067
21	6	0	-1.780107	2.009731	0.944175
22	6	0	-0.087818	2.611530	-0.642014
23	6	0	-2.212105	3.336217	0.978293
24	1	0	-2.305109	1.277442	1.554224
25	6	0	-0.517886	3.941143	-0.624140
26	1	0	0.762835	2.359322	-1.284817
27	6	0	-1.586227	4.306878	0.193199
28	1	0	-3.046565	3.615265	1.618792
29	1	0	-0.019953	4.685822	-1.241842
30	1	0	-1.929277	5.338362	0.219022
31	6	0	-2.640873	-0.983404	-0.144031
32	6	0	-3.066140	-0.412483	-1.351653
33	6	0	-3.585574	-1.147979	0.875876
34	6	0	-4.380637	0.004823	-1.523432
35	1	0	-2.344346	-0.259046	-2.150754

36	6	0	-4.907101	-0.731170	0.707452
37	1	0	-3.284879	-1.613894	1.811447
38	6	0	-5.309360	-0.149558	-0.491634
39	1	0	-4.681495	0.466171	-2.460732
40	1	0	-5.621912	-0.865654	1.515678
41	1	0	-6.336113	0.181343	-0.624376
42	6	0	3.160864	-0.422788	0.054963
43	6	0	3.290392	0.616291	0.994569
44	6	0	4.071181	-0.458671	-1.014559
45	6	0	4.273726	1.592499	0.854149
46	1	0	2.601311	0.674683	1.833776
47	6	0	5.060480	0.510975	-1.148334
48	1	0	4.015311	-1.270167	-1.735226
49	6	0	5.164257	1.544506	-0.216920
50	1	0	4.341422	2.394034	1.584965
51	1	0	5.759650	0.454964	-1.978815
52	1	0	5.936591	2.301723	-0.321967

```
SCF Done:  E(RPBE1PBE) =  -5691.92155228     A.U. after    1 cycles
             Convg  =    0.1814D-08             -V/T =  2.0042
Zero-point correction=                           0.436081 (Hartree/Particle)
 Thermal correction to Energy=                   0.460080
 Thermal correction to Enthalpy=                 0.461040
 Thermal correction to Gibbs Free Energy=        0.381232
 Sum of electronic and zero-point Energies=          -5691.485472
 Sum of electronic and thermal Energies=             -5691.461472
 Sum of electronic and thermal Enthalpies=           -5691.460512
 Sum of electronic and thermal Free Energies=        -5691.540320
                    1                    2                    3
Frequencies --    25.8777              35.0033              37.0649
```

PhCOD$_{3,7}$-Rh(I)-Ph-CH-si-confU-CR-TS (217a)

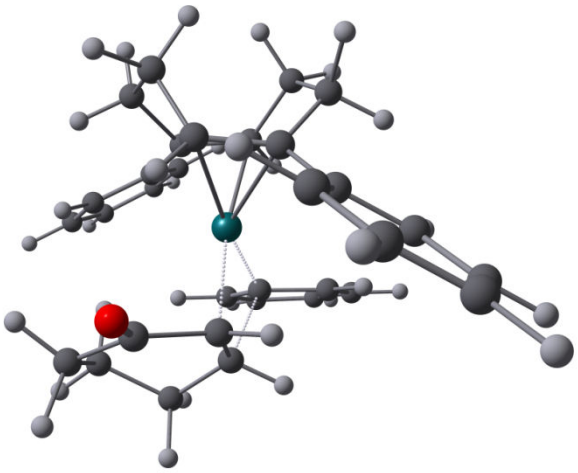


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.018006	-0.323037	-0.060951
2	6	0	-1.187810	-1.402088	1.484909
3	1	0	-1.696950	-0.629350	2.058770

4	6	0	-0.336308	-2.371764	2.277179
5	1	0	-0.543786	-2.232568	3.343301
6	1	0	-0.637896	-3.399543	2.051950
7	6	0	1.167802	-2.177978	2.050970
8	1	0	1.540120	-1.470838	2.795599
9	1	0	1.716451	-3.113117	2.241053
10	6	0	1.566936	-1.661661	0.674461
11	6	0	1.049886	-2.204844	-0.506933
12	1	0	1.583324	-1.996749	-1.433402
13	6	0	0.119737	-3.397566	-0.513763
14	1	0	0.318102	-3.994696	-1.409724
15	1	0	0.348745	-4.050189	0.333860
16	6	0	-1.359902	-2.998540	-0.518263
17	1	0	-1.681664	-2.883045	-1.556220
18	1	0	-1.982713	-3.809346	-0.109825
19	6	0	-1.707412	-1.710790	0.219369
20	6	0	-0.340744	2.063940	1.484858
21	6	0	-0.964632	2.883397	2.424181
22	6	0	-1.035876	1.559576	0.368620
23	6	0	-2.297120	3.259701	2.253035
24	1	0	-0.402846	3.236857	3.286158
25	6	0	-2.369087	1.961588	0.211771
26	6	0	-2.992365	2.798838	1.135774
27	1	0	-2.782267	3.912522	2.974244
28	1	0	-2.939817	1.626838	-0.651419
29	1	0	-4.028637	3.089588	0.979107
30	6	0	-0.149395	1.661860	-1.474325
31	6	0	0.682518	0.582456	-1.924335
32	1	0	0.219088	-0.187131	-2.544288
33	6	0	0.518588	3.018910	-1.349476
34	6	0	1.961288	2.914650	-0.873794
35	1	0	1.986877	2.509905	0.142060
36	1	0	2.406014	3.914262	-0.818564
37	1	0	-1.132391	1.692964	-1.938934
38	6	0	2.105539	0.741443	-2.205561
39	6	0	2.790014	2.026687	-1.793030
40	1	0	3.758047	1.771074	-1.351959
41	1	0	3.010104	2.552215	-2.732363
42	8	0	2.726216	-0.117624	-2.838262
43	1	0	0.505136	3.449188	-2.362575
44	1	0	-0.064463	3.689013	-0.713647
45	1	0	0.703451	1.806559	1.641201
46	6	0	-2.999110	-1.121994	-0.243637
47	6	0	-3.232747	-0.855846	-1.602820
48	6	0	-4.044997	-0.889093	0.658006
49	6	0	-4.454517	-0.353350	-2.039147
50	1	0	-2.438045	-1.019891	-2.327128
51	6	0	-5.271557	-0.387955	0.224764
52	1	0	-3.899282	-1.111145	1.711388
53	6	0	-5.482582	-0.114712	-1.124984
54	1	0	-4.604823	-0.143918	-3.095306
55	1	0	-6.066949	-0.216931	0.945837
56	1	0	-6.439084	0.273976	-1.464475
57	6	0	2.870387	-0.927934	0.669154
58	6	0	3.131945	0.099421	1.592105
59	6	0	3.907062	-1.306651	-0.194987
60	6	0	4.368724	0.733389	1.638575
61	1	0	2.354140	0.410450	2.285018
62	6	0	5.149925	-0.677870	-0.147111
63	1	0	3.745037	-2.110181	-0.906028
64	6	0	5.388329	0.344800	0.767934
65	1	0	4.539155	1.530839	2.357635
66	1	0	5.934568	-0.993107	-0.829691

```
     67          1           0        6.358666    0.833010    0.806246
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -6000.24811089     A.U. after    1 cycles
             Convg  =    0.3533D-08             -V/T =  2.0047
Zero-point correction=                           0.567276 (Hartree/Particle)
 Thermal correction to Energy=                    0.597648
 Thermal correction to Enthalpy=                  0.598608
 Thermal correction to Gibbs Free Energy=         0.506907
 Sum of electronic and zero-point Energies=          -5999.680835
 Sum of electronic and thermal Energies=             -5999.650463
 Sum of electronic and thermal Enthalpies=           -5999.649503
 Sum of electronic and thermal Free Energies=        -5999.741204
                    1                    2                    3
Frequencies --  -308.6206               27.6181              39.8904
```

PhCOD$_{3,7}$-Rh(I)-Ph-CH-re-confU-CR-TS (219a)

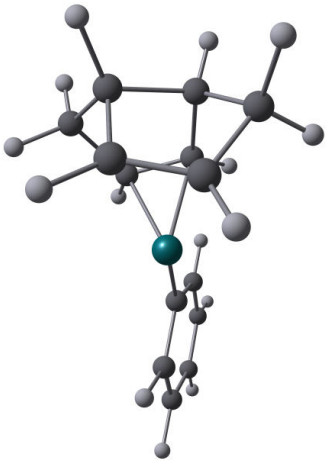


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.217107	-0.085703	-0.063707
2	6	0	0.799975	-0.380733	-2.031834
3	1	0	1.361154	0.541860	-2.166705
4	6	0	-0.196601	-0.703531	-3.123411
5	1	0	0.012177	-0.055778	-3.981391
6	1	0	-0.035292	-1.723860	-3.481601
7	6	0	-1.655076	-0.489103	-2.708143
8	1	0	-1.925301	0.548166	-2.919887
9	1	0	-2.328098	-1.096389	-3.332526
10	6	0	-1.977849	-0.769646	-1.249329
11	6	0	-1.451781	-1.867341	-0.558943
12	1	0	-1.933493	-2.134883	0.379790
13	6	0	-0.659844	-2.966490	-1.231355
14	1	0	-0.914742	-3.918631	-0.754052
15	1	0	-0.972478	-3.069359	-2.273968
16	6	0	0.854023	-2.771836	-1.125541
17	1	0	1.189404	-3.211049	-0.183038
18	1	0	1.375097	-3.341372	-1.910326
19	6	0	1.346188	-1.333785	-1.174671
20	6	0	0.447854	2.745719	-0.581776
21	6	0	1.256992	3.746833	-1.110383
22	6	0	0.975704	1.712000	0.218217
23	6	0	2.623440	3.769702	-0.817648

