

Supporting Information

The Structure of Dichlorotris(triphenylphosphine) ruthenium(II): A DFT Study of Interaction Energies and Substitution Mechanism

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Table S1. Selected geometric parameters for the $[\text{RuCl}_2(\text{PPh}_3)_3]$ complex calculated with the ten DFT methods using the def2-tzvpp on Ru, P and Cl atoms and def2-sv(p) basis set on C and H atoms. Distances in Å and bond angles in °.

Bond distance	PBE0	B3P86	PBE	B3PW91	wB97X-D	Exp. ¹
Ru–Cl(1)	2.376	2.379	2.390	2.383	2.399	2.373
Ru–Cl(2)	2.383	2.386	2.398	2.391	2.403	2.392
Ru–P(1)	2.382	2.384	2.383	2.396	2.393	2.356
Ru–P(2)	2.411	2.415	2.421	2.430	2.399	2.433
Ru–P(3)	2.213	2.212	2.213	2.220	2.221	2.212
Bond angle						
P(1)–Ru–P(2)	158.49	158.28	157.85	158.06	159.72	160.12
P(1)–Ru–P(3)	100.43	100.58	100.72	100.75	100.06	98.27
P(2)–Ru–P(3)	100.38	100.49	100.71	100.52	99.55	101.08
P(1)–Ru–Cl(2)	91.68	91.60	91.68	91.31	91.78	92.05
P(1)–Ru–Cl(1)	85.63	85.67	85.57	85.64	85.72	86.29

Cl(1)–Ru–Cl(2)	155.12	155.23	153.82	154.79	153.98	159.24
P(2)–Ru–Cl(1)	82.47	82.53	82.13	82.31	82.77	83.63
P(3)–Ru–Cl(1)	109.20	109.02	109.42	109.35	109.97	107.46
Bond distance	M06-L	MN12-L	B3LYP-D3	CAM-B3LYP	B3LYP	Exp. ¹
Ru–Cl(1)	2.416	2.394	2.418	2.399	2.416	2.373
Ru–Cl(2)	2.423	2.404	2.424	2.404	2.422	2.392
Ru–P(1)	2.371	2.398	2.397	2.421	2.437	2.356
Ru–P(2)	2.443	2.420	2.424	2.445	2.478	2.433
Ru–P(3)	2.202	2.246	2.226	2.244	2.250	2.212
Bond angle						
P(1)–Ru–P(2)	159.61	160.58	158.90	158.23	157.35	160.12
P(1)–Ru–P(3)	99.22	98.86	100.13	100.73	101.19	98.27
P(2)–Ru–P(3)	99.80	99.09	100.12	100.45	100.89	101.08
P(1)–Ru–Cl(2)	91.72	91.34	91.72	91.31	91.16	92.05
P(1)–Ru–Cl(1)	84.90	85.01	85.33	85.56	8.57	86.29
Cl(1)–Ru–Cl(2)	156.23	158.00	1154.40	155.47	15.87	159.24
P(2)–Ru–Cl(1)	82.66	82.77	82.58	82.77	82.42	83.63
P(3)–Ru–Cl(1)	106.78	106.73	108.87	109.17	109.28	107.46

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Table S2. Calculated energies (in kcal mol⁻¹) for the first dissociation energy (D_e) and absolute energies (in a.u.) of the [RuCl₂(PPh₃)₂] and PPh₃ fragments in the [RuCl₂(PPh₃)₃] complex, using the M06-L method with the def2-tzvp basis set for the Ru, P and Cl atoms and def2-sv(p) for C and H atoms.

	[RuCl ₂ (PPh ₃) ₃]		
Absolute energy (a.u.)	-4122.66917		
[RuCl ₂ (PPh ₃) ₂] fragment	[RuCl ₂ (PPh ₃) ₂](1)	[RuCl ₂ (PPh ₃) ₂](2)	[RuCl ₂ (PPh ₃) ₂](3)
Absolute energies (a.u.)	-3086.90577	-3086.91185	-3086.85856
PPh ₃ group	PPh ₃ (1)	PPh ₃ (2)	PPh ₃ (3)
Absolute energies (a.u.)	-1035.67761	-1035.67776	-1035.67746
Dissociation energy (D_e , kcal·mol ⁻¹), computed according to Eq. 2.	53.82	49.92	83.55

Table S3. Bond reorganization energies (R_e) for the three PPh_3 groups in the $[RuCl_2(PPh_3)_3]$ complex calculated with the M06-L method.

Group	R_e
$PPh_3(1)$	$\Delta E = 2.23 \text{ kcal mol}^{-1}$
$PPh_3(2)$	$\Delta E = 2.13 \text{ kcal mol}^{-1}$
$PPh_3(3)$	$\Delta E = 2.32 \text{ kcal mol}^{-1}$

Table S4. CDA analysis obtained with AOMix for the $[RuCl_2(PPh_3)_2\text{piperidine}]$ complex based on the M06-L/def2-tzvpp method. Donation (Σ -D) and back-donation (Σ -BD). $P_x = PPh_3(1), PPh_3(2)$ or piperidine. steric, orbital and interaction energies in $\text{kcal}\cdot\text{mol}^{-1}$.

	Σ -D	Σ -RD	ΔE_{steric}	$\Delta E_{\text{orbital}}$	$\Delta E_{\text{interaction}}$
	$P_x \rightarrow Ru$	$Ru \rightarrow P_x$			
$PPh_3(1)$ (basal)	0.403	0.410	39.07	-101.00	61.93
$PPh_3(2)$ (apical)	0.129	0.428	118.81	-196.20	77.40
Piperidine	0.379	0.111	0.440	-40.60	40.16

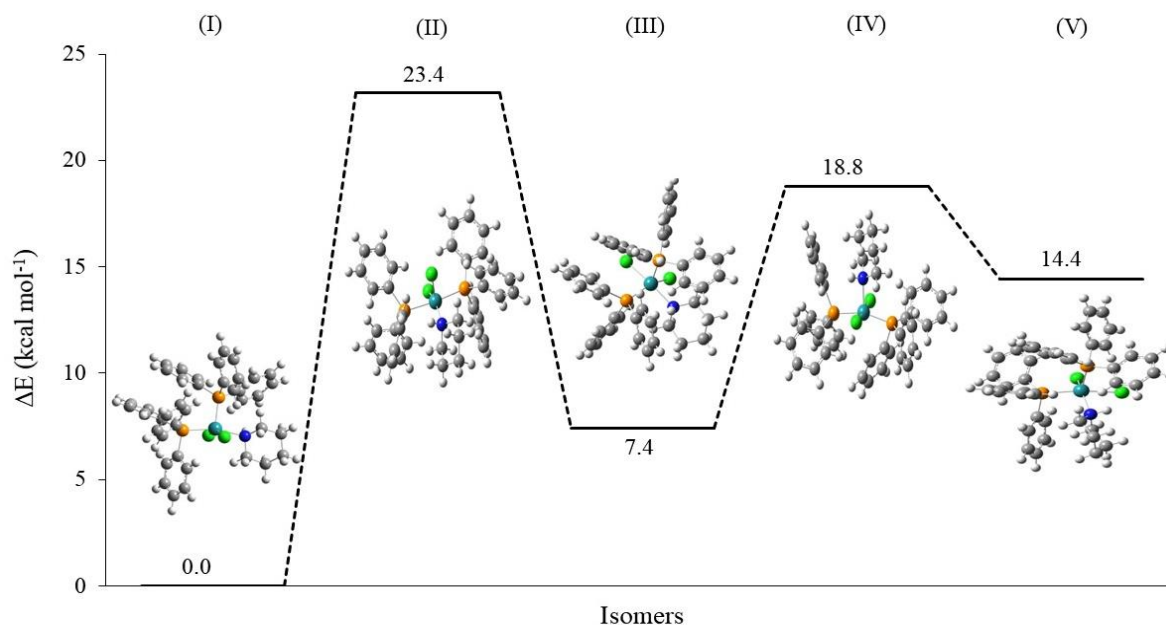
Table S5. Absolute and relative energies for decomposition of $[RuCl_2(PPh_3)_4]$ in $[RuCl_2(PPh_3)_3]$ and PPh_3 , calculated with the M06-L method based on the equation: $[RuCl_2(PPh_3)_4] \rightarrow [RuCl_2(PPh_3)_3] + PPh_3$.

	E (a.u.)	H (a.u.)	G (a.u.)
$[RuCl_2(PPh_3)_4]$	-5158.35624	-5157.17658	-5157.34860
$[RuCl_2(PPh_3)_3]$	-4122.66917	-4121.78281	-4121.92654
PPh_3	-1035.68116	-1035.39116	-1035.45314
ΔE (a.u.)	0.00591	0.00261	-0.03108
E_f ($\text{kcal}\cdot\text{mol}^{-1}$)	3.71	+1.64	-19.50

Table S6. Calculation of the relative basicity of the piperidine and PPh_3 molecules, computed with the M06-L method, based on the reaction: $C_5H_{11}N-H + PPh_3 \rightarrow H-PPh_3 + C_5H_{11}N$.

	ΔE (a.u.)	ΔH (a.u.)	ΔG (a.u.)
$C_5H_{11}N-H$	-252.08465	-251.904152	-251.939457
PPh_3	-1035.68112	-1035.392019	-1035.451704
$H-PPh_3$	-1036.06827	-1035.76724	-1035.83039
$C_5H_{11}N$	-251.71249	-251.54716	-251.58226
ΔE (a.u.)	0.01499	0.01823	0.02149
ΔE (kcal mol^{-1})	-9.40	-11.44	-13.48

Figure S1. Relative (in kcal mol⁻¹) and total (in a.u.) energies of the five possible isomers of the [RuCl₂(PPh₃)₂(pip)] complex using the M06-L method.