24	1	0	0.818576	4.521815	-1.735506
25	6	0	2.343203	1.764551	0.513222
26	6	0	3.156750	2.779194	0.002960
27	1	0	3.257876	4.558359	-1.214196
28	1	0	2.801537	0.999295	1.134424
29	1	0	4.217120	2.783060	0.245026
30	6	0	-0.301470	1.421857	1.835753
31	6	0	-1.348146	0.452806	1.689815
32	1	0	-0.622044	2.773967	-0.784334
33	6	0	2.736477	-1.175652	-0.654477
34	6	0	3.137699	-1.741126	0.566364
35	6	0	3.717159	-0.534444	-1.425011
36	6	0	4.449609	-1.634020	1.017837
37	1	0	2.411400	-2.259992	1.185730
38	6	0	5.033316	-0.430866	-0.981234
39	1	0	3.449446	-0.120401	-2.392616
40	6	0	5.406637	-0.973824	0.246514
41	1	0	4.726070	-2.069196	1.974964
42	1	0	5.770928	0.070959	-1.602421
43	1	0	6.433515	-0.895451	0.593871
44	6	0	-3.251815	-0.126408	-0.800718
45	6	0	-3.514937	1.232295	-1.042241
46	6	0	-4.249640	-0.881149	-0.170915
47	6	0	-4.713641	1.817284	-0.648400
48	1	0	-2.760089	1.852554	-1.519078
49	6	0	-5.453591	-0.299563	0.221778
50	1	0	-4.083437	-1.937106	0.016633
51	6	0	-5.692502	1.052172	-0.012121
52	1	0	-4.883996	2.874658	-0.835269
53	1	0	-6.207195	-0.909463	0.713153
54	1	0	-6.630742	1.506443	0.295327
55	6	0	0.644238	1.265834	3.002527
56	1	0	1.528143	1.895624	2.880909
57	1	0	0.104196	1.645855	3.883047
58	6	0	1.016031	-0.190203	3.224965
59	6	0	-1.400503	-0.739324	2.546311
60	8	0	-2.397188	-1.464081	2.591038
61	1	0	-2.317839	0.794812	1.338456
62	1	0	-0.613591	2.445987	1.654991
63	6	0	-0.228865	-1.034445	3.466170
64	1	0	1.548329	-0.554467	2.339732
65	1	0	1.706495	-0.286374	4.070296
66	1	0	-0.611867	-0.853685	4.479608
67	1	0	-0.018138	-2.107194	3.413811

```
 ----------------------------------------------------------------------SCF Done:
E(RPBE1PBE) =  -6000.25260315     A.U. after    1 cycles
            Convg  =    0.5132D-08             -V/T =  2.0047
Zero-point correction=                           0.567466 (Hartree/Particle)
 Thermal correction to Energy=                    0.597959
 Thermal correction to Enthalpy=                  0.598919
 Thermal correction to Gibbs Free Energy=         0.506719
 Sum of electronic and zero-point Energies=          -5999.685137
 Sum of electronic and thermal Energies=             -5999.654645
 Sum of electronic and thermal Enthalpies=           -5999.653685
 Sum of electronic and thermal Free Energies=        -5999.745884
                    1                      2                      3
Frequencies --  -279.2888               31.5767                34.3350
```

[3.3.0]BOD-Rh(I)-Ph (220)

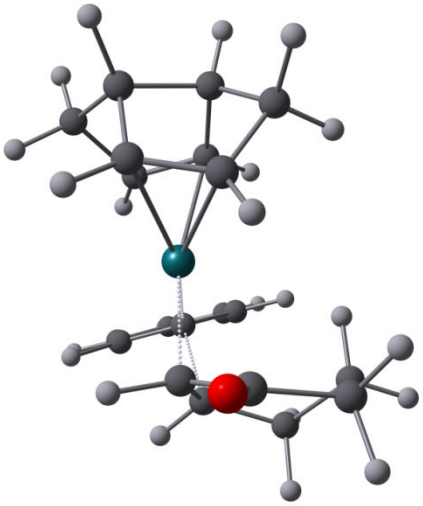


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.216829	-0.532717	-0.078285
2	6	0	-0.725877	1.452844	-0.634421
3	6	0	-1.079995	1.202105	0.715221
4	6	0	1.715954	0.000055	0.010458
5	1	0	0.145920	2.032401	-0.924899
6	6	0	-1.968041	1.435349	-1.494520
7	6	0	-2.558320	0.852422	0.814653
8	6	0	2.536034	-1.038071	-0.461163
9	6	0	2.350453	1.137040	0.531973
10	6	0	-2.875773	0.520996	-0.669725
11	1	0	-1.798796	1.062957	-2.510186
12	1	0	-2.385845	2.449884	-1.576585
13	6	0	-2.726962	-0.471589	1.568660
14	1	0	-3.155255	1.676880	1.222738
15	6	0	3.929885	-0.959363	-0.405947
16	1	0	2.088719	-1.940382	-0.890572
17	6	0	3.742156	1.224690	0.595224
18	1	0	1.758807	1.972304	0.904995
19	6	0	-2.379183	-0.907764	-0.738208
20	1	0	-3.938857	0.603232	-0.926584
21	6	0	-2.232631	-1.444134	0.520815
22	1	0	-2.154849	-0.498805	2.501638
23	1	0	-3.779640	-0.674479	1.814517
24	6	0	4.537438	0.177523	0.125983
25	1	0	4.539086	-1.779420	-0.780518
26	1	0	4.210410	2.113287	1.014078
27	1	0	-2.081422	-2.504663	0.716970
28	1	0	5.621304	0.248775	0.172470
29	1	0	-0.541481	1.596122	1.575494
30	1	0	-2.361628	-1.478458	-1.664761

SCF Done: E(RPBE1PBE) = -5229.15182477 A.U. after 1 cycles
Convg = 0.3130D-08 -V/T = 2.0032
Zero-point correction= 0.250954 (Hartree/Particle)
Thermal correction to Energy= 0.263827
Thermal correction to Enthalpy= 0.264787
Thermal correction to Gibbs Free Energy= 0.209446
Sum of electronic and zero-point Energies= -5228.900871

```
 Sum of electronic and thermal Energies=            -5228.887998
 Sum of electronic and thermal Enthalpies=          -5228.887038
 Sum of electronic and thermal Free Energies=       -5228.942379
                      1                      2                      3
Frequencies --    13.4140               60.5274               76.2054
```

[3.3.0]BOD-Rh(I)-Ph-CH-si-confU-CR-TS (222a)

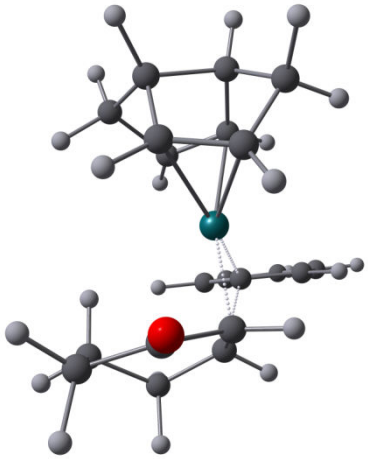


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.270329	-0.247558	-0.265038
2	6	0	-0.662117	-2.293452	-0.058353
3	6	0	-0.047531	-1.964407	1.137181
4	6	0	-1.765414	0.432997	-0.155015
5	1	0	-1.728661	-2.198846	-0.236758
6	6	0	0.215483	-3.221218	-0.862392
7	6	0	1.344531	-2.557776	1.209599
8	6	0	-2.588551	0.111037	-1.250359
9	6	0	-2.369636	0.496784	1.110871
10	6	0	1.589022	-2.865289	-0.291286
11	1	0	0.152518	-3.063519	-1.944035
12	1	0	-0.056076	-4.267937	-0.661092
13	6	0	2.358668	-1.473993	1.573937
14	1	0	1.382279	-3.441400	1.858271
15	6	0	-3.939560	-0.181286	-1.084549
16	1	0	-2.164102	0.090840	-2.253651
17	6	0	-3.725420	0.213799	1.280568
18	1	0	-1.773918	0.753096	1.984650
19	6	0	2.013193	-1.493983	-0.778597
20	1	0	2.359841	-3.624122	-0.472234
21	6	0	2.400991	-0.690038	0.285448
22	1	0	2.054956	-0.882495	2.443972
23	1	0	3.351902	-1.895422	1.788305
24	6	0	-4.517496	-0.131732	0.185982
25	1	0	-4.546069	-0.438289	-1.950149
26	1	0	-4.162909	0.260597	2.275485
27	1	0	3.015753	0.195435	0.164967
28	1	0	-5.574076	-0.349107	0.318525
29	6	0	-0.527331	1.972488	-0.698506
30	6	0	0.784989	1.621064	-1.176573
31	1	0	-1.254821	2.157944	-1.482383

32	1	0	0.893025	1.361786	-2.231899
33	6	0	1.986998	2.229349	-0.601137
34	8	0	3.067890	2.210349	-1.193009
35	6	0	1.869973	2.938795	0.735495
36	1	0	2.715592	2.628788	1.357710
37	6	0	-0.606710	2.951114	0.451755
38	1	0	-1.582990	2.900951	0.939008
39	6	0	0.532556	2.744865	1.437657
40	1	0	2.029795	4.003649	0.519788
41	1	0	0.473172	1.729200	1.851871
42	1	0	0.443548	3.440581	2.278946
43	1	0	-0.527753	3.956324	0.011561
44	1	0	-0.569067	-1.592002	2.015554
45	1	0	2.280311	-1.303442	-1.816010

```
SCF Done:  E(RPBE1PBE) =  -5537.49527826     A.U. after    1 cycles
             Convg  =    0.2015D-08             -V/T =  2.0039
Zero-point correction=                           0.381681 (Hartree/Particle)
 Thermal correction to Energy=                    0.401009
 Thermal correction to Enthalpy=                  0.401969
 Thermal correction to Gibbs Free Energy=         0.333736
 Sum of electronic and zero-point Energies=          -5537.113597
 Sum of electronic and thermal Energies=             -5537.094269
 Sum of electronic and thermal Enthalpies=           -5537.093309
 Sum of electronic and thermal Free Energies=        -5537.161543
                    1                    2                    3
Frequencies --  -283.1400               29.9927              46.6979
```

[3.3.0]BOD-Rh(I)-Ph-CH-re-confU-CR-TS (224a)



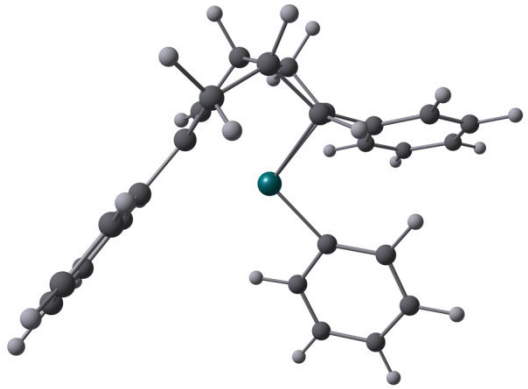
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.279952	-0.166119	-0.190566
2	6	0	0.063573	-1.676094	1.455372
3	6	0	0.024499	-2.327898	0.234487
4	6	0	1.828765	0.249796	-0.194945
5	1	0	0.984140	-1.414523	1.968207
6	6	0	-1.254925	-1.833201	2.173678
7	6	0	-1.360452	-2.877596	-0.045354
8	6	0	2.619297	0.305285	0.962515
9	6	0	2.418963	-0.274902	-1.360967
10	6	0	-2.189527	-2.065181	0.984530
11	1	0	-1.543650	-0.964513	2.774591

12	1	0	-1.218685	-2.704427	2.844312
13	6	0	-1.844959	-2.405435	-1.419613
14	1	0	-1.412290	-3.964012	0.095053
15	6	0	3.930493	-0.172258	0.966899
16	1	0	2.207822	0.709722	1.885045
17	6	0	3.720459	-0.769514	-1.355555
18	1	0	1.852067	-0.287663	-2.291081
19	6	0	-2.374838	-0.771082	0.221207
20	1	0	-3.146842	-2.528093	1.252745
21	6	0	-2.120750	-0.948418	-1.132877
22	1	0	-1.105278	-2.571532	-2.209451
23	1	0	-2.773685	-2.911956	-1.721033
24	6	0	4.486960	-0.717751	-0.189060
25	1	0	4.516409	-0.121958	1.882080
26	1	0	4.144424	-1.181363	-2.268684
27	1	0	-2.442123	-0.239988	-1.892096
28	1	0	5.508919	-1.087529	-0.185801
29	6	0	0.772410	1.941535	-0.633273
30	1	0	1.537571	2.105351	-1.386285
31	6	0	-0.547412	1.709961	-1.161406
32	1	0	-0.648375	1.505151	-2.227988
33	6	0	-1.740359	2.292758	-0.543861
34	8	0	-2.833893	2.285918	-1.114421
35	6	0	0.888594	2.863566	0.558625
36	1	0	1.852472	2.739695	1.057650
37	6	0	-1.596237	2.963245	0.811138
38	1	0	-2.461029	2.686274	1.421826
39	6	0	-0.275749	2.688182	1.521167
40	1	0	0.878977	3.888018	0.157748
41	1	0	-0.268493	1.659641	1.909333
42	1	0	-0.165581	3.356669	2.382096
43	1	0	-1.696355	4.039777	0.616342
44	1	0	0.903345	-2.644813	-0.322298
45	1	0	-2.927591	0.070107	0.632298

SCF Done: E(RPBE1PBE) = -5537.49840970 A.U. after 1 cycles
Convg = 0.3817D-08 -V/T = 2.0039
Zero-point correction= 0.381565 (Hartree/Particle)
Thermal correction to Energy= 0.400881
Thermal correction to Enthalpy= 0.401841
Thermal correction to Gibbs Free Energy= 0.333546
Sum of electronic and zero-point Energies= -5537.116845
Sum of electronic and thermal Energies= -5537.097528
Sum of electronic and thermal Enthalpies= -5537.096568
Sum of electronic and thermal Free Energies= -5537.164864

	1	2	3
Frequencies --	-291.4621	29.3499	45.4634

(*R*)-3,7-diphenyl[3.3.0]BOD-Rh(I)-Ph (225)

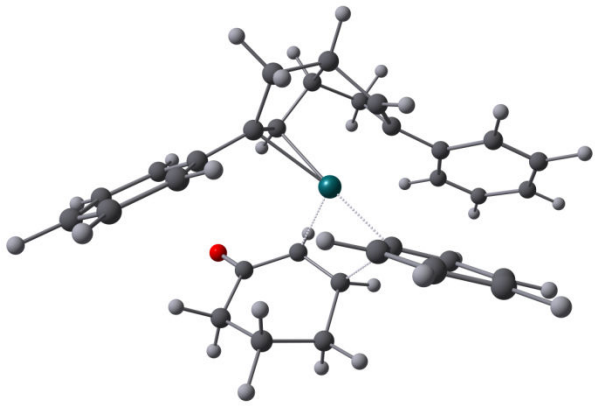


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.319562	-0.068384	0.128620
2	6	0	0.550424	-1.487627	-1.139424
3	1	0	0.883170	-1.067782	-2.087750
4	6	0	-0.452188	-2.633478	-1.107323
5	6	0	-1.856950	-2.105464	-1.404267
6	1	0	-1.871828	-1.462898	-2.290169
7	1	0	-2.580926	-2.918265	-1.561691
8	6	0	-2.164024	-1.371203	-0.111215
9	6	0	-1.412448	-1.917953	0.915133
10	1	0	-1.616558	-1.797454	1.976567
11	6	0	-0.462202	-2.973185	0.404816
12	6	0	0.949657	-2.673865	0.897720
13	1	0	0.995297	-2.485630	1.975458
14	1	0	1.643508	-3.499181	0.678710
15	6	0	1.330930	-1.468954	0.047720
16	6	0	0.766930	1.581060	-0.220742
17	6	0	1.780630	1.938202	-1.118092
18	6	0	0.189841	2.601690	0.551408
19	6	0	2.190686	3.266082	-1.244845
20	1	0	2.265342	1.179803	-1.728831
21	6	0	0.599712	3.932530	0.439220
22	1	0	-0.611049	2.369458	1.262691
23	6	0	1.606467	4.266885	-0.465419
24	1	0	2.973579	3.523400	-1.955593
25	1	0	0.136107	4.702358	1.052648
26	1	0	1.934163	5.298963	-0.563389
27	6	0	2.721712	-0.966178	0.169647
28	6	0	3.196894	-0.457121	1.386366
29	6	0	3.618781	-1.068465	-0.900781
30	6	0	4.516128	-0.040223	1.521275
31	1	0	2.511086	-0.360128	2.224690
32	6	0	4.943137	-0.650461	-0.768735
33	1	0	3.279115	-1.487790	-1.844904
34	6	0	5.396873	-0.131683	0.441389
35	1	0	4.859047	0.367100	2.469092
36	1	0	5.621568	-0.735146	-1.614174
37	1	0	6.427394	0.197657	0.545250
38	6	0	-3.275173	-0.416440	0.036279
39	6	0	-4.080762	-0.078695	-1.062926
40	6	0	-3.553831	0.202005	1.270453
41	6	0	-5.122988	0.836435	-0.935787

42	1	0	-3.894107	-0.539080	-2.028546
43	6	0	-4.590168	1.118924	1.395189
44	1	0	-2.952140	-0.038463	2.143390
45	6	0	-5.382229	1.442204	0.291604
46	1	0	-5.733053	1.079038	-1.801990
47	1	0	-4.783843	1.583594	2.358524
48	1	0	-6.192587	2.159391	0.389548
49	1	0	-0.800095	-3.992338	0.629621
50	1	0	-0.147907	-3.469471	-1.749032

```
 ---------------------------------------------------------------------SCF Done:
E(RPBE1PBE) =  -5690.73629452     A.U. after    1 cycles
            Convg  =    0.3942D-08             -V/T =  2.0042
Zero-point correction=                          0.413062 (Hartree/Particle)
 Thermal correction to Energy=                   0.436131
 Thermal correction to Enthalpy=                 0.437091
 Thermal correction to Gibbs Free Energy=        0.357460
 Sum of electronic and zero-point Energies=          -5690.323233
 Sum of electronic and thermal Energies=             -5690.300163
 Sum of electronic and thermal Enthalpies=           -5690.299203
 Sum of electronic and thermal Free Energies=        -5690.378835
                    1                      2                      3
Frequencies --    21.5620               23.9718                27.5713
```

(*R*)-3,7-diphenyl[3.3.0]BOD-Rh(I)-Ph-CH-si-confU-CR-TS (227a)

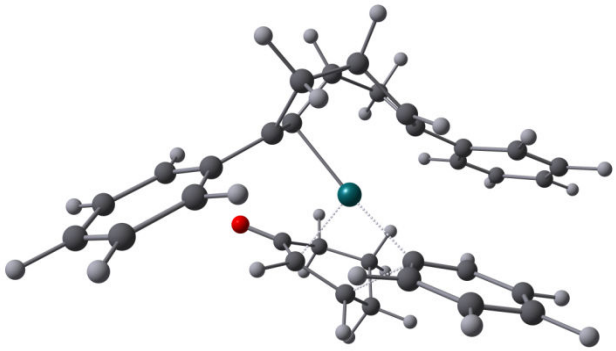


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.024668	-0.324997	0.100193
2	6	0	1.176537	-1.600182	-1.371137
3	1	0	1.518142	-0.971500	-2.190179
4	6	0	0.193125	-2.730255	-1.579515
5	6	0	-1.166106	-2.168569	-1.968356
6	1	0	-1.099436	-1.424942	-2.768238
7	1	0	-1.863271	-2.950942	-2.302926
8	6	0	-1.661519	-1.613898	-0.642707
9	6	0	-1.005805	-2.265415	0.403190
10	1	0	-1.381456	-2.315716	1.422904
11	6	0	0.020236	-3.242798	-0.128145
12	6	0	1.367370	-2.999760	0.539567
13	1	0	1.291586	-2.924043	1.628424
14	1	0	2.091674	-3.796525	0.314029
15	6	0	1.824349	-1.722009	-0.145427
16	6	0	0.412368	1.948496	-1.538809
17	6	0	1.074645	2.721444	-2.490598
18	6	0	1.059581	1.517542	-0.363003

19	6	0	2.392417	3.127269	-2.273936
20	1	0	0.553588	3.018189	-3.398333
21	6	0	2.380039	1.941407	-0.164163
22	6	0	3.037376	2.736898	-1.101294
23	1	0	2.904501	3.748332	-3.004480
24	1	0	2.911896	1.656157	0.741276
25	1	0	4.062096	3.048153	-0.911905
26	6	0	0.107838	1.683436	1.405030
27	6	0	-0.758712	0.626332	1.866714
28	1	0	-0.328739	-0.109732	2.549848
29	6	0	-0.544388	3.042321	1.209418
30	6	0	-1.966354	2.931732	0.677275
31	1	0	-1.954239	2.480366	-0.319137
32	1	0	-2.396205	3.932053	0.556648
33	1	0	1.059931	1.731135	1.929069
34	6	0	-2.181378	0.839048	2.124654
35	6	0	-2.840448	2.098361	1.605208
36	1	0	-3.786558	1.815465	1.133467
37	1	0	-3.107267	2.677348	2.499624
38	8	0	-2.822125	0.047454	2.820249
39	1	0	-0.570536	3.507016	2.206742
40	1	0	0.070159	3.686523	0.576380
41	1	0	-0.620242	1.665308	-1.729800
42	6	0	3.114683	-1.125278	0.252824
43	6	0	3.437711	-0.971822	1.610245
44	6	0	4.076427	-0.766942	-0.700909
45	6	0	4.670100	-0.455395	1.999875
46	1	0	2.708714	-1.244525	2.369399
47	6	0	5.312724	-0.256995	-0.313468
48	1	0	3.855107	-0.894588	-1.756730
49	6	0	5.614814	-0.094500	1.038066
50	1	0	4.895510	-0.336413	3.056652
51	1	0	6.044607	0.012419	-1.070702
52	1	0	6.580137	0.302820	1.340621
53	6	0	-2.976020	-0.936564	-0.612442
54	6	0	-3.314925	-0.012668	-1.615854
55	6	0	-3.952749	-1.269937	0.335728
56	6	0	-4.578504	0.566055	-1.663761
57	1	0	-2.576956	0.256251	-2.367759
58	6	0	-5.220545	-0.694886	0.286244
59	1	0	-3.721372	-1.989513	1.114082
60	6	0	-5.540680	0.223507	-0.712053
61	1	0	-4.815662	1.282021	-2.446679
62	1	0	-5.960486	-0.967178	1.033932
63	1	0	-6.531489	0.668730	-0.749946
64	1	0	-0.323236	-4.282691	-0.063334
65	1	0	0.571221	-3.490589	-2.274378