Isomers	(I)	(II)	(III)	(IV)	(V)
E (a.u.)	-3338.69382	-3338.65678	-3338.68209	-3338.66389	-3338.67091
ΔE (kcal mol ⁻¹)	0	23.2	7.4	18.8	14.4

Table S7. Cartesian coordinates of all species computed in the present study calculated with the M06-L method and the def2-tzvp basis set on Ru, Cl, P and N and def2-svp(p) on C and H.

Dimer [Ru₂Cl₄(PPh₃)₄]

C	-1.69217900	3.36180200	-0.29369000	H	-6.33525700	-3.25822000	3.47074500	C	1.57941800	-1.68796100	-2.55189000
C	-3.64030700	2.55691000	4.70142800	H	-4.65601400	-1.90917400	-2.71516800	C	1.33029400	-3.02287200	1.01966400
C	-3.59828700	1.27899400	4.14607600	H	-6.86750000	-1.23870400	-3.62184000	C	4.50961800	5.28191700	0.42895500
C	-3.29987300	1.11999100	2.79444100	H	-8.45200400	0.08314900	-2.21747400	C	0.67680800	-4.05861100	0.33693100
C	-4.37061400	2.44541800	-0.54866600	H	-7.78497700	0.77093800	0.08935900	C	-0.12396500	-4.97824600	1.01671800
C	-5.34131500	3.13693600	0.19303900	H	-5.57273100	0.12568300	0.98595900	C	-0.25829100	-4.90148000	2.39963400
C	-6.51411500	3.58622100	-0.41247700	H	-3.23047800	0.11335800	2.37221000	C	0.38501200	-3.87398200	3.09218000
C	-6.74239600	3.35000000	-1.76647000	H	-3.78375400	0.39310900	4.76468400	C	1.14258400	-2.92741000	2.41030800
C	-5.79435300	2.64654100	-2.50793400	H	-3.86453200	2.68911200	5.76646800	C	4.42886400	4.00479600	-0.11851400
C	-4.62372800	2.19150800	-1.90589600	H	-3.41116900	4.67730900	4.33034000	C	3.56176300	1.50361400	-1.94157100
C	-0.64668800	3.77931100	0.54429300	H	-2.90972500	4.39042200	1.92049500	C	2.86947000	2.58581900	-2.50520500
C	0.24511000	4.76245000	0.12361600	H	-5.19570200	3.32950000	1.26071900	C	2.64897800	2.64975500	-3.87908700
C	-4.97359600	-0.96572500	-0.79265600	H	-3.90211200	1.61272400	-2.49342000	P	3.67052000	1.28183900	-0.13531200
C	-5.34529400	-1.32572200	-2.09450100	H	-5.96984700	2.43250400	-3.56886900	P	2.41720800	-1.81042100	0.15449700
C	-6.58868400	-0.94822700	-2.60205200	H	-7.66553800	3.70438400	-2.24091900	Ru	1.87057400	0.24463100	0.73120000
C	0.12847000	5.32037200	-1.15060700	H	-7.25691200	4.12662400	0.18657000	H	1.58380500	-2.09214100	2.96501300
C	-7.47347800	-0.20937600	-1.81774600	H	-2.59070700	3.60277500	-2.25445700	H	0.27931900	-3.78999000	4.18054300
C	-7.10440800	0.17223600	-0.52702800	H	-0.52033700	3.31775000	1.53304100	H	-0.88112200	-5.62691600	2.93672000
C	-5.85931900	-0.19281100	-0.02621000	H	1.04934000	5.08929100	0.79174900	H	-0.64619100	-5.75729300	0.44819200
C	-3.76220200	-2.12559600	1.52045200	H	0.84050500	6.08722400	-1.48015500	H	0.77763200	-4.16013800	-0.74621100
C	-5.06718100	-2.44514800	1.92690000	H	-0.98960700	5.31953500	-3.00520000	H	3.45657900	-4.19609000	-1.21027700
C	-5.30666800	-3.01982300	3.17495600	Cl	0.50627400	1.16490100	-1.05086800	H	1.10527800	-0.73446900	-2.30016700
C	-4.24712200	-3.29200600	4.03879200	Cl	2.73124000	0.03399400	2.95673700	H	0.87117700	-1.60899600	-4.58452500
C	-2.94303900	-3.01050100	3.63221600	C	3.69322400	2.99622100	0.52382900	H	1.97353000	-3.76553000	-5.23245800
C	-2.70206200	-2.44262700	2.38282300	C	3.11617100	1.63544700	-4.71472300	H	3.26272600	-5.04965100	-3.51809300
C	-2.90615800	-2.92945400	-1.00596800	C	3.80483000	0.55294500	-4.16751700	H	3.62770700	-2.74257400	2.70043300
C	-0.89108000	4.89355200	-1.99979600	C	4.01763800	0.48776500	-2.79298100	H	5.90998600	-3.41727200	3.32360900
C	-3.78935600	-4.02064100	-0.98653500	C	5.43053800	0.85646200	0.15137100	H	7.74044900	-3.41263700	1.62200100

C	-3.48364000	-5.19622000	-1.66537000	C	6.43028500	1.06807700	-0.81045100	H	7.23743100	-2.70685200	-0.72261900
C	-2.28161500	-5.30456400	-2.37050100	C	7.76973300	0.82781100	-0.50421800	H	4.94718900	-2.06909300	-1.36070400
C	-1.38906200	-4.23635900	-2.38084100	C	8.13149900	0.38938800	0.76858500	H	4.54610400	-0.37735000	-2.37344900
C	-1.69898300	-3.05877400	-1.69823000	C	7.14503600	0.19345600	1.73520300	H	4.16690300	-0.25689100	-4.81189200
C	-1.79824200	3.92631800	-1.57142500	C	5.80570600	0.42245800	1.43172600	H	2.93761300	1.68549700	-5.79516200
C	-3.05184200	2.22556000	1.97549800	C	3.05104800	3.29506500	1.73144700	H	2.09155400	3.49619900	-4.29706400
C	-3.09552900	3.50794100	2.54458800	C	3.15219000	4.56988200	2.29224400	H	2.46849700	3.37564100	-1.85961500
C	-3.38413400	3.66991800	3.89842100	C	4.10552000	-2.36455000	0.61819500	H	6.17324100	1.43639000	-1.80968800
P	-2.76046100	1.95961000	0.19122200	C	4.40771500	-2.74155300	1.93457100	H	5.03437100	0.25922000	2.19402700
P	-3.33857900	-1.38387100	-0.11220000	C	5.70159500	-3.11898100	2.28950900	H	7.41797500	-0.14987100	2.74018800
Ru	-1.68298100	0.12423800	-0.39665900	C	3.87564000	5.56626400	1.64130500	H	9.18563000	0.20443000	1.00825100
H	-0.98143700	-2.22894300	-1.72567800	C	6.72245600	-3.11788300	1.34015500	H	8.53763000	0.99528300	-1.26899100
H	-0.43867200	-4.31062300	-2.92397000	C	6.44220300	-2.72764600	0.03170200	H	4.95288100	3.78574900	-1.05781800
H	-2.04297200	-6.22761800	-2.91219600	C	5.14827500	-2.35529300	-0.32221100	H	2.48668400	2.51803900	2.26279500
H	-4.18972500	-6.03471300	-1.64794100	C	2.31046200	-2.38785400	-1.58609200	H	2.65373800	4.78150800	3.24556700
H	-4.73732400	-3.94635100	-0.43795200	C	2.90333100	-3.61076300	-1.95396700	H	3.95313800	6.56833600	2.07967800
H	-5.91728700	-2.25743900	1.26362200	C	2.78746800	-4.09789900	-3.25233000	H	5.08643600	6.05910000	-0.08612400
H	-1.67051400	-2.23234500	2.07883400	C	2.06385800	-3.38058800	-4.20946400	Cl	-0.44693100	-0.00059500	1.73237400
H	-2.09781200	-3.23444600	4.29310500	C	1.45219300	-2.18215100	-3.85236200	Cl	-2.11753500	0.04867000	-2.74293300
H	-4.43645700	-3.73347900	5.02446100								

Piperidine

N	-0.00194200	-1.46547200	-0.18569700
C	1.20544500	-0.75231900	0.22609900
C	1.25353700	0.70248600	-0.22769200
C	0.00195600	1.44608800	0.22043400
C	1.25170200	0.70586400	-0.22743100
C	-1.20742700	-0.74927600	0.22584700
H	0.00213900	1.52311000	1.32741000
H	2.08487000	-1.31359700	-0.13753100
H	2.16625200	1.19760500	0.15558000
H	-2.16302000	1.20336800	0.15608000
H	-1.24922500	-0.79148500	1.33298400
H	1.32704300	0.73555400	-1.33449300
H	0.00334600	2.48570500	-0.15665200
H	1.24703600	-0.79427000	1.33325900
H	-2.08837700	-1.30814200	-0.13793200
H	-1.32530200	0.73933400	-1.33420200
H	-0.00202600	-1.53593600	-1.20817300