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5999.06449019     A.U. after    1 cycles
             Convg  =    0.3456D-08             -V/T =  2.0047
Zero-point correction=                           0.543983 (Hartree/Particle)
 Thermal correction to Energy=                    0.573380
 Thermal correction to Enthalpy=                  0.574340
 Thermal correction to Gibbs Free Energy=         0.483939
 Sum of electronic and zero-point Energies=          -5998.520507
 Sum of electronic and thermal Energies=             -5998.491110
 Sum of electronic and thermal Enthalpies=           -5998.490150
 Sum of electronic and thermal Free Energies=        -5998.580552
                    1                    2                    3
Frequencies --  -307.9995               26.5507              33.9785
```

(*R*)-3,7-diphenyl[3.3.0]BOD-Rh(I)-Ph-CH-re-confU-CR-TS (229a)

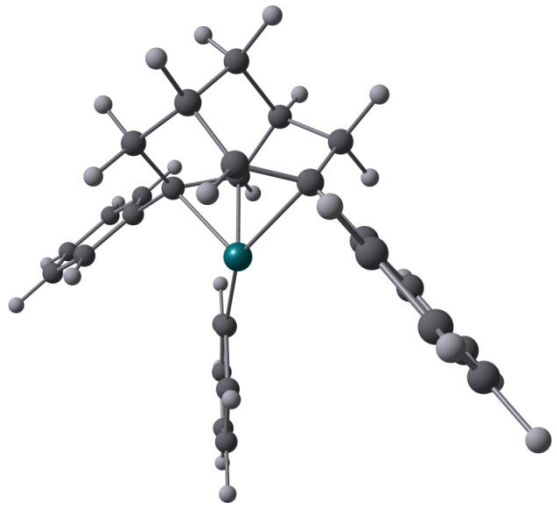


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.231991	-0.060196	-0.056858
2	6	0	0.780626	-0.183766	-2.088495
3	1	0	1.130595	0.815915	-2.335564
4	6	0	-0.304583	-0.865352	-2.888522
5	6	0	-1.627174	-0.130872	-2.732147
6	1	0	-1.527402	0.949272	-2.875855
7	1	0	-2.386701	-0.488674	-3.442659
8	6	0	-2.046465	-0.541306	-1.330944
9	6	0	-1.392836	-1.725089	-0.983952
10	1	0	-1.735935	-2.404110	-0.206847
11	6	0	-0.468093	-2.179202	-2.090069
12	6	0	0.919383	-2.487133	-1.538323
13	1	0	0.878412	-3.099125	-0.632212
14	1	0	1.546032	-3.020717	-2.268011
15	6	0	1.493845	-1.096388	-1.327066
16	6	0	0.269508	2.783407	-0.022358
17	6	0	0.991308	3.918283	-0.378377
18	6	0	0.899706	1.661423	0.555600
19	6	0	2.363165	3.986427	-0.117371
20	1	0	0.479336	4.761892	-0.836283
21	6	0	2.270671	1.753462	0.819626
22	6	0	2.992558	2.903202	0.490364
23	1	0	2.927465	4.879999	-0.371861
24	1	0	2.800941	0.918668	1.271055
25	1	0	4.058838	2.939891	0.702012
26	6	0	-0.243271	0.965743	2.107360
27	6	0	-1.343486	0.106697	1.756555
28	1	0	-0.808737	2.772073	-0.177477
29	6	0	2.879601	-0.952622	-0.841431
30	6	0	3.409830	-1.861563	0.087689
31	6	0	3.738721	0.026633	-1.362999
32	6	0	4.735808	-1.777682	0.503053
33	1	0	2.777445	-2.645810	0.494743
34	6	0	5.066800	0.107513	-0.957019
35	1	0	3.365504	0.728824	-2.102176
36	6	0	5.572144	-0.790128	-0.016504
37	1	0	5.118825	-2.490433	1.228941
38	1	0	5.711434	0.873690	-1.380206
39	1	0	6.610170	-0.727996	0.299530
40	6	0	-3.320447	-0.018429	-0.790550
41	6	0	-3.672774	1.325845	-0.991725
42	6	0	-4.232654	-0.848825	-0.125512
43	6	0	-4.883837	1.828912	-0.526974
44	1	0	-2.983186	1.990598	-1.505680
45	6	0	-5.446231	-0.347535	0.337230

46	1	0	-3.986753	-1.891806	0.040229
47	6	0	-5.778182	0.992227	0.141765
48	1	0	-5.131544	2.875169	-0.687744
49	1	0	-6.135608	-1.009545	0.854745
50	1	0	-6.726319	1.381023	0.504049
51	6	0	0.741850	0.457461	3.133426
52	1	0	1.640722	1.077497	3.156751
53	1	0	0.255171	0.576306	4.113084
54	6	0	1.069617	-1.008136	2.903749
55	6	0	-1.407073	-1.270879	2.265188
56	8	0	-2.433875	-1.950033	2.189275
57	1	0	-2.309972	0.561596	1.550610
58	1	0	-0.521559	2.006375	2.246743
59	6	0	-0.197198	-1.849812	2.979506
60	1	0	1.531907	-1.114771	1.914618
61	1	0	1.803170	-1.360997	3.637323
62	1	0	-0.511408	-1.956859	4.026551
63	1	0	-0.041985	-2.867995	2.609123
64	1	0	-0.005083	-1.013416	-3.933840
65	1	0	-0.898216	-3.002580	-2.673941

```
SCF Done:  E(RPBE1PBE) =  -5999.07277675     A.U. after    1 cycles
             Convg  =    0.3057D-08             -V/T =  2.0047
Zero-point correction=                           0.544004 (Hartree/Particle)
 Thermal correction to Energy=                    0.573494
 Thermal correction to Enthalpy=                  0.574454
 Thermal correction to Gibbs Free Energy=         0.483340
 Sum of electronic and zero-point Energies=          -5998.528773
 Sum of electronic and thermal Energies=             -5998.499283
 Sum of electronic and thermal Enthalpies=           -5998.498323
 Sum of electronic and thermal Free Energies=        -5998.589437
                     1                      2                      3
Frequencies --  -288.8292               26.4565                33.3534
```

(*R*)-3,7-diphenylBND-Rh(I)-Ph (230)



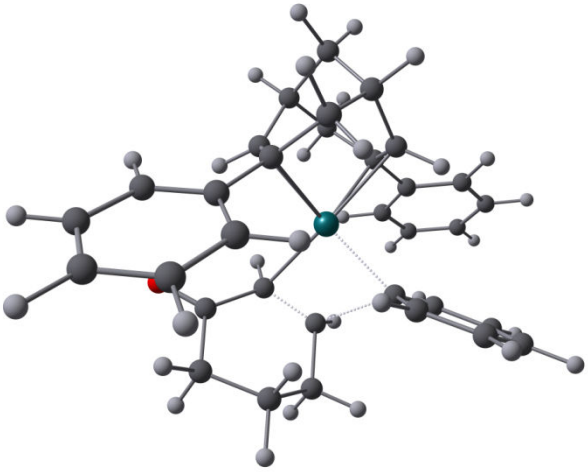
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.323144	0.040285	-0.123133
2	6	0	-0.584792	-1.358113	1.158716

3	1	0	-1.084804	-0.844853	1.980343
4	6	0	0.456335	-2.400890	1.581092
5	1	0	0.205537	-2.771286	2.581821
6	6	0	1.836981	-1.747911	1.604928
7	1	0	1.855417	-0.926960	2.328452
8	1	0	2.608645	-2.465774	1.920700
9	6	0	2.135145	-1.227261	0.213195
10	6	0	1.507479	-1.787268	-0.888329
11	1	0	1.824486	-1.486460	-1.886700
12	6	0	0.542406	-2.954168	-0.817678
13	1	0	0.831241	-3.710966	-1.556762
14	6	0	-0.860494	-2.440484	-1.133282
15	1	0	-0.901682	-2.000670	-2.136748
16	1	0	-1.585296	-3.268830	-1.125180
17	6	0	-1.256158	-1.396288	-0.101001
18	6	0	-0.799004	1.676353	0.190501
19	6	0	-1.875115	2.001557	1.025702
20	6	0	-0.224635	2.711014	-0.564243
21	6	0	-2.349973	3.311249	1.107576
22	1	0	-2.362887	1.229741	1.617708
23	6	0	-0.698308	4.023876	-0.497116
24	1	0	0.621273	2.503102	-1.229304
25	6	0	-1.767353	4.326340	0.345375
26	1	0	-3.183793	3.542762	1.767532
27	1	0	-0.236251	4.804390	-1.098264
28	1	0	-2.145280	5.343995	0.407249
29	6	0	-2.662504	-0.919086	-0.238980
30	6	0	-3.105578	-0.290971	-1.411414
31	6	0	-3.598019	-1.160828	0.774093
32	6	0	-4.429771	0.105728	-1.554774
33	1	0	-2.391364	-0.077378	-2.203052
34	6	0	-4.928445	-0.763215	0.634352
35	1	0	-3.283317	-1.674355	1.679524
36	6	0	-5.349566	-0.125488	-0.529402
37	1	0	-4.745849	0.610144	-2.464433
38	1	0	-5.636172	-0.958084	1.436510
39	1	0	-6.384094	0.189030	-0.639634
40	6	0	3.223246	-0.229036	0.037117
41	6	0	3.362603	0.845297	0.933073
42	6	0	4.125597	-0.311606	-1.036393
43	6	0	4.348660	1.811390	0.747292
44	1	0	2.681270	0.942848	1.774287
45	6	0	5.116149	0.648810	-1.216593
46	1	0	4.061803	-1.151359	-1.723261
47	6	0	5.230477	1.718248	-0.327604
48	1	0	4.425266	2.640633	1.445599
49	1	0	5.807967	0.557988	-2.050143
50	1	0	6.004061	2.468222	-0.469150
51	6	0	0.510367	-3.556063	0.584407
52	1	0	-0.363095	-4.210326	0.684657
53	1	0	1.401058	-4.165517	0.775597

SCF Done: SCF Done: E(RPBE1PBE) = -5730.00586033 A.U. after 1 cycles
Convg = 0.3780D-08 -V/T = 2.0043
Zero-point correction= 0.443854 (Hartree/Particle)
Thermal correction to Energy= 0.467497
Thermal correction to Enthalpy= 0.468457
Thermal correction to Gibbs Free Energy= 0.389342
Sum of electronic and zero-point Energies= -5729.562007
Sum of electronic and thermal Energies= -5729.538363
Sum of electronic and thermal Enthalpies= -5729.537403
Sum of electronic and thermal Free Energies= -5729.616518
1 2 3

Frequencies -- 27.0539 33.6567 35.8953

(*R*)-3,7-diphenylBND-Rh(I)-Ph-CH-si-confU-CR-TS (232a)

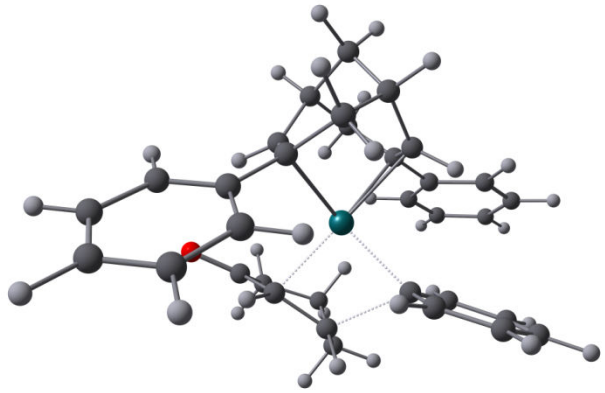


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.029419	-0.221135	-0.139407
2	6	0	-1.232443	-1.547375	1.263145
3	1	0	-1.701501	-0.871055	1.976575
4	6	0	-0.266704	-2.570070	1.840731
5	6	0	1.111814	-1.934805	1.958323
6	1	0	1.061283	-1.052477	2.604852
7	1	0	1.830624	-2.625724	2.424168
8	6	0	1.604997	-1.544613	0.576702
9	6	0	1.042575	-2.138345	-0.559014
10	1	0	1.538104	-1.991268	-1.517723
11	6	0	0.030113	-3.271676	-0.494701
12	6	0	-1.322414	-2.747996	-0.956251
13	1	0	-1.255829	-2.373639	-1.982678
14	1	0	-2.075050	-3.551039	-0.963945
15	6	0	-1.774000	-1.641523	-0.020576
16	6	0	-0.403041	1.955645	1.641430
17	6	0	-1.061041	2.668140	2.642020
18	6	0	-1.054658	1.593174	0.445530
19	6	0	-2.382172	3.079201	2.459413
20	1	0	-0.534837	2.912091	3.562447
21	6	0	-2.377289	2.025069	0.280516
22	6	0	-3.032711	2.757669	1.268937
23	1	0	-2.892509	3.651495	3.229922
24	1	0	-2.912780	1.795771	-0.637938
25	1	0	-4.059941	3.075131	1.104970
26	6	0	-0.102746	1.868857	-1.318423
27	6	0	0.769997	0.845020	-1.835582
28	1	0	0.348815	0.148475	-2.563873
29	6	0	0.538953	3.219047	-1.045261
30	6	0	1.963518	3.093619	-0.523148
31	1	0	1.957112	2.597801	0.451990
32	1	0	2.385759	4.090892	-0.357941
33	1	0	-1.056765	1.939992	-1.836599
34	6	0	2.197309	1.065748	-2.058557
35	6	0	2.842758	2.310636	-1.489806
36	1	0	3.796527	2.022464	-1.037580

37	1	0	3.093212	2.930549	-2.361516
38	8	0	2.851951	0.297549	-2.766996
39	1	0	0.558380	3.739238	-2.015064
40	1	0	-0.079852	3.821606	-0.376324
41	1	0	0.630826	1.663446	1.807751
42	6	0	-3.068070	-1.007909	-0.388852
43	6	0	-3.340488	-0.636958	-1.715616
44	6	0	-4.084445	-0.838255	0.560494
45	6	0	-4.571701	-0.095916	-2.073613
46	1	0	-2.572529	-0.749612	-2.476616
47	6	0	-5.317565	-0.296012	0.205963
48	1	0	-3.911481	-1.145562	1.587930
49	6	0	-5.568048	0.080331	-1.112351
50	1	0	-4.753491	0.192073	-3.106041
51	1	0	-6.088761	-0.175174	0.962568
52	1	0	-6.531448	0.499212	-1.390949
53	6	0	2.938845	-0.880516	0.552294
54	6	0	3.290851	0.075400	1.520822
55	6	0	3.923901	-1.269348	-0.366307
56	6	0	4.566876	0.627350	1.562055
57	1	0	2.558372	0.396694	2.256166
58	6	0	5.201990	-0.717309	-0.329361
59	1	0	3.693243	-2.021118	-1.113758
60	6	0	5.532517	0.231772	0.635282
61	1	0	4.808636	1.368443	2.319879
62	1	0	5.942480	-1.034745	-1.058520
63	1	0	6.531571	0.658657	0.667013
64	6	0	-0.137468	-3.787592	0.930944
65	1	0	-0.616544	-2.868743	2.836101
66	1	0	0.358558	-4.078707	-1.160189
67	1	0	0.723965	-4.390540	1.240593
68	1	0	-1.025946	-4.426734	0.990545

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5999.06449019     A.U. after    1 cycles
             Convg  =    0.3456D-08             -V/T =  2.0047
Zero-point correction=                           0.574216 (Hartree/Particle)
 Thermal correction to Energy=                    0.604420
 Thermal correction to Enthalpy=                  0.605380
 Thermal correction to Gibbs Free Energy=         0.513606
 Sum of electronic and zero-point Energies=          -6037.758434
 Sum of electronic and thermal Energies=             -6037.728229
 Sum of electronic and thermal Enthalpies=           -6037.727269
 Sum of electronic and thermal Free Energies=        -6037.819043
                    1                    2                    3
Frequencies --  -307.3640               23.8075              34.9076
```

(*R*)-3,7-diphenylBND-Rh(I)-Ph-CH-re-confU-CR-TS (234a)



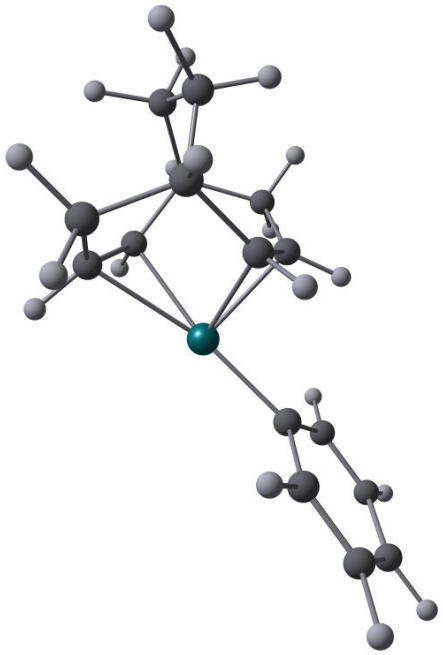
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.215439	-0.002010	0.025497
2	6	0	-0.814400	1.430622	-1.417727
3	1	0	-1.317021	0.780063	-2.131485
4	6	0	0.268303	2.326054	-1.996666
5	6	0	1.579252	1.557482	-2.065826
6	1	0	1.461173	0.667081	-2.692243
7	1	0	2.368656	2.166007	-2.531902
8	6	0	2.003528	1.166039	-0.663740
9	6	0	1.452679	1.829313	0.438124
10	1	0	1.904774	1.663531	1.414240
11	6	0	0.562076	3.056155	0.321729
12	6	0	-0.850579	2.692306	0.759017
13	1	0	-0.834292	2.308046	1.784561
14	1	0	-1.502243	3.578919	0.765639
15	6	0	-1.419754	1.650384	-0.184860
16	6	0	-0.414722	-2.108607	-1.888539
17	6	0	-1.201248	-2.670548	-2.889062
18	6	0	-0.973629	-1.661160	-0.673574
19	6	0	-2.572757	-2.848011	-2.684620
20	1	0	-0.741161	-2.992066	-3.820987
21	6	0	-2.345692	-1.861170	-0.483065
22	6	0	-3.134753	-2.448896	-1.474844
23	1	0	-3.189016	-3.304849	-3.454830
24	1	0	-2.825030	-1.539964	0.438277
25	1	0	-4.199657	-2.581137	-1.297681
26	6	0	0.235428	-2.245806	0.880379
27	6	0	1.336546	-1.381414	1.211062
28	1	0	0.660466	-2.029742	-2.042979
29	6	0	-2.821801	1.237680	0.090946
30	6	0	-3.311322	1.146444	1.404017
31	6	0	-3.734899	1.032173	-0.954682
32	6	0	-4.639755	0.819656	1.661371
33	1	0	-2.648231	1.327340	2.244695
34	6	0	-5.065068	0.710480	-0.702412
35	1	0	-3.405185	1.138414	-1.983414
36	6	0	-5.525271	0.593446	0.608264
37	1	0	-4.985094	0.746953	2.689631
38	1	0	-5.746856	0.558212	-1.535294
39	1	0	-6.564384	0.344644	0.807252
40	6	0	3.283890	0.407591	-0.581889
41	6	0	3.599972	-0.578586	-1.531060
42	6	0	4.240666	0.699353	0.399165
43	6	0	4.811352	-1.261084	-1.488199
44	1	0	2.882696	-0.833357	-2.306370
45	6	0	5.454536	0.018327	0.444650
46	1	0	4.035892	1.467670	1.136790
47	6	0	5.747395	-0.966390	-0.496325
48	1	0	5.025337	-2.026120	-2.230451
49	1	0	6.175207	0.261730	1.220971
50	1	0	6.695297	-1.496944	-0.460614
51	6	0	-0.719030	-2.617734	1.990435
52	1	0	-1.627341	-3.075475	1.592411
53	1	0	-0.211828	-3.392453	2.584945
54	6	0	-1.029159	-1.421049	2.872791
55	6	0	1.427122	-0.748400	2.533960
56	8	0	2.454364	-0.184250	2.918361
57	1	0	2.294555	-1.557589	0.727774
58	1	0	0.505737	-3.080107	0.239602
59	6	0	0.249484	-0.866319	3.486631

60	1	0	-1.512188	-0.652260	2.258286
61	1	0	-1.740909	-1.693272	3.660185
62	1	0	0.598209	-1.533861	4.286391
63	1	0	0.095202	0.109227	3.958092
64	6	0	0.490014	3.552000	-1.117774
65	1	0	1.415817	4.058907	-1.412969
66	1	0	-0.034163	2.624542	-3.007648
67	1	0	0.955436	3.838462	0.981515
68	1	0	-0.329941	4.271911	-1.222700

SCF Done: E(RPBE1PBE) = -6038.33984393 A.U. after 17 cycles
Convg = 0.9515D-08 -V/T = 2.0048
Zero-point correction= 0.574673 (Hartree/Particle)
Thermal correction to Energy= 0.604858
Thermal correction to Enthalpy= 0.605818
Thermal correction to Gibbs Free Energy= 0.514052
Sum of electronic and zero-point Energies= -6037.765171
Sum of electronic and thermal Energies= -6037.734986
Sum of electronic and thermal Enthalpies= -6037.734026
Sum of electronic and thermal Free Energies= -6037.825792

	1	2	3
Frequencies --	-290.7990	31.2049	31.6277

BDD-Rh(I)-Ph (235)



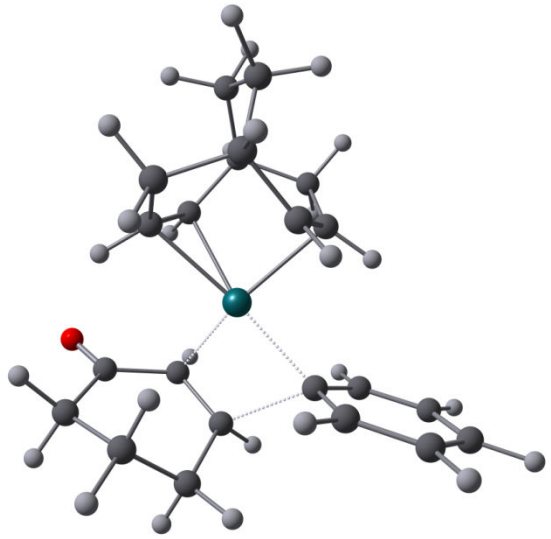
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.166776	-0.011378	-0.686588
2	6	0	0.502502	-0.823582	1.122458
3	6	0	0.663222	0.590698	1.142881
4	6	0	-2.070607	-0.008786	-0.025268
5	1	0	-0.345003	-1.218878	1.683902
6	6	0	1.584785	-1.836181	0.839483
7	6	0	1.987648	1.342914	0.973561
8	6	0	-2.844376	-1.183732	-0.031171