Phosphine

C	-0.99948500	-1.26492300	-0.39747400	C	2.64029600	0.79141000	-0.51836600
C	-0.96216800	-1.42199100	0.99514800	P	0.08441300	-0.06074300	-1.24032800
C	-1.85097900	-2.28243800	1.63364300	H	-3.60357500	-3.36399400	-1.08655800
C	-2.80152600	-2.98313000	0.88844300	H	-3.50714700	-3.65456300	1.39181700
C	-2.85623300	-2.82374800	-0.49521900	H	-1.80836600	-2.40133700	2.72269200
C	-1.95568000	-1.97171700	-1.13503300	H	-0.22711300	-0.86046500	1.58651900
C	-0.56932300	1.46366400	-0.44611100	H	-2.01304700	-1.85485500	-2.22840200
C	-1.79604200	1.96814000	-0.90781200	H	-0.05440100	3.68031700	2.10634400
C	-2.37463100	3.08757700	-0.31438800	H	0.96832400	1.69721900	1.07510400
C	-1.74737200	3.71982000	0.75962600	H	-2.20183800	4.60246100	1.22508400
C	-0.54652100	3.20782600	1.24782500	H	-3.32962600	3.46689800	-0.69669900
C	0.03573900	2.08757000	0.65490300	H	-2.29975100	1.48128500	-1.74969900
C	1.72109600	-0.26868400	-0.47710700	H	3.77814100	-2.66005700	0.83547400
C	2.14765900	-1.50947400	0.01862600	H	1.44925100	-2.35158400	0.05171700
C	3.46142200	-1.68224700	0.45399500	H	2.32533000	1.77480200	-0.88402400
C	4.36842000	-0.62411400	0.39904100	H	4.65288200	1.45943600	-0.13067000
C	3.95240400	0.61674200	-0.08467400	H	5.40228300	-0.76613000	0.73583000

[RuCl₂(PPh₃)₂(piperidine)]

Cl	0.45976200	1.42379300	2.27041200	C	3.76937600	-2.23641200	-0.06613600	H	-4.30243900	1.48366100	1.39826500
Cl	0.46387300	1.21162000	-2.46836700	C	5.08358900	-2.30078600	-0.53056000	H	-4.39078100	-1.02430000	0.33661800
Ru	0.40678700	0.83391200	-0.06267400	C	5.47216700	-1.57110200	-1.65268900	H	-1.54785400	-0.06598000	-2.77902700
C	-3.77492000	-0.48313100	4.13194000	C	4.52999200	-0.78817800	-2.32060100	H	-2.91624200	-1.33356100	-4.40586100
C	-2.57212500	-1.07793900	3.75154700	C	3.21852600	-0.71756700	-1.85494500	H	-5.02183400	-2.46456700	-3.66982600
C	-1.98559500	-0.74664300	2.53148700	C	-2.64686900	2.72114900	-1.53837900	H	-5.73679800	-2.29731400	-1.28358900
C	-2.88262800	-0.42120300	-1.11087600	C	-2.60152400	0.16586500	1.66730400	H	-2.77994300	2.00410400	-2.35567200
C	-4.05931900	-1.06988000	-0.70626100	C	-3.80873000	0.76068000	2.06006400	H	-1.78509000	2.88497900	1.75987500
C	-4.82130800	-1.79654200	-1.62113200	C	-4.39024200	0.44066100	3.28573500	H	-2.15293200	5.30011900	1.32482100
C	-4.42239500	-1.88982700	-2.95342500	P	-1.83032600	0.52650200	0.05486700	H	-2.81971200	6.07789400	-0.95326900
C	-3.25065000	-1.25501800	-3.36452800	P	1.09731200	-1.24292500	-0.07611800	H	-3.13441100	4.41090400	-2.78515900
C	-2.48400700	-0.53356000	-2.45293500	H	2.48560100	-0.09754500	-2.38711000	N	2.34110100	1.93893200	-0.21570800
C	-2.09341100	3.21860400	0.76164700	H	4.81729100	-0.22081300	-3.21416000	C	3.47644900	1.68838700	0.69548500
C	-2.27527800	2.27309600	-0.26248500	H	6.50741800	-1.61807500	-2.01049200	C	4.67358300	2.56341900	0.36338200
C	-2.29281200	4.57565000	0.51388300	H	5.81123300	-2.92947500	-0.00399100	C	4.29491900	4.03798600	0.36913700
C	0.13296400	-2.39996800	-1.10568600	H	3.49262900	-2.81972700	0.81850800	C	3.10359200	4.28293000	-0.54434700
C	0.55099000	-2.78914000	-2.38456900	H	0.36050100	-4.01679800	0.94225500	C	1.94700700	3.36988000	-0.19006300
C	-0.23874300	-3.63708000	-3.16171100	H	2.25933100	-0.42781500	2.42112800	H	4.03145400	4.34126200	1.40235500
C	-2.66554400	5.00990400	-0.75844600	H	2.54503800	-1.49391500	4.63085800	H	3.73694100	0.61772900	0.63619600
C	-1.44930800	-4.12027400	-2.66766800	H	1.68900600	-3.80920900	5.03023900	H	5.49064200	2.36069200	1.08009000
C	-1.87987900	-3.73634400	-1.39757300	H	0.61208800	-5.06146400	3.15669600	H	2.76993800	5.34141500	-0.48606300
C	-1.10280800	-2.87142300	-0.63375900	H	1.50597400	-2.43190000	-2.78535200	H	1.57328800	3.57344900	0.83064700
C	1.24516800	-2.12054300	1.52942900	H	0.10354100	-3.92821400	-4.16173300	H	5.06244200	2.27798500	-0.63581200
C	0.81199000	-3.43547000	1.75175000	H	-2.06601700	-4.79100400	-3.27781200	H	5.15566300	4.66524900	0.07319100
C	0.96542900	-4.03496900	3.00315700	H	-2.83822300	-0.09582200	-1.00521600	H	3.10747500	1.88258100	1.71903100
C	1.57316800	-3.33895300	4.04646900	H	-1.46583400	-2.55872800	0.35531700	H	1.10107000	3.49716400	-0.89106800
C	2.04833600	-2.04583600	3.82477400	H	-1.01562100	-1.17929500	2.25986400	H	3.39346000	4.11548000	-1.60053500
C	1.88705700	-1.44456000	2.57948400	H	-2.07210800	-1.79065600	4.41766900	H	2.63271200	1.72593300	-1.18125900
C	2.81793800	-1.43248100	-0.71376500	H	-4.23135900	-0.73186300	5.09734700				
C	-2.84224300	4.07851600	-1.78225200	H	-5.33187500	0.91754000	3.58238000				

[RuCl₂(PPh₃)₃(piperidine)]

Cl	0.13673700	0.71138400	2.49479500	C	0.04053700	-5.45045300	2.04776300	H	-3.24810000	2.28219700	-4.46489600
Cl	-0.08597000	0.32243500	-2.37834700	C	0.01361300	-5.06583200	3.39051300	H	-4.63862700	0.34967800	-5.22996800
C	-3.16410400	2.05599400	0.75936200	C	0.00890000	-3.71160900	3.71200600	H	-5.05585600	-1.55788700	-3.66718300
C	-4.93872500	-2.21958700	2.86942600	C	0.02408000	-2.74452800	2.70169500	H	-4.36576900	2.65989500	-0.94990700
C	-3.57192500	-2.04087600	3.07266900	C	1.56871800	-2.60279100	-0.93512100	H	-2.16607300	1.71632700	2.65552900
C	-2.83876000	-1.23739700	2.19943700	C	-4.67248300	3.96536700	0.72773700	H	-3.22305100	3.64070500	3.79096800
C	-3.21024600	0.42667000	-1.58825200	C	2.54178800	-3.30861900	-0.20471100	H	-4.84189500	5.09927200	2.56310500
C	-3.96153100	-0.66094700	-2.04055300	C	3.65062500	-3.88128300	-0.82653100	H	-5.38997200	4.58830500	0.18047300
C	-4.47238200	-0.68913300	-3.33927100	C	3.80814600	-3.78598800	-2.20735900	H	4.22942000	5.34481000	-0.41765100
C	-4.23595700	0.37011800	-4.21040300	C	2.87569300	-3.05920600	-2.94370000	H	4.10905600	5.80893200	2.03386000
C	-3.46577400	1.45329700	-3.78179000	C	1.79058600	-2.45120600	-2.31532100	H	3.31961600	4.01221700	3.58645400
C	-2.95089700	1.47164700	-2.49122800	C	-4.07968900	2.87692100	0.08416500	H	2.61330700	1.81845700	2.69409700
C	2.99332000	2.33147800	0.62433400	C	-3.45310000	-0.61419400	1.11179100	H	3.55345700	3.15173100	-1.30640200
C	-2.86888000	2.35147900	2.10193500	C	-4.84080500	-0.75005900	0.94941000	H	5.89264800	-1.27676200	-2.97477700
C	2.96208600	2.59442900	2.00499700	C	-5.57313500	-1.56016100	1.81298200	H	4.68942400	-1.11151600	-0.84147200
C	3.35655600	3.83139200	2.50580600	P	-2.43974100	0.49143300	0.06367800	H	5.22276100	0.14194500	-4.92134700
C	3.79668600	4.83445200	1.64009100	P	2.43019600	0.66119700	0.07392800	H	3.29427600	1.71558800	-4.68564500
C	3.85884100	4.57698800	0.27214900	P	0.06405800	-1.91960000	-0.07961200	H	2.09213300	1.89500900	-2.54214300
C	3.46698300	3.33411800	-0.23029000	Ru	-0.01233400	0.38375500	0.04856400	H	6.70708200	-0.43810800	2.36610700
C	3.33625200	0.45305900	-1.50411300	H	1.13314700	-1.82008700	-2.91442300	H	5.30845300	0.75530300	0.71129900
C	2.94545100	1.21521900	-2.61878900	H	3.00433400	-2.93150800	-4.02502400	H	1.83765500	-1.35697800	2.10310500
C	3.61865100	1.10774500	-3.83303800	H	4.66442600	-4.25853600	-2.70405100	H	3.22080700	-2.56223400	3.78287200
C	4.69168800	0.22619200	-3.96559000	H	4.38487300	-4.42360500	-0.21851200	H	5.67854800	-2.10662200	3.91372800
C	5.07128400	-0.55623600	-2.87789600	H	2.43649700	-3.44106900	0.87457700	C	0.16371400	3.49786600	-1.42884300
C	-3.46532100	3.43510300	2.74157800	H	0.08159400	-4.80994700	-0.00062500	C	-0.55303100	4.82335300	-1.63724100
C	4.39613800	-0.44965300	-1.66262500	H	0.03010500	-1.68450500	2.97786600	C	-0.36466200	5.75001600	-0.44672700
C	3.47302400	-0.26516600	1.26698900	H	-0.00664800	-3.39234700	4.76107800	C	-0.77658200	5.03933500	0.83242500
C	4.84780600	0.00887600	1.37032100	H	-0.00093300	-5.82421600	4.18230600	C	-0.03109000	3.72312000	0.07675800
C	5.63433000	-0.65621500	2.30511500	H	0.04921500	-6.51284500	1.77747500	N	-0.26430300	2.82275100	-0.18072400
C	5.05787800	-1.58946400	3.17236400	H	-0.68774900	-2.20165000	-3.02004900	H	0.70425500	6.03866200	-0.37576800
C	3.69139700	-1.84481800	3.09954600	H	-2.46237600	-3.41851800	-4.16990800	H	-0.00712800	2.80656700	-2.26954600
C	2.91161500	-1.18081900	2.15131500	H	-4.23598700	-4.61753800	-2.87424600	H	-0.19533500	5.29224700	-2.57323900
C	-1.33654500	-2.72070100	-1.01439400	H	-4.17828100	-4.52970600	-0.36730900	H	-0.58240100	5.66922800	1.72083500
C	-1.41791500	-2.73770800	-2.41585500	H	-2.36146100	-3.38387900	0.78783200	H	1.04945900	3.91740600	1.02638000
C	-2.44147500	-3.41965000	-3.07367300	H	-1.77083000	-1.06935400	2.36256900	H	-1.63704300	4.62935800	-1.78585800
C	-4.36919000	4.24896200	2.05741700	H	-3.06470600	-2.53242300	3.91171300	H	-0.93325500	6.68863800	-0.58359000
C	-3.43447000	-4.07944200	-2.35360300	H	-5.51990400	-2.85757200	3.54576000	H	1.25271300	3.66617900	-1.34945100
C	-3.40034000	-4.03437300	-0.96098500	H	-6.65417000	-1.67053200	1.66688500	H	-0.30706900	3.18237500	1.89577900
C	-2.36530300	-3.36944500	-0.30510000	H	-5.35861800	-0.21478200	0.14485400	H	-1.86989600	4.84976700	0.82131200
C	0.04595900	-3.11201900	1.35328600	H	-4.13899200	-1.51821600	-1.38385800	H	-1.28718200	2.76778400	-0.25368300
C	0.05759400	-4.48629000	1.04702900	H	-2.31949400	2.31549200	-2.18604500				