9	6	0	-2.736444	1.195751	0.265547
10	6	0	2.621871	-1.331665	-0.175159
11	1	0	1.099285	-2.738766	0.449385
12	1	0	2.085225	-2.142930	1.771879
13	6	0	2.168803	1.806464	-0.479769
14	1	0	1.912139	2.243148	1.594617
15	6	0	-4.220985	-1.154623	0.204836
16	1	0	-2.369524	-2.145674	-0.225610
17	6	0	-4.113680	1.232216	0.498916
18	1	0	-2.176168	2.129619	0.305136
19	6	0	1.935127	-0.617950	-1.332205
20	1	0	3.113973	-2.210754	-0.608485
21	6	0	1.783171	0.746315	-1.482455
22	1	0	1.530735	2.679165	-0.660154
23	1	0	3.202394	2.147450	-0.645712
24	6	0	-4.863004	0.055970	0.468160
25	1	0	-4.793394	-2.080235	0.187612
26	1	0	-4.602091	2.181571	0.710813
27	1	0	1.540661	1.111326	-2.483051
28	1	0	-5.933801	0.081054	0.655355
29	6	0	3.718244	-0.494749	0.495606
30	6	0	3.199951	0.551282	1.480080
31	1	0	4.316661	-0.011708	-0.285903
32	1	0	4.400328	-1.169834	1.027368
33	1	0	2.934589	0.075439	2.431527
34	1	0	4.013258	1.251906	1.707549
35	1	0	1.771125	-1.228757	-2.221318
36	1	0	-0.092872	1.136831	1.708545

SCF Done: E(RPBE1PBE) = -5307.68291866 A.U. after 1 cycles
Convg = 0.2607D-08 -V/T = 2.0034
Zero-point correction= 0.310904 (Hartree/Particle)
Thermal correction to Energy= 0.325789
Thermal correction to Enthalpy= 0.326749
Thermal correction to Gibbs Free Energy= 0.267323
Sum of electronic and zero-point Energies= -5307.372014
Sum of electronic and thermal Energies= -5307.357130
Sum of electronic and thermal Enthalpies= -5307.356170
Sum of electronic and thermal Free Energies= -5307.415596

	1	2	3
Frequencies --	14.3759	48.6681	54.7888

BDD-Rh(I)-Ph-CH-si-confU-CR-TS (237a)

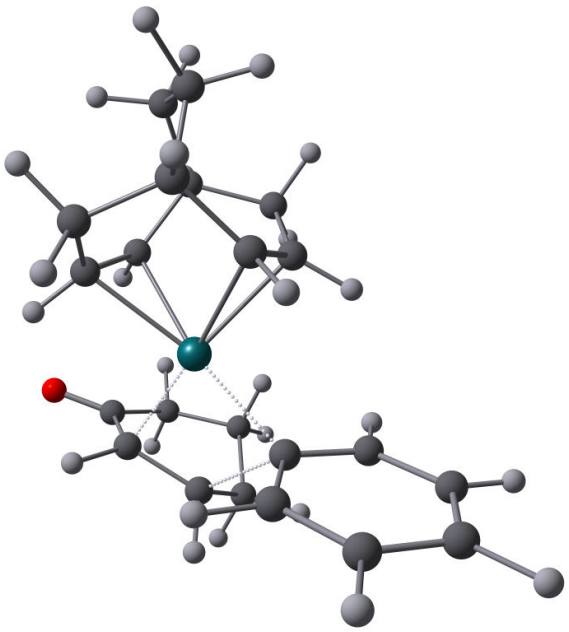


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.058745	0.112170	-0.285651
2	6	0	0.896590	-1.934686	-0.297945
3	6	0	1.003557	-1.475331	1.006784
4	6	0	-1.895726	-0.796124	-0.149184
5	1	0	0.045959	-2.575761	-0.523576
6	6	0	1.971991	-1.908902	-1.352573
7	6	0	2.268617	-0.968983	1.688245
8	6	0	-2.285811	-1.583630	-1.249112
9	6	0	-2.364280	-1.181351	1.117295
10	6	0	2.917589	-0.710474	-1.203686
11	1	0	1.476551	-1.861429	-2.329494
12	1	0	2.541248	-2.851722	-1.347747
13	6	0	2.309850	0.562283	1.666269
14	1	0	2.195089	-1.282558	2.736502
15	6	0	-3.065690	-2.725554	-1.087765
16	1	0	-1.975926	-1.293614	-2.252669
17	6	0	-3.154232	-2.319528	1.283365
18	1	0	-2.098904	-0.595462	1.994933
19	6	0	2.124695	0.561185	-0.917774
20	1	0	3.404116	-0.553361	-2.173567
21	6	0	1.906545	1.133703	0.333652
22	1	0	1.620801	0.957615	2.422066
23	1	0	3.309670	0.926229	1.950810
24	6	0	-3.505791	-3.101170	0.183459
25	1	0	-3.340168	-3.318685	-1.957291
26	1	0	-3.493256	-2.596937	2.279148
27	1	0	1.688122	2.199251	0.344121
28	1	0	-4.124242	-3.985569	0.312227
29	6	0	4.031804	-0.972850	-0.183858
30	6	0	3.551573	-1.592975	1.126932
31	1	0	4.550952	-0.027869	0.014574
32	1	0	4.776574	-1.639814	-0.635905
33	1	0	3.386157	-2.668840	0.995958
34	1	0	4.349046	-1.496427	1.874379
35	6	0	-2.064373	1.180009	-0.633314
36	6	0	-0.886541	1.826698	-1.152986

37	1	0	-2.760969	0.840518	-1.393729
38	1	0	-0.672628	1.720997	-2.218255
39	6	0	-0.368680	3.064288	-0.571530
40	8	0	0.443981	3.771364	-1.171967
41	6	0	-0.889053	3.495203	0.787813
42	1	0	-0.037870	3.835905	1.385779
43	6	0	-2.734583	1.829965	0.556302
44	1	0	-3.398794	1.126879	1.063908
45	6	0	-1.716885	2.438620	1.508924
46	1	0	-1.501519	4.387486	0.600726
47	1	0	-1.057574	1.645094	1.886941
48	1	0	-2.218929	2.879924	2.376726
49	1	0	-3.375098	2.628127	0.152585
50	1	0	2.005393	1.231949	-1.768795
51	1	0	0.203843	-1.772866	1.683777

```
SCF Done:  E(RPBE1PBE) =  -5616.02681306     A.U. after    1 cycles
             Convg  =    0.4976D-08             -V/T =  2.0040
Zero-point correction=                           0.441462 (Hartree/Particle)
 Thermal correction to Energy=                    0.462845
 Thermal correction to Enthalpy=                  0.463805
 Thermal correction to Gibbs Free Energy=         0.391560
 Sum of electronic and zero-point Energies=          -5615.585351
 Sum of electronic and thermal Energies=             -5615.563968
 Sum of electronic and thermal Enthalpies=           -5615.563008
 Sum of electronic and thermal Free Energies=        -5615.635253
                    1                    2                    3
Frequencies --  -290.7532               27.2788              43.8892
```

BDD-Rh(I)-Ph-CH-re-confU-CR-TS (239a)

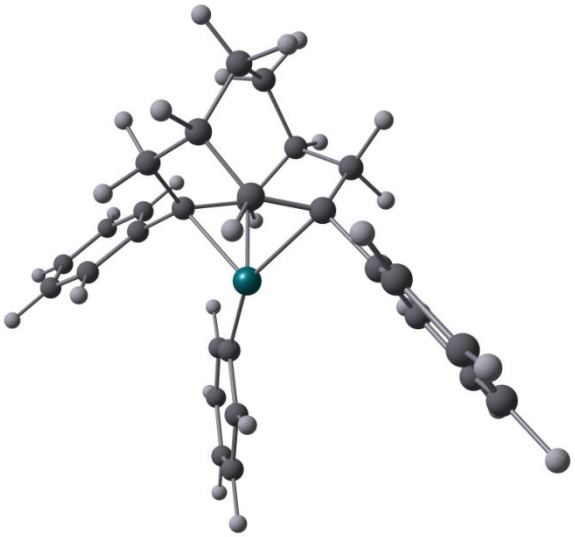


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.046431	0.123137	-0.257023
2	6	0	-0.759945	-1.333338	1.263561
3	6	0	-0.959911	-1.892505	0.008171

4	6	0	1.936104	-0.719842	-0.144596
5	1	0	0.136909	-1.642789	1.798036
6	6	0	-1.787256	-0.615472	2.097909
7	6	0	-2.282069	-1.992251	-0.746653
8	6	0	2.513630	-1.093450	1.078630
9	6	0	2.250108	-1.500553	-1.273788
10	6	0	-2.805944	0.148517	1.243328
11	1	0	-1.256947	0.090145	2.748043
12	1	0	-2.301346	-1.320286	2.770187
13	6	0	-2.411780	-0.851947	-1.765949
14	1	0	-2.237876	-2.931737	-1.310316
15	6	0	3.338239	-2.214673	1.179510
16	1	0	2.307511	-0.513787	1.976248
17	6	0	3.060811	-2.628110	-1.175602
18	1	0	1.856881	-1.215125	-2.248822
19	6	0	-2.099121	0.892411	0.116404
20	1	0	-3.255253	0.920790	1.878890
21	6	0	-1.976495	0.478112	-1.207965
22	1	0	-1.784600	-1.070239	-2.638039
23	1	0	-3.444279	-0.792230	-2.144159
24	6	0	3.612574	-2.991772	0.055120
25	1	0	3.763352	-2.482930	2.144291
26	1	0	3.274071	-3.218091	-2.064212
27	1	0	-1.791191	1.262195	-1.942505
28	1	0	4.256848	-3.863588	0.132998
29	6	0	-3.951505	-0.747542	0.759081
30	6	0	-3.500613	-2.086266	0.179168
31	1	0	-4.535168	-0.192937	0.015115
32	1	0	-4.631900	-0.937675	1.598577
33	1	0	-3.269486	-2.788978	0.988503
34	1	0	-4.336049	-2.528241	-0.378189
35	6	0	2.035823	1.267437	-0.609209
36	1	0	2.768749	0.958484	-1.348456
37	6	0	0.840115	1.847475	-1.162156
38	1	0	0.663177	1.736467	-2.232888
39	6	0	0.202123	3.019690	-0.566261
40	8	0	-0.672326	3.654473	-1.162100
41	6	0	2.642366	1.955668	0.592431
42	1	0	3.346237	1.298138	1.107633
43	6	0	0.671552	3.479977	0.802501
44	1	0	-0.211109	3.748213	1.391129
45	6	0	1.573260	2.491187	1.532796
46	1	0	3.233636	2.795843	0.199158
47	1	0	0.973195	1.651780	1.910291
48	1	0	2.033513	2.972723	2.402586
49	1	0	1.213450	4.418955	0.625735
50	1	0	-0.181188	-2.568967	-0.342540
51	1	0	-1.975514	1.960426	0.286947

```
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5616.02870558     A.U. after    1 cycles
             Convg  =    0.3922D-08             -V/T =  2.0040
Zero-point correction=                           0.441879 (Hartree/Particle)
 Thermal correction to Energy=                    0.463142
 Thermal correction to Enthalpy=                  0.464102
 Thermal correction to Gibbs Free Energy=         0.392225
 Sum of electronic and zero-point Energies=          -5615.586827
 Sum of electronic and thermal Energies=             -5615.565564
 Sum of electronic and thermal Enthalpies=           -5615.564604
 Sum of electronic and thermal Free Energies=        -5615.636481
                    1                    2                    3
Frequencies --  -288.4716               24.8589              51.9817
```

(*S*)-3,7-diphenylBDD-Rh(I)-Ph (240)

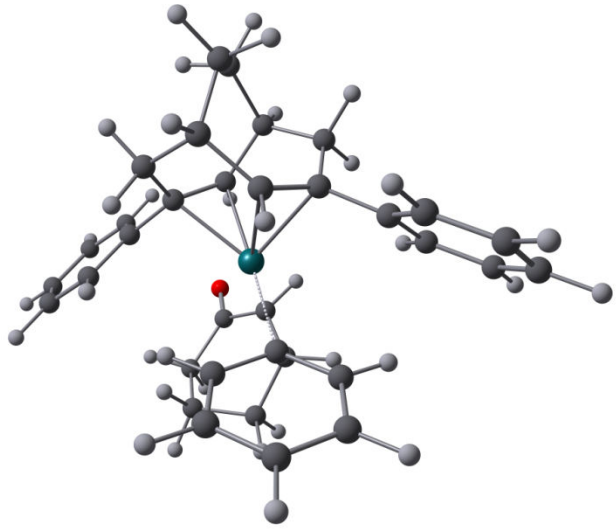


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.289653	0.206330	-0.161256
2	6	0	-0.584413	-1.175006	1.141300
3	1	0	-1.148597	-0.639570	1.905282
4	6	0	0.436328	-2.162429	1.721641
5	1	0	0.259731	-2.173787	2.803624
6	6	0	1.869918	-1.656676	1.509315
7	1	0	2.082852	-0.884856	2.254444
8	1	0	2.598418	-2.459933	1.697698
9	6	0	2.097075	-1.056924	0.134670
10	6	0	1.492383	-1.527649	-1.021985
11	1	0	1.847100	-1.113803	-1.966584
12	6	0	0.603386	-2.750851	-1.161935
13	1	0	0.823928	-3.172385	-2.150406
14	6	0	-0.868923	-2.325555	-1.174839
15	1	0	-1.113978	-1.903015	-2.155916
16	1	0	-1.523481	-3.204412	-1.062219
17	6	0	-1.233166	-1.283310	-0.127247
18	6	0	-0.855162	1.827655	0.184676
19	6	0	-1.979888	2.121611	0.966115
20	6	0	-0.236384	2.892274	-0.488799
21	6	0	-2.457011	3.428403	1.075982
22	1	0	-2.506537	1.326995	1.491083
23	6	0	-0.711022	4.203244	-0.394123
24	1	0	0.649541	2.711670	-1.109064
25	6	0	-1.827623	4.473484	0.395811
26	1	0	-3.329179	3.634340	1.693511
27	1	0	-0.211998	5.007029	-0.931693
28	1	0	-2.206348	5.489241	0.480131
29	6	0	-2.659268	-0.848488	-0.258357
30	6	0	-3.126729	-0.200472	-1.410293
31	6	0	-3.585483	-1.156665	0.745461
32	6	0	-4.465298	0.149487	-1.542555
33	1	0	-2.422164	0.067087	-2.194204
34	6	0	-4.930637	-0.806825	0.616941
35	1	0	-3.251232	-1.683676	1.636051
36	6	0	-5.375953	-0.149847	-0.526696
37	1	0	-4.799862	0.671563	-2.435494
38	1	0	-5.629989	-1.053453	1.412145

39	1	0	-6.421701	0.128400	-0.628397
40	6	0	3.190859	-0.047720	0.014616
41	6	0	3.288402	1.025610	0.917332
42	6	0	4.145477	-0.131747	-1.011536
43	6	0	4.284524	1.989409	0.781698
44	1	0	2.563842	1.124169	1.722398
45	6	0	5.147841	0.825584	-1.141077
46	1	0	4.112052	-0.970670	-1.701686
47	6	0	5.220248	1.893724	-0.247134
48	1	0	4.327175	2.818815	1.482765
49	1	0	5.881018	0.732545	-1.938285
50	1	0	6.002545	2.641246	-0.348078
51	6	0	0.252383	-3.601726	1.227226
52	6	0	0.876950	-3.858418	-0.139987
53	1	0	0.696569	-4.290367	1.956688
54	1	0	-0.819086	-3.833686	1.203395
55	1	0	1.961168	-3.989273	-0.042717
56	1	0	0.490951	-4.806149	-0.535274

```
SCF Done:  E(RPBE1PBE) =  -5769.26169799     A.U. after    1 cycles
             Convg  =    0.5417D-08             -V/T =  2.0044
Zero-point correction=                           0.473210 (Hartree/Particle)
 Thermal correction to Energy=                    0.498014
 Thermal correction to Enthalpy=                  0.498974
 Thermal correction to Gibbs Free Energy=         0.417884
 Sum of electronic and zero-point Energies=          -5768.788488
 Sum of electronic and thermal Energies=             -5768.763684
 Sum of electronic and thermal Enthalpies=           -5768.762724
 Sum of electronic and thermal Free Energies=        -5768.843814
                    1                    2                    3
Frequencies --    26.9122              33.1652              40.7357
```

(*S*)-3,7-diphenylBDD-Rh(I)-Ph-CH-si-confU-CR-TS (242a)



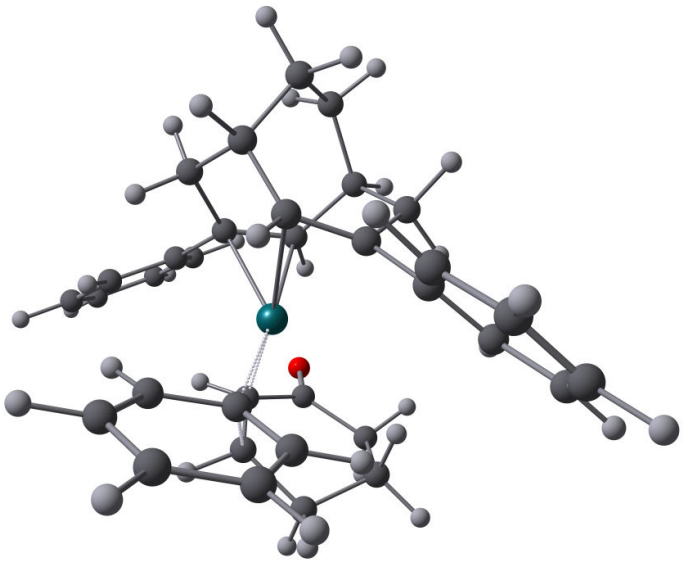
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	0.021423	0.095163	-0.158843
2	6	0	1.229752	1.414616	1.175950
3	1	0	1.750065	0.736096	1.851422
4	6	0	0.355654	2.451443	1.872068

5	1	0	0.646945	2.424889	2.928922
6	6	0	-1.115076	2.035549	1.808766
7	1	0	-1.281491	1.248537	2.549574
8	1	0	-1.774940	2.864260	2.109417
9	6	0	-1.561785	1.508967	0.455538
10	6	0	-1.033554	1.951427	-0.763153
11	1	0	-1.587470	1.666776	-1.657007
12	6	0	-0.070800	3.115751	-0.956972
13	1	0	-0.347795	3.572814	-1.914434
14	6	0	1.359753	2.598738	-1.108196
15	1	0	1.483407	2.203272	-2.120517
16	1	0	2.085892	3.422798	-1.025707
17	6	0	1.739917	1.502555	-0.126024
18	6	0	0.356012	-2.004364	1.727977
19	6	0	0.991531	-2.675024	2.771394
20	6	0	1.028260	-1.703410	0.527074
21	6	0	2.311679	-3.104154	2.629632
22	1	0	0.448552	-2.871811	3.693378
23	6	0	2.349545	-2.152768	0.404250
24	6	0	2.983502	-2.843484	1.436025
25	1	0	2.805145	-3.643324	3.434279
26	1	0	2.901704	-1.971868	-0.515140
27	1	0	4.010442	-3.176358	1.303610
28	6	0	0.090761	-2.068189	-1.246218
29	6	0	-0.774160	-1.070724	-1.815140
30	1	0	-0.346332	-0.399420	-2.562208
31	6	0	-0.552917	-3.402141	-0.910254
32	6	0	-1.981195	-3.250965	-0.405061
33	1	0	-1.979199	-2.713829	0.547990
34	1	0	-2.406821	-4.239323	-0.199795
35	1	0	1.054508	-2.160959	-1.742261
36	6	0	-2.201898	-1.289297	-2.026842
37	6	0	-2.853498	-2.507446	-1.409011
38	1	0	-3.807463	-2.196727	-0.972565
39	1	0	-3.102455	-3.163372	-2.254346
40	8	0	-2.854370	-0.543355	-2.761543
41	1	0	-0.564986	-3.969545	-1.853464
42	1	0	0.060869	-3.970762	-0.207797
43	1	0	-0.677438	-1.696330	1.866441
44	6	0	3.030607	0.841515	-0.483106
45	6	0	3.263612	0.344078	-1.775592
46	6	0	4.079458	0.771311	0.442657
47	6	0	4.487397	-0.220656	-2.121224
48	1	0	2.467853	0.372076	-2.515959
49	6	0	5.306811	0.206326	0.100691
50	1	0	3.935980	1.174336	1.441240
51	6	0	5.517731	-0.294337	-1.182263
52	1	0	4.636655	-0.608974	-3.125635
53	1	0	6.103493	0.165124	0.839249
54	1	0	6.475485	-0.731952	-1.451336
55	6	0	-2.896859	0.834553	0.496510
56	6	0	-3.218710	-0.099141	1.496765
57	6	0	-3.908720	1.191613	-0.405564
58	6	0	-4.488089	-0.660654	1.583114
59	1	0	-2.465992	-0.399498	2.220633
60	6	0	-5.181750	0.631672	-0.322741
61	1	0	-3.702842	1.926555	-1.176921
62	6	0	-5.480443	-0.295911	0.672065
63	1	0	-4.703481	-1.386232	2.363607
64	1	0	-5.942531	0.925942	-1.040709
65	1	0	-6.474536	-0.730216	0.739137
66	6	0	-0.178084	4.216060	0.103674
67	6	0	0.567375	3.891297	1.393131