[RuCl₂(PPh₃)₂]

Cl	-0.48615900	1.97244800	-2.34703100	C	-3.43289400	2.08814500	0.67024900
Cl	-0.02785800	-2.66391300	-1.49998200	C	-3.72578900	3.36405600	1.14995500
C	-3.04201300	-0.45669300	-1.19248100	P	-1.66924400	0.00270800	-0.07473600
C	-2.69319300	4.25427000	1.44785300	P	1.81219400	-0.01837200	-0.22294100
C	-1.36774900	3.86633600	1.25486700	Ru	0.11903300	-0.24829400	-1.61133500
C	-1.07882500	2.59487900	0.76470200	H	2.43581300	-2.46945300	-1.66214700
C	-2.00304600	-1.00329100	1.42751100	H	4.53946800	-3.47851000	-2.49592400
C	-2.70075000	-0.49022900	2.53247100	H	6.72948900	-2.34212700	-2.07577800
C	-2.95992200	-1.28881200	3.64571600	H	6.77982300	-0.20116700	-0.79144900
C	-2.52686500	-2.61333300	3.68032200	H	4.68790300	0.81437100	0.02423900
C	-1.81845500	-3.12732900	2.59624500	H	2.96284700	1.18701500	2.27378900
C	-1.55050100	-2.33123800	1.48517200	H	1.91667000	2.48716600	-1.71579200
C	-3.59812700	0.50465700	-2.05217400	H	2.72423000	4.75678600	-1.18241100
C	-4.58154700	0.14533700	-2.97075500	H	3.59906100	5.27982800	1.10272800
C	1.54224900	-0.81987900	1.39866800	H	3.71536600	3.46800100	2.81943900
C	1.99811400	-2.11966900	1.65688200	H	2.55417300	-2.67046500	0.89028200
C	1.75964800	-2.72374100	2.89066600	H	2.12600700	-3.74077200	3.07351300
C	-5.00978700	-1.18012900	-3.05942700	H	0.88263700	-2.51385700	4.85906800
C	1.06712500	-2.03806900	3.88850100	H	0.02863200	-0.21003900	4.40676900
C	0.59337600	-0.75120900	3.63871100	H	0.42935400	0.85558000	2.22158900
C	0.81899400	-0.15519400	2.40152400	H	-0.03795700	2.31432800	0.57061100
C	2.35699600	1.67268500	0.24241000	H	-0.54986500	4.56422000	1.46916500
C	2.87937000	1.96957600	1.51221800	H	-2.92512200	5.25805100	1.82332800
C	3.31854700	3.25649900	1.81945800	H	-4.77053300	3.66439600	1.29278600
C	3.25871300	4.26627800	0.85872000	H	-4.25144400	1.39242200	0.44669300
C	2.77023900	3.97592300	-0.41431600	H	-3.04291900	0.54931400	2.54217800
C	2.32386100	2.69088300	-0.72087900	H	-0.96396300	-2.74110600	0.65596200
C	3.40626200	-0.75829500	-0.76182800	H	-1.45044100	-4.16022600	2.61631100
C	-4.44619200	-2.14603000	-2.22530200	H	-2.73438100	-3.24012200	4.55599900
C	4.64150900	-0.13749300	-0.51548300	H	-3.50885100	-0.86532600	4.49543900
C	5.82532900	-0.70655200	-0.98222800	H	-3.03363300	-2.55804500	-0.65079700
C	5.79764800	-1.90404300	-1.69854000	H	-3.25054600	1.54228900	-2.00424100
C	4.57825700	-2.53935400	-1.93090300	H	-5.00855100	0.90934900	-3.63110400
C	3.39325600	-1.97061500	-1.46605300	H	-5.78167800	-1.46304200	-3.78538500
C	-3.46950800	-1.78869800	-1.29758100	H	-4.77076200	-3.19076300	-2.29274500
C	-2.10337000	1.68649000	0.47695900				

Table S8. Cartesian coordinates of the [RuCl₂(PPh₃)₃] complex for the 10 computational models used. For all models, the def2-tzvp basis set was used for Ru, Cl, P and N, while def2-sv(p) was used for the C and H atoms.

M06L

Cl	0.04511300	1.05083200	2.20987500	C	-1.91074900	5.50276800	-0.48536700	H	-0.36473500	-2.62804600	-3.04163300
Cl	-0.03152500	0.83563700	-2.51994400	C	-3.68609400	-3.31485900	-2.72952100	H	-2.28217000	-3.43259600	-4.37261800
C	-2.25058900	2.73403400	-0.16976400	C	-3.86285900	-2.97160500	-1.39020300	H	-4.53495900	-3.67717300	-3.32160800
C	-4.45692500	0.23133600	4.09108000	C	-2.78586700	-2.50071900	-0.64513700	H	-4.85091400	-3.05497400	-0.92275100
C	-3.47525100	-0.65095800	3.64117900	C	-0.26797900	-2.69687300	1.35239400	H	-2.94821700	-2.22684700	0.40581400
C	-2.82443500	-0.41114800	2.43317600	C	-0.97948800	-3.90553500	1.43191600	H	-2.02143800	-1.08217300	2.10959000
C	-3.66265600	0.43362100	-1.14789700	C	-1.04571100	-4.61648100	2.62925200	H	-3.19821200	-1.52450200	4.24290000
C	-4.99646800	0.25991800	-0.74573700	C	-0.38909500	-4.14114800	3.76466600	H	-4.96392500	0.05186700	5.04663800
C	-5.98156000	-0.08246900	-1.67125600	C	0.34503800	-2.95837300	3.68965500	H	-5.55041900	2.05340400	3.67673700
C	-5.65614700	-0.26060600	-3.01493200	C	0.40623800	-2.24238200	2.49459300	H	-4.40939900	2.46203600	1.51380300
C	-4.33235800	-0.10764100	-3.42167900	C	1.33018400	-2.59263200	-0.98301300	H	-5.28249300	0.37968600	0.30386700
C	-3.34350400	0.22684200	-2.49954400	C	-2.16513000	4.69683900	-1.59538400	H	-2.30276000	0.31076000	-2.83032700
C	2.63792000	2.52335800	0.43173400	C	1.83962500	-3.80534200	-0.49136500	H	-4.05476600	-0.26648800	-4.47069000
C	-1.97108800	3.54982600	0.93879000	C	2.96517500	-4.38762900	-1.07204400	H	-6.43332300	-0.52722400	-3.74132800
C	3.86512700	2.99925300	0.91438100	C	3.59873100	-3.77305500	-2.15313600	H	-7.01675300	-0.21028200	-1.33253400
C	4.06176700	4.36122700	1.12506900	C	3.08878800	-2.57917200	-2.66218200	H	-2.53108500	2.70105200	-2.32136900
C	3.03866200	5.26703900	0.83767900	C	1.96404800	-1.99478100	-2.08147200	H	-1.86953000	3.10020900	1.93247400
C	1.81932100	4.80574000	0.34439700	C	-2.33454500	3.32221000	-1.44060500	H	-1.59982900	5.54757100	1.65800800
C	1.61912800	3.43925400	0.14703000	C	-3.15382700	0.69935400	1.64835300	H	-1.78256200	6.58494400	-0.60920000
C	3.66128600	0.61338200	-1.28212200	C	-4.13915200	1.58277800	2.11205400	H	-2.23637900	5.14077000	-2.59498900
C	3.33720300	1.12178400	-2.55058700	C	-4.78438000	1.35169300	3.32619300	H	1.01395800	5.51017100	0.10937100
C	4.26724800	1.09641000	-3.58713300	P	-2.33807200	0.91833100	0.03139800	H	3.19595900	6.34054900	0.99560900
C	5.54382800	0.57424000	-3.37648300	P	2.39774600	0.75437800	0.04661900	H	5.02393700	4.72088300	1.50828700
C	5.88759000	0.09776300	-2.11263300	P	-0.11253800	-1.75174100	-0.21464100	H	4.67770200	2.29197800	1.12608900
C	-1.81286200	4.92465800	0.78125100	Ru	-0.01997200	0.44629400	-0.12882100	H	0.65111800	3.09073500	-0.24526300
C	4.95796600	0.12095700	-1.07300900	H	1.57447600	-1.04927500	-2.47926900	H	6.89485200	-0.29366000	-1.92636400
C	3.14260200	-0.14734900	1.43822000	H	3.57790200	-2.08171600	-3.50839300	H	5.26555900	-0.24103900	-0.08659900
C	3.15961300	0.38755500	2.73469800	H	4.49183500	-4.22694900	-2.59911700	H	6.27501800	0.55218700	-4.19325700
C	3.59182300	-0.38560900	3.81209400	H	3.35673000	-5.32856400	-0.66683200	H	3.98875900	1.49310000	-4.57056700
C	4.00970800	-1.70148800	3.61424200	H	1.37430900	-4.29561500	0.37038400	H	2.33897000	1.53524200	-2.72977100
C	4.00457700	-2.24089900	2.32747000	H	-1.47939900	-4.31342400	0.54700000	H	3.59533300	0.04801500	4.81902400
C	3.57475500	-1.46958800	1.25017900	H	0.96300200	-1.30109500	2.46068500	H	2.81894500	1.41376400	5.90457600
C	-1.50718700	-2.38653700	-1.21308400	H	0.87291100	-2.57609200	4.57115700	H	3.58808300	-1.90305100	0.24424600
C	-1.34703800	-2.71878900	-2.56508300	H	-0.44621400	-4.69788600	4.70776800	H	4.33371900	-3.27286000	2.15530500
C	-2.42855300	-3.17633800	-3.31672600	H	-1.61330400	-5.55363900	2.67087700	H	4.34216500	-2.30818200	4.46504300

B3LYP

Cl	0.04524500	1.21147100	2.20110500	C	-2.28865700	5.53405500	-0.84350500	H	-0.36172300	-3.02074700	-2.84502100
Cl	0.00289700	0.67348500	-2.48986000	C	-3.62523400	-3.84880000	-2.35395700	H	-2.24601600	-4.08810000	-4.00619400
C	-2.38410900	2.75958400	-0.33995100	C	-3.78778200	-3.35518900	-1.05633300	H	-4.46015400	-4.33495300	-2.86813700
C	-4.63470900	0.55903000	4.07680400	C	-2.72104500	-2.73556200	-0.40236800	H	-4.75211700	-3.44600700	-0.54777300
C	-3.64809000	-0.36181700	3.71342500	C	-0.19402700	-2.72306200	1.53412700	H	-2.87401000	-2.37026000	0.61521500
C	-2.96465900	-0.21725000	2.50239000	C	-0.68736300	-4.04332800	1.59760200	H	-2.16876300	-0.91949500	2.25303700
C	-3.69677200	0.33043300	-1.16957900	C	-0.72827300	-4.73692700	2.80918600	H	-3.39164600	-1.18995400	4.38097000
C	-5.04428800	0.19274300	-0.78768400	C	-0.27317900	-4.12816100	3.98479500	H	-5.16442200	0.45332200	5.02892800
C	-6.01381700	-0.21062600	-1.71084600	C	0.22583900	-2.82483300	3.93369400	H	-5.69894600	2.35559100	3.49823600
C	-5.65792200	-0.48555300	-3.03410800	C	0.26627500	-2.12851900	2.71911500	H	-4.50299100	2.59954100	1.35075500
C	-4.32041600	-0.36736100	-3.42123500	C	1.39537800	-2.68538600	-0.85974400	H	-5.35340900	0.39508200	0.23808500
C	-3.34749500	0.02871300	-2.49858200	C	-2.62541700	4.64287600	-1.86674700	H	-2.30515500	0.10410900	-2.81325500
C	2.69055500	2.66905900	-0.00800000	C	2.02645300	-3.79081400	-0.25839100	H	-4.02219700	-0.59202700	-4.44996400
C	-2.02440200	3.66328800	0.67852100	C	3.06939600	-4.46073900	-0.90639700	H	-6.41861400	-0.79678000	-3.75739800
C	3.99794900	3.19277100	-0.03396900	C	3.49566800	-4.04690100	-2.17136200	H	-7.05564300	-0.30756000	-1.38843200
C	4.21560600	4.56864400	-0.11702300	C	2.88531000	-2.94365400	-2.77385400	H	-2.94521700	2.59150400	-2.42996900
C	3.12854100	5.44847600	-0.19008900	C	1.85558700	-2.26062000	-2.11991900	H	-1.76872000	3.28962700	1.67240000
C	1.82806300	4.94113300	-0.17317900	C	-2.67439800	3.26800100	-1.61792500	H	-1.71729700	5.72422000	1.23912400
C	1.61216400	3.56102300	-0.07885800	C	-3.26282900	0.83821500	1.62755900	H	-2.25965600	6.61100900	-1.03797700
C	3.66303200	0.35544700	-1.23382100	C	-4.25409000	1.76202600	2.00643600	H	-2.85722100	5.01697100	-2.86878400
C	3.43415600	0.79679700	-2.55197400	C	-4.93310000	1.62426200	3.22083800	H	0.96746400	5.61314600	-0.23414300
C	4.35792900	0.53158500	-3.56491300	P	-2.39664000	0.94048900	0.00335100	H	3.29851000	6.52743000	-0.26351900
C	5.53171700	-0.17695300	-3.28362900	P	2.42123500	0.84212500	0.05305800	H	5.23946500	4.95558600	-0.13228400
C	5.77309400	-0.61179900	-1.97864100	P	-0.06028300	-1.82801100	-0.08740400	H	4.85775800	2.51907500	0.00735800
C	-1.98694500	5.03853100	0.42959100	Ru	-0.01679300	0.42163100	-0.08090900	H	0.58450800	3.19453100	-0.05793100
C	4.84911100	-0.34522800	-0.96113900	H	1.40405300	-1.38540800	-2.59268300	H	6.69137400	-1.15834200	-1.74085000
C	3.21563400	0.33230300	1.63460800	H	3.22109600	-2.59479800	-3.75457900	H	5.07390800	-0.68259300	0.05127900
C	3.54874500	1.25859200	2.63669200	H	4.30745300	-4.57604900	-2.68051600	H	6.25762800	-0.38159300	-4.07724500
C	4.11435200	0.83357900	3.84284600	H	3.54539800	-5.31655200	-0.41695800	H	4.15870300	0.88678700	-4.58099800
C	4.35687500	-0.52400100	4.07064000	H	1.70840900	-4.14297400	0.72348000	H	2.52335000	1.35005900	-2.78771000
C	4.01714100	-1.45715300	3.08624600	H	-1.03832500	-4.54375300	0.69326900	H	4.36169400	1.57295900	4.61107300
C	3.44405200	-1.03276800	1.88388500	H	0.64000600	-1.10461100	2.70409000	H	3.35594400	2.32152500	2.48488900
C	-1.46342100	-2.60720100	-1.02029500	H	0.58690900	-2.33403700	4.84256000	H	3.17535200	-1.78035700	1.13412900
C	-1.31859900	-3.09743400	-2.32871900	H	-0.30900600	-4.67041700	4.93521800	H	4.19040300	-2.52473100	3.25406100
C	-2.38873500	-3.71029700	-2.98881100	H	-1.11808800	-5.75959000	2.83299600	H	4.80265300	-0.85459700	5.01419200