68	1	0	-1.237572	4.403634	0.314234
69	1	0	0.218771	5.149954	-0.313355
70	1	0	0.235717	4.580057	2.180131
71	1	0	1.641875	4.069065	1.266663

```
SCF Done:  E(RPBE1PBE) =  -6077.58768160     A.U. after    1 cycles
            Convg  =    0.3315D-08             -V/T =  2.0049
Zero-point correction=                           0.603528 (Hartree/Particle)
 Thermal correction to Energy=                    0.634925
 Thermal correction to Enthalpy=                  0.635885
 Thermal correction to Gibbs Free Energy=         0.541877
 Sum of electronic and zero-point Energies=          -6076.984153
 Sum of electronic and thermal Energies=             -6076.952757
 Sum of electronic and thermal Enthalpies=           -6076.951797
 Sum of electronic and thermal Free Energies=        -6077.045804
                     1                      2                      3
Frequencies --  -310.2644               22.8058                32.1573
```

(*S*)-3,7-diphenylBDD-Rh(I)-Ph-CH-re-confU-CR-TS (244a)



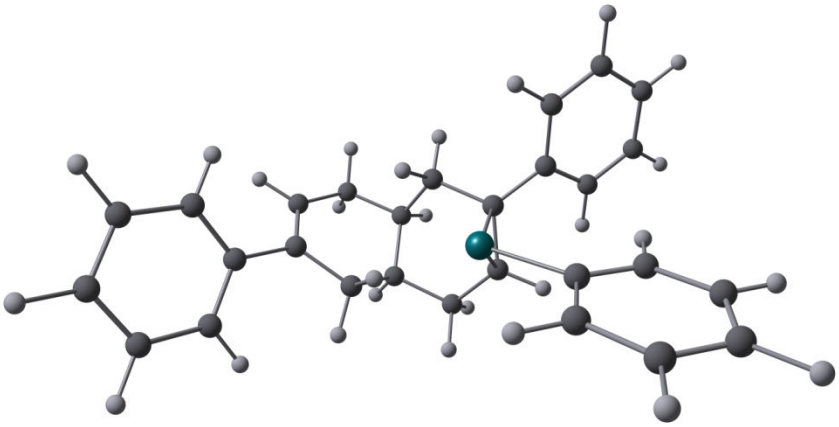
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.191600	-0.128778	-0.029427
2	6	0	0.788255	1.560460	1.077101
3	1	0	1.367305	1.048819	1.844255
4	6	0	-0.250848	2.526274	1.631406
5	1	0	0.029716	2.682856	2.680107
6	6	0	-1.638729	1.887516	1.636474
7	1	0	-1.695030	1.182775	2.471432
8	1	0	-2.416035	2.641161	1.836745
9	6	0	-1.988723	1.138822	0.364260
10	6	0	-1.477134	1.469572	-0.895978
11	1	0	-1.963922	0.989570	-1.743502
12	6	0	-0.692855	2.724902	-1.253424
13	1	0	-1.017594	2.993385	-2.265906
14	6	0	0.801871	2.419700	-1.339860
15	1	0	0.984626	1.882500	-2.275222
16	1	0	1.387590	3.348964	-1.416030
17	6	0	1.347015	1.579966	-0.199275

18	6	0	0.545981	-1.723142	2.325611
19	6	0	1.373441	-2.015391	3.405417
20	6	0	1.060478	-1.552175	1.023812
21	6	0	2.745610	-2.193597	3.207961
22	1	0	0.945092	-2.126958	4.399214
23	6	0	2.434741	-1.752398	0.846004
24	6	0	3.266427	-2.069833	1.922548
25	1	0	3.394468	-2.440115	4.044595
26	1	0	2.882793	-1.641756	-0.138133
27	1	0	4.331123	-2.208506	1.749091
28	6	0	-0.177089	-2.528177	-0.311073
29	6	0	-1.282771	-1.787207	-0.850300
30	1	0	-0.527150	-1.642361	2.494402
31	6	0	2.764121	1.156230	-0.406288
32	6	0	3.230232	0.700726	-1.650397
33	6	0	3.709808	1.305030	0.619642
34	6	0	4.566549	0.365095	-1.846765
35	1	0	2.542297	0.591924	-2.483250
36	6	0	5.048757	0.974958	0.427244
37	1	0	3.397642	1.699916	1.581603
38	6	0	5.485465	0.494633	-0.805670
39	1	0	4.891208	0.003037	-2.819112
40	1	0	5.754839	1.102773	1.243878
41	1	0	6.530536	0.238658	-0.959158
42	6	0	-3.256988	0.354461	0.483597
43	6	0	-3.509156	-0.477079	1.587287
44	6	0	-4.268772	0.485632	-0.476028
45	6	0	-4.709991	-1.167411	1.712872
46	1	0	-2.745165	-0.613085	2.348365
47	6	0	-5.474545	-0.201769	-0.352553
48	1	0	-4.113351	1.135466	-1.331341
49	6	0	-5.702303	-1.033508	0.740415
50	1	0	-4.871181	-1.815455	2.570817
51	1	0	-6.238540	-0.083682	-1.116559
52	1	0	-6.641957	-1.570996	0.837079
53	6	0	0.774805	-3.175068	-1.289186
54	1	0	1.689160	-3.504172	-0.790572
55	1	0	0.269352	-4.082878	-1.651749
56	6	0	1.072041	-2.256405	-2.461923
57	6	0	-1.386088	-1.524762	-2.291317
58	8	0	-2.421247	-1.090051	-2.801606
59	1	0	-2.237990	-1.837296	-0.333820
60	1	0	-0.437294	-3.162718	0.530987
61	6	0	-0.212863	-1.880179	-3.188682
62	1	0	1.564346	-1.354499	-2.081428
63	1	0	1.773734	-2.731389	-3.156663
64	1	0	-0.563163	-2.729943	-3.790048
65	1	0	-0.064160	-1.056422	-3.893887
66	6	0	-0.246826	3.905104	0.965887
67	6	0	-0.990861	3.935146	-0.363618
68	1	0	0.791972	4.227823	0.827716
69	1	0	-0.703135	4.631132	1.650307
70	1	0	-0.721908	4.850548	-0.905318
71	1	0	-2.072555	3.989587	-0.193035

SCF Done: E(RPBE1PBE) = -6077.59338140 A.U. after 1 cycles
Convg = 0.2718D-08 -V/T = 2.0049
Zero-point correction= 0.604175 (Hartree/Particle)
Thermal correction to Energy= 0.635564
Thermal correction to Enthalpy= 0.636524
Thermal correction to Gibbs Free Energy= 0.542621
Sum of electronic and zero-point Energies= -6076.989207
Sum of electronic and thermal Energies= -6076.957818

```
 Sum of electronic and thermal Enthalpies=          -6076.956858
 Sum of electronic and thermal Free Energies=       -6077.050760
                      1                      2                      3
Frequencies --   -285.3976               29.2843                39.3836
```

(1*S*,6*S*)-3,8-diphenylbicyclo[4.4.0]deca-3,8-diene-Rh(I)-Ph (245)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	45	0	-0.553179	0.780189	0.118156
2	6	0	3.288665	-2.215477	0.023044
3	6	0	3.312100	-0.916074	-0.321688
4	6	0	-2.110184	1.932831	-0.076343
5	1	0	4.109377	-2.617136	0.616497
6	6	0	2.210561	-3.180032	-0.375374
7	6	0	1.329163	-1.364849	-1.859041
8	6	0	-1.703585	3.264132	0.115328
9	6	0	-3.468914	1.671933	-0.285046
10	6	0	0.950019	-2.488483	-0.891480
11	1	0	1.966344	-3.823271	0.480671
12	1	0	2.603577	-3.859865	-1.145279
13	6	0	0.072170	-0.743510	-2.467170
14	1	0	1.914834	-1.813266	-2.672690
15	6	0	-2.629430	4.308752	0.110223
16	1	0	-0.648479	3.508409	0.272745
17	6	0	-4.394296	2.717969	-0.293109
18	1	0	-3.817927	0.650817	-0.418556
19	6	0	-1.145023	-1.182722	-0.229240
20	1	0	0.347665	-3.222930	-1.442877
21	6	0	-1.035735	-0.478078	-1.469573
22	1	0	0.321168	0.177465	-3.008782
23	1	0	-0.326900	-1.438213	-3.222936
24	6	0	-3.982086	4.036834	-0.097933
25	1	0	-2.293774	5.332395	0.261959
26	1	0	-5.449009	2.497942	-0.445549
27	1	0	-1.967291	-0.157357	-1.937461
28	1	0	-4.708174	4.845697	-0.105665
29	6	0	4.381701	-0.012434	0.167979
30	6	0	4.954605	0.964454	-0.660341
31	6	0	4.850058	-0.107998	1.487931
32	6	0	5.969772	1.797211	-0.195155
33	1	0	4.625390	1.063957	-1.691020
34	6	0	5.864091	0.723954	1.955750

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     35          1           0        4.395551   -0.831120    2.160408
     36          6           0        6.430984    1.681457    1.115410
     37          1           0        6.404900    2.537588   -0.861634
     38          1           0        6.203569    0.632503    2.984448
     39          1           0        7.218982    2.335038    1.479941
     40          6           0       -2.455672   -1.630485    0.311749
     41          6           0       -2.653830   -1.759202    1.696054
     42          6           0       -3.514688   -1.979454   -0.537520
     43          6           0       -3.868361   -2.196719    2.211186
     44          1           0       -1.849649   -1.485597    2.375665
     45          6           0       -4.735971   -2.417455   -0.023328
     46          1           0       -3.378307   -1.921227   -1.614407
     47          6           0       -4.920209   -2.525656    1.352597
     48          1           0       -4.001285   -2.273716    3.287494
     49          1           0       -5.541813   -2.682052   -0.703600
     50          1           0       -5.870748   -2.865975    1.754837
     51          6           0        2.227682   -0.327327   -1.184882
     52          1           0        2.658087    0.317858   -1.959284
     53          1           0        1.627837    0.378092   -0.571230
     54          6           0        0.086431   -1.953898    0.254585
     55          1           0        0.719906   -1.326370    0.909885
     56          1           0       -0.230884   -2.786230    0.891726
 ---------------------------------------------------------------------
SCF Done:  E(RPBE1PBE) =  -5769.24715717     A.U. after    1 cycles
             Convg  =    0.2285D-08             -V/T =  2.0043
Zero-point correction=                           0.471593 (Hartree/Particle)
 Thermal correction to Energy=                    0.497237
 Thermal correction to Enthalpy=                  0.498197
 Thermal correction to Gibbs Free Energy=         0.412595
 Sum of electronic and zero-point Energies=          -5768.775564
 Sum of electronic and thermal Energies=             -5768.749920
 Sum of electronic and thermal Enthalpies=           -5768.748960
 Sum of electronic and thermal Free Energies=        -5768.834563
                     1                      2                      3
Frequencies --    17.9324                26.5048                29.6624
```

Gaussian 09 reference:

Gaussian 09, Revision **A.02**, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

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