B3LYP-D3

Cl	0.03945800	1.18811300	2.18243600	C	-2.23527400	5.47708400	-0.83403300	H	-0.29504500	-2.97561700	-2.83126800
Cl	0.00827800	0.64299600	-2.47190900	C	-3.57307800	-3.76524200	-2.40038600	H	-2.17096100	-4.02317200	-4.02616000
C	-2.34365800	2.71369700	-0.33251400	C	-3.75433500	-3.27039300	-1.10923600	H	-4.40312300	-4.24401000	-2.92834600
C	-4.59244400	0.52332700	4.05585000	C	-2.69610200	-2.66157000	-0.43922400	H	-4.72816800	-3.35103800	-0.61843700
C	-3.59729600	-0.38684900	3.70129200	C	-0.20354100	-2.67514700	1.51705800	H	-2.86099900	-2.29062100	0.57553500
C	-2.91268200	-0.24019700	2.49535200	C	-0.71557000	-3.98431700	1.56705000	H	-2.10690100	-0.93371000	2.24769900
C	-3.65386300	0.30327700	-1.15620100	C	-0.76006800	-4.68716900	2.76935800	H	-3.33509800	-1.20912700	4.37308200
C	-4.99325200	0.14743000	-0.76843600	C	-0.29004500	-4.09762600	3.94484500	H	-5.12404300	0.41574500	5.00626700
C	-5.95921300	-0.25785700	-1.68917800	C	0.22721300	-2.80425300	3.90499600	H	-5.67357000	2.30364800	3.47035700
C	-5.60575600	-0.51588600	-3.01316800	C	0.27158400	-2.09820000	2.70062000	H	-4.47128600	2.55250900	1.32559000
C	-4.27419000	-0.38133300	-3.40424600	C	1.40367600	-2.63103400	-0.83380100	H	-5.29588300	0.33543900	0.26296000
C	-3.30451400	0.01628800	-2.48449700	C	-2.53953600	4.58733700	-1.86440900	H	-2.26044200	0.10150000	-2.79701400
C	2.63140000	2.64295600	-0.01601200	C	2.02049300	-3.73569200	-0.22567700	H	-3.97802800	-0.59498600	-4.43548100
C	-2.01394100	3.61373400	0.69385100	C	3.07422900	-4.39816500	-0.85571400	H	-6.36577300	-0.82867700	-3.73588700
C	3.93191300	3.17094400	-0.06547900	C	3.52129600	-3.97771700	-2.10791200	H	-6.99829800	-0.36986300	-1.36422700
C	4.13776700	4.54456800	-0.15772800	C	2.92083000	-2.87713600	-2.71740800	H	-2.84220400	2.53532900	-2.43338000
C	3.04529400	5.41350000	-0.21688500	C	1.88124900	-2.20014600	-2.08090000	H	-1.78494300	3.23671200	1.69384800
C	1.75130800	4.89959600	-0.17629200	C	-2.59493600	3.21628400	-1.61659600	H	-1.72527800	5.67205100	1.26087700
C	1.54685000	3.52229500	-0.07225100	C	-3.22029000	0.80688000	1.61996400	H	-2.20258300	6.55355900	-1.02853200
C	3.61059200	0.33746400	-1.21283700	C	-4.21943600	1.72042100	1.98803900	H	-2.74172800	4.96077900	-2.87258700
C	3.39717900	0.79729400	-2.52337500	C	-4.89934800	1.58007400	3.19759800	H	0.88546800	5.56522800	-0.22706700
C	4.31495600	0.51681500	-3.53268400	P	-2.36200300	0.90819200	0.00688100	H	3.20638500	6.49283000	-0.29847900
C	5.46532500	-0.22376000	-3.25296500	P	2.37450700	0.82850400	0.05720500	H	5.15776500	4.93919800	-0.19179100
C	5.69059900	-0.67501200	-1.95413700	P	-0.05199400	-1.78139300	-0.08736200	H	4.79449000	2.49941500	-0.03588400
C	-1.97040200	4.98522500	0.44508200	Ru	-0.01632800	0.42761900	-0.08479500	H	0.52207500	3.14541700	-0.03082900
C	4.77291200	-0.39377600	-0.94003700	H	1.43249800	-1.32144100	-2.55383300	H	6.59338800	-1.24681100	-1.71854800
C	3.16210000	0.33747800	1.63292500	H	3.27375700	-2.52393000	-3.69014900	H	4.98232600	-0.74347600	0.07230200
C	3.50318100	1.27570500	2.61546200	H	4.34379600	-4.50241900	-2.60344300	H	6.18852400	-0.44044500	-4.04533400
C	4.07081400	0.86604000	3.82171600	H	3.54301800	-5.25524700	-0.36252500	H	4.13000300	0.88605600	-4.54598800
C	4.30696100	-0.48648400	4.06628400	H	1.68030000	-4.09029100	0.74898300	H	2.49984000	1.37587700	-2.75389900
C	3.95816100	-1.43049800	3.10034200	H	-1.07817000	-4.46752400	0.65717900	H	4.32551900	1.61422600	4.57830500
C	3.38230100	-1.02197600	1.89774800	H	0.65599200	-1.07639700	2.68922200	H	3.31327200	2.33705000	2.44510300
C	-1.43122000	-2.54801700	-1.03586000	H	0.59926800	-2.32831100	4.81685800	H	3.10249500	-1.77750600	1.15881300
C	-1.26515900	-3.04027300	-2.33654800	H	-0.32898900	-4.64838300	4.88981800	H	4.12681700	-2.49589000	3.28326400
C	-2.32720100	-3.64135900	-3.01274800	H	-1.16515100	-5.70355100	2.78601200	H	4.75594300	-0.80552200	5.01183600

B3P86

Cl	0.04728400	1.20163700	2.17818600	C	-2.27491600	5.49497600	-0.85600900	H	-0.32184600	-2.99634200	-2.83195000
Cl	-0.00322500	0.64169900	-2.47895700	C	-3.59030700	-3.81407900	-2.36815900	H	-2.19769200	-4.06933900	-4.00457300
C	-2.35547900	2.72843600	-0.34561400	C	-3.76600400	-3.31006300	-1.07850800	H	-4.42012100	-4.30568600	-2.88587000
C	-4.60067300	0.57253900	4.06872400	C	-2.70733100	-2.68540800	-0.42098900	H	-4.73523300	-3.39728200	-0.57845600
C	-3.60917900	-0.34485600	3.71817200	C	-0.20121500	-2.68502900	1.52320600	H	-2.86835800	-2.30975800	0.59275100
C	-2.92541500	-0.20938700	2.50889700	C	-0.71259300	-3.99583800	1.58210200	H	-2.12289000	-0.90815600	2.26506800
C	-3.67181700	0.31010800	-1.15226600	C	-0.75386700	-4.69307400	2.78923200	H	-3.34927800	-1.16400600	4.39560300
C	-5.01274900	0.16405900	-0.76061200	C	-0.28107900	-4.09696900	3.96171800	H	-5.13129900	0.47377300	5.02136700
C	-5.98483500	-0.23844700	-1.67802000	C	0.23575200	-2.80256100	3.91348200	H	-5.67608000	2.35431400	3.47121200
C	-5.63685700	-0.50374900	-3.00324300	C	0.27663700	-2.10218300	2.70419100	H	-4.47781800	2.58271100	1.32236200
C	-4.30432400	-0.37977100	-3.39839800	C	1.39309200	-2.65121700	-0.84646400	H	-5.31289000	0.35769700	0.27071600
C	-3.32854100	0.01449600	-2.48166900	C	-2.58424800	4.59910300	-1.88108700	H	-2.28530900	0.09248000	-2.79885700
C	2.66054200	2.64440300	0.00732600	C	1.99793900	-3.77186800	-0.25221300	H	-4.01215000	-0.59907900	-4.43021500
C	-2.02001900	3.63534400	0.67472900	C	3.03708600	-4.44672800	-0.89576800	H	-6.40146300	-0.81384200	-3.72322400
C	3.96774100	3.16236200	0.00130900	C	3.48307700	-4.02273700	-2.14852600	H	-7.02422700	-0.34243900	-1.34928000
C	4.18912100	4.53547500	-0.07876300	C	2.89667900	-2.90533000	-2.74357500	H	-2.87874000	2.54337500	-2.44191300
C	3.10621100	5.41534900	-0.17023700	C	1.87111300	-2.21676200	-2.09353900	H	-1.77798800	3.26417700	1.67411400
C	1.80633200	4.91195200	-0.17424000	C	-2.62598000	3.22706200	-1.62888900	H	-1.74134500	5.69878700	1.23369200
C	1.58574400	3.53481200	-0.08163600	C	-3.22971200	0.83345000	1.62527600	H	-2.25338300	6.57180700	-1.05354600
C	3.63212200	0.35785600	-1.22506500	C	-4.22598400	1.75412700	1.98970000	H	-2.80177700	4.96821000	-2.88837900
C	3.40317400	0.81717400	-2.53441700	C	-4.90479600	1.62513300	3.20251800	H	0.94898500	5.58666500	-0.25102600
C	4.32818400	0.56929500	-3.54745600	P	-2.37114000	0.92012600	0.00603600	H	3.27931300	6.49412300	-0.24254100
C	5.50248100	-0.13708600	-3.27329500	P	2.39020800	0.82580800	0.05584000	H	5.21394200	4.92072800	-0.07846200
C	5.74407500	-0.58676800	-1.97552300	P	-0.05776700	-1.79235200	-0.08831900	H	4.82449200	2.48425400	0.05459700
C	-1.99060700	5.00774000	0.42190900	Ru	-0.01707500	0.42488100	-0.08766700	H	0.55674900	3.16709800	-0.07696500
C	4.81882100	-0.33847300	-0.95785800	H	1.43189500	-1.32889000	-2.55836100	H	6.66539700	-1.13099600	-1.74338000
C	3.17965900	0.30782000	1.62684200	H	3.24731000	-2.55056200	-3.71723900	H	5.04293300	-0.68469700	0.05283800
C	3.49613300	1.22667600	2.63779200	H	4.29305700	-4.55741800	-2.65527600	H	6.23093500	-0.32790900	-4.06834600
C	4.06821300	0.79634100	3.83618800	H	3.49522100	-5.31597600	-0.41251700	H	4.12984700	0.93777500	-4.55920200
C	4.33329900	-0.55800200	4.04561000	H	1.66120500	-4.12983600	0.72262500	H	2.48938000	1.37143900	-2.76142600
C	4.00794400	-1.48339200	3.05219600	H	-1.07712800	-4.48568200	0.67616200	H	4.30384000	1.52978700	4.61402000
C	3.42757800	-1.05457300	1.85736700	H	0.66145800	-1.08051500	2.68712800	H	3.28459900	2.28845600	2.49634300
C	-1.44628000	-2.56578100	-1.02766900	H	0.61011900	-2.32131300	4.82229800	H	3.16699900	-1.79638100	1.09760600
C	-1.28698300	-3.06589400	-2.32778600	H	-0.31747000	-4.64315200	4.91217000	H	4.19850900	-2.55013900	3.20713200
C	-2.34971000	-3.68179800	-2.99199700	H	-1.15857700	-5.71019100	2.81179900	H	4.78615200	-0.89288900	4.98455000

B3PW91

Cl	0.03528000	1.19377800	2.20068900	C	-2.24757700	5.48555900	-0.81587000	H	-0.30800400	-2.97498800	-2.85099900
Cl	-0.00391700	0.63599800	-2.49155600	C	-3.57706400	-3.76994700	-2.41041300	H	-2.18558100	-4.00953400	-4.04433200
C	-2.37758600	2.72421000	-0.32166000	C	-3.75109400	-3.28947500	-1.11509400	H	-4.41011700	-4.24002700	-2.93983300
C	-4.60401000	0.49033800	4.06440500	C	-2.68987200	-2.69074400	-0.44504700	H	-4.72254500	-3.37196100	-0.62162400
C	-3.61150000	-0.41326200	3.69536900	C	-0.19245600	-2.69880000	1.51167200	H	-2.85048900	-2.33039500	0.57240100
C	-2.93612400	-0.25398800	2.48788600	C	-0.70594800	-4.00452200	1.57653500	H	-2.13160400	-0.94339000	2.23346500
C	-3.69050200	0.31456200	-1.15940300	C	-0.74842600	-4.69561500	2.78277200	H	-3.34317000	-1.24094500	4.35683600
C	-5.03032700	0.16652300	-0.77733200	C	-0.27300500	-4.09761200	3.94986500	H	-5.12927400	0.37310600	5.01626700
C	-5.99451500	-0.23982100	-1.69669300	C	0.24724100	-2.80884900	3.89642100	H	-5.68897700	2.27306000	3.50309600
C	-5.63917600	-0.50634200	-3.01608400	C	0.28798000	-2.11491900	2.68662300	H	-4.50374300	2.54182300	1.35742300
C	-4.30849000	-0.37696600	-3.40358500	C	1.41343100	-2.65762400	-0.84389000	H	-5.33844800	0.36203800	0.24912100
C	-3.34157000	0.02163500	-2.48408800	C	-2.55922400	4.60233500	-1.84642800	H	-2.30029800	0.10295000	-2.79829300
C	2.64591600	3.52391000	-0.00261900	C	2.03334300	-3.75914100	-0.23797000	H	-4.01015400	-0.59625900	-4.43212300
C	-2.04293200	3.61893900	0.70460200	C	3.09311700	-4.41374500	-0.86186800	H	-6.39757900	-0.82079400	-3.73857400
C	3.93797800	3.20256800	-0.02230400	C	3.54644100	-3.98723400	-2.10724100	H	-7.03398900	-0.34582400	-1.37395500
C	4.12930800	4.57672500	-0.10142000	C	2.94366700	-2.89031900	-2.71595900	H	-2.87435300	2.55847200	-2.42120300
C	3.02918600	5.43179900	-0.17711200	C	1.89557000	-2.22431800	-2.08586300	H	-1.81704500	3.24072500	1.70313000
C	1.74335600	4.90296500	-0.16759200	C	-2.62502800	3.23287500	-1.60161200	H	-1.73583500	5.67077700	1.27665500
C	1.55478200	3.52391000	-0.07697700	C	-3.24936400	0.79785200	1.62390600	H	-2.20489600	6.56136600	-1.06074600
C	3.64470000	0.36947200	-1.22345900	C	-4.24531900	1.70449500	2.00855600	H	-2.75761300	4.97913700	-2.85317400
C	3.40794500	0.80272800	-2.53634500	C	-4.91660600	1.55319000	3.21904400	H	0.87117300	5.55751100	-0.23141800
C	4.32654900	0.54267400	-3.54748600	P	-2.39904200	0.91578000	0.00741100	H	3.17866400	6.51276900	-0.24752500
C	5.50253600	-0.15259900	-3.26758100	P	2.40551200	0.84075000	0.05259900	H	5.14404400	4.98364700	-0.11207800
C	5.75202100	-0.57754000	-1.96694200	C	-0.04496600	-1.81420600	-0.09588900	H	4.80783200	2.54301600	0.02031200
C	-1.98770100	4.98875800	0.46002900	Ru	-0.01490000	0.42932200	-0.08595000	H	0.53438600	3.13841500	-0.06005200
C	4.83252800	-0.31507200	-0.95140200	H	1.44575600	-1.35233800	-2.56415700	H	6.67482000	-1.11443000	-1.73062300
C	3.19090200	0.33381800	1.62520300	H	3.30099300	-2.53087300	-3.68383100	H	5.06206700	-0.64554300	0.06130100
C	3.51026400	1.25322900	2.62891800	H	4.37525400	-4.50443200	-2.59835400	H	6.22635400	-0.35471500	-0.46210600
C	4.06772400	0.82641800	3.83199200	H	3.56285400	-5.26879100	-0.36804500	H	4.12136400	0.89116200	-4.56332500
C	4.31419000	-0.52598300	4.05289200	H	1.69495100	-4.11860300	0.73351000	H	2.49044900	1.34484200	-2.76959300
C	3.98846700	-1.45257400	3.06510900	H	-1.07255000	-4.49600800	0.67440800	H	4.30546900	1.56610100	4.60541000
C	3.42474800	-1.02545300	1.86584100	H	0.67798800	-1.09804700	2.66801600	H	3.31017200	2.31455500	2.48070700
C	-1.42965600	-2.57099100	-1.04465300	H	0.62550700	-2.32605100	4.80109600	H	3.16620300	-1.76848400	1.10894900
C	-1.27186500	-3.04827300	-2.34927400	H	-0.30946900	-4.63967900	4.89899600	H	4.16597400	-2.51890200	3.22847100
C	-2.33618900	-3.64069400	-3.02621700	H	-1.15549900	-5.71000000	2.81005700	H	4.75418300	-0.85882000	4.99698100

CAM-B3LYP

Cl	0.03185500	1.03175600	2.21820900	C	-1.61593600	5.46185100	-0.42318100	H	-0.38724500	-2.49027700	-3.09517400
Cl	-0.06728400	0.80094300	-2.52206700	C	-3.71160200	-3.17080900	-2.78153800	H	-2.33085900	-3.22003900	-4.44508600
C	-2.20685000	2.74019300	-0.13320500	C	-3.87518800	-2.88529200	-1.42874400	H	-4.56844600	-3.50401700	-3.37973700
C	-4.48626500	0.25461400	4.09107100	C	-2.78894900	-2.45590600	-0.67542700	H	-4.86125800	-2.97887900	-0.95785200
C	-3.49726500	-0.61997900	3.64932800	C	-0.28466500	-2.73930000	1.29591700	H	-2.93501400	-2.21872300	0.38895500
C	-2.84847000	-0.38274800	2.44154500	C	-0.97046200	-3.96306300	1.33327800	H	-2.03371300	-1.04374000	2.11920300
C	-3.72457600	0.49475300	-1.13581700	C	-1.00297400	-4.71964300	2.50101400	H	-3.21087300	-1.48545000	4.25767600
C	-5.04946000	0.28379400	-0.72366900	C	-0.34085800	-4.27314300	3.64360400	H	-4.99073400	0.07605900	5.04828600
C	-6.03571300	-0.05329100	-1.64760200	C	0.36269600	-3.07246300	3.60933700	H	-5.59827700	2.06308000	3.67097900
C	-5.72330700	-0.18772600	-2.99758200	C	0.39208100	-2.30838600	2.44449300	H	-4.45796400	2.47065800	1.50108800
C	-4.40915800	-0.00079600	-3.41392900	C	1.32621500	-2.59367600	-1.01093000	H	-5.32734600	0.36389300	0.33194700
C	-3.41654000	0.32253100	-2.49462300	C	-1.86469100	4.67789800	-1.54762300	H	-2.37975500	0.41620200	-2.83527200
C	2.65220400	2.49738800	0.50506100	C	1.83533500	-3.81337300	-0.54010900	H	-4.13964400	-0.12934900	-4.46940600
C	-1.93370400	3.53266900	0.99292200	C	2.99614100	-4.34976100	-1.09001800	H	-6.50409700	-0.44917800	-3.72210700
C	3.88406600	2.91878900	1.02147700	C	3.66631500	-3.68190500	-2.11468300	H	-7.06420700	-0.21250300	-1.30129500
C	4.12436500	4.26577700	1.26195900	C	3.15480500	-2.48409100	-2.60749500	H	-2.34345600	2.71589600	-2.29952000
C	3.14155700	5.20956400	0.96538700	C	1.99161800	-1.94696600	-2.06098600	H	-1.93058600	3.07674700	1.98964500
C	1.92065100	4.80290800	0.43472200	C	-2.15995500	3.32515400	-1.40651500	H	-1.44492900	5.49511400	1.73461400
C	1.67117100	3.44998000	0.20996900	C	-3.19181900	0.71912400	1.65335300	H	-1.38976000	6.52926100	-0.53790300
C	3.64636700	0.63508300	-1.26353700	C	-4.18372400	1.59756700	2.10971800	H	-1.83126400	5.12286000	-2.54885500
C	3.30981700	1.17496400	-2.51354000	C	-4.82577900	1.36727100	3.32260900	H	1.15146900	5.54306900	0.18810600
C	4.22052300	1.15029200	-3.56462500	P	-2.39136300	0.93504200	0.04038400	H	3.33284500	6.27434000	1.14465800
C	5.48873300	0.60122500	-3.38292400	P	2.39116400	0.75295000	0.06466000	H	5.08900000	4.58530500	1.67381200
C	5.84789500	0.10444700	-2.13296100	P	-0.11370300	-1.77038700	-0.23840200	H	4.66506100	2.17406800	1.23314900
C	-1.65042800	4.88640500	0.84595000	Ru	-0.02423100	0.48172100	-0.12544300	H	0.70003800	3.14743400	-0.22100300
C	4.93812400	0.12538600	-1.07820700	H	1.60505400	-0.99181500	-2.43858800	H	6.85328600	-0.30209400	-1.96984200
C	3.10711600	-0.21200100	1.42118900	H	3.67355400	-1.94016000	-3.40869700	H	5.25259500	-0.25673200	-0.10074900
C	3.08767600	0.25292600	2.74364700	H	4.59143500	-4.09953900	-2.52987300	H	6.20551500	0.57788000	-4.21258300
C	3.46425400	-0.58741400	3.78878200	H	3.38938100	-5.29793600	-0.70360000	H	3.93495100	1.56993600	-4.53655300
C	3.86675900	-1.89657900	3.53247000	H	1.34623000	-4.34246300	0.28491800	H	2.31744200	1.61632200	-2.66290300
C	3.91086700	-2.36139700	2.21939300	H	-1.47293700	-4.34158100	0.43534500	H	3.43940200	-0.21070700	4.81822900
C	3.53621400	-1.52473400	1.17340300	H	0.92858800	-1.35252400	2.43574300	H	2.75225100	1.27432900	2.95645500
C	-1.51684300	-2.33294000	-1.25265100	H	0.89382800	-2.71242000	4.49893200	H	3.59742700	-1.89485800	0.14269600
C	-1.36906200	-2.59934400	-2.61835300	H	-0.37209600	-4.86884300	4.56401400	H	4.23932900	-3.38503700	2.00079700
C	-2.46217600	-3.01138300	-3.37671200	H	-1.54803700	-5.67102600	2.51629400	H	4.15797200	-2.55492900	4.36001200

MN12-L

Cl	0.04300900	1.19136600	2.17657000	C	-2.19472800	5.48064600	-0.83164400	H	-0.30032600	-2.96643500	-2.84059100
Cl	0.00937600	0.64626900	-2.47059500	C	-3.58486400	-3.73478500	-2.42295500	H	-2.17926500	-3.99894700	-4.04440200
C	-2.32979000	2.72000400	-0.32773900	C	-3.76756200	-3.24186100	-1.13172200	H	-4.41669200	-4.20594100	-2.95541900
C	-4.57825500	0.51896900	4.05996500	C	-2.70782900	-2.64203000	-0.45673000	H	-4.74439200	-3.31535100	-0.64524700
C	-3.58551600	-0.39080700	3.69951200	C	-0.22008500	-2.67251200	1.50759600	H	-2.87432700	-2.27062000	0.55791800
C	-2.90407000	-0.23967800	2.49289700	C	-0.74750400	-3.97495000	1.55977600	H	-2.09889100	-0.93246600	2.24059900
C	-3.65394900	0.31755900	-1.15365500	C	-0.79803800	-4.67503000	2.76303200	H	-3.32208300	-1.21656000	4.36706400
C	-4.99370200	0.17054200	-0.76513500	C	-0.31784400	-4.08992300	3.93624000	H	-5.10791400	0.40818600	5.01131500
C	-5.96159600	-0.23226200	-1.68439800	C	0.21610900	-2.80387200	3.89376000	H	-5.65820700	2.30330400	3.48548300
C	-5.60977300	-0.49610500	-3.00726400	C	0.26563800	-2.10025600	2.68867800	H	-4.46103700	2.56003800	1.33832400
C	-4.27802300	-0.37009500	-3.39895300	C	1.39281700	-2.63420900	-0.83700200	H	-5.29529200	0.36260000	0.26611100
C	-3.30635600	0.02474600	-2.48074000	C	-2.49077700	4.59183000	-1.86466400	H	-2.26155200	0.10179800	-2.79348700
C	2.63911000	2.62973000	-0.00806200	C	1.99953700	-3.74508200	-0.23078100	H	-3.98286800	-0.58975100	-4.42944900
C	-2.00910100	3.61897100	0.70190100	C	3.05532200	-4.40780200	-0.85619500	H	-6.37171400	-0.80736500	-3.72891900
C	3.94274800	3.15060200	-0.03742700	C	3.51396700	-3.98192600	-2.10202200	H	-7.00139000	-0.33783500	-1.35897800
C	4.15691800	4.52256900	-0.12789500	C	2.92227500	-2.87658500	-2.71038500	H	-2.79889200	2.54136700	-2.43537000
C	3.07009200	5.39651900	-0.20609300	C	1.88054600	-2.19946000	-0.87282700	H	-1.79640400	3.24184200	1.70562600
C	1.77335800	4.88974300	-0.18639100	C	-2.55939300	3.22015100	-1.61574100	H	-1.71262000	5.67582000	1.26957700
C	1.56012600	3.51387200	-0.08368200	C	-3.21249800	0.81104400	1.62295500	H	-2.15093900	6.55670800	-1.02747200
C	3.61335100	0.32820400	-1.20811300	C	-4.20890100	1.72458300	1.99701100	H	-2.67564600	4.96516800	-2.87637800
C	3.40430100	0.79477700	-2.51651600	C	-4.88565100	1.57927200	3.20736500	H	0.91179100	5.55994400	-0.25227600
C	4.32418700	0.51783800	-3.52429800	P	-2.35772600	0.91417800	0.00864300	H	3.23810400	6.47507100	-0.28665100
C	5.47276400	-0.22493800	-3.24473400	P	2.37376500	0.81630700	0.05969900	H	5.17941400	4.91222600	-0.14600100
C	5.69441600	-0.68141200	-1.94760600	P	-0.06069000	-1.77802100	-0.09479400	H	4.80117500	2.47393600	0.00644900
C	-1.95211400	4.98931700	0.45157400	Ru	-0.01536800	0.43095000	-0.08707900	H	0.53228000	3.14312500	-0.05915400
C	4.77434500	-0.40419500	-0.93501500	H	1.43841500	-1.31674800	-2.55033400	H	6.59640600	-1.25482400	-1.71198800
C	3.15439200	0.31603400	1.63573400	H	3.28459000	-2.51872400	-3.67824800	H	4.98112600	-0.75834800	0.07655900
C	3.48638400	1.24740400	2.62732200	H	4.33901200	-4.50668400	-2.59373000	H	6.19795100	-0.43896100	-0.43627000
C	4.04467300	0.82926500	3.83451800	H	3.51706700	-5.26956700	-0.36412600	H	4.14241800	0.89188300	-4.53662100
C	4.27981800	-0.52449300	4.07106700	H	1.65112700	-4.10294100	0.74020700	H	2.50839100	1.37633800	-2.74638400
C	3.94029700	-1.46157500	3.09576300	H	-1.11779300	-4.45477600	0.65078900	H	4.29245300	1.57207500	4.59891500
C	3.37430400	-1.04471100	1.89182500	H	0.66274600	-1.08317200	2.67431500	H	3.29535300	2.30989300	2.46333900
C	-1.44062300	-2.53540900	-1.04885300	H	0.59759300	-2.33156700	4.80395100	H	3.10038900	-1.79513300	1.14517900
C	-1.27284800	-3.02612700	-2.34942300	H	-0.36154900	-4.63916700	4.88211400	H	4.10775100	-2.52847700	3.27239000
C	-2.33636700	-3.61828800	-3.03048400	H	-1.21590800	-5.68635800	2.78234700	H	4.72114000	-0.84996000	5.01825900

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Cl	0.05063600	1.19890800	2.18692600	C	-2.20419800	5.52799800	-0.84968700	H	-0.33735300	-2.96318400	-2.86550700
Cl	0.01890000	0.68455200	-2.48198800	C	-3.63342200	-3.77130800	-2.41056300	H	-2.23499400	-4.01033200	-4.06328700
C	-2.32963000	2.74772400	-0.33637900	C	-3.80516000	-3.28720000	-1.10401000	H	-4.47377400	-4.24946800	-2.94064100
C	-4.59567000	0.54429300	4.09064500	C	-2.73570200	-2.67881000	-0.43127700	H	-4.78260700	-3.37478400	-0.60215500
C	-3.60369200	-0.37945900	3.72445300	C	-0.21924400	-2.69808800	1.52160000	H	-2.89401500	-2.31568500	0.59636300
C	-2.91730600	-0.23082900	2.50924900	C	-0.73175600	-4.01772300	1.56624100	H	-2.11315000	-0.93494900	2.24977400
C	-3.66439700	0.32963700	-1.15758200	C	-0.78087200	-4.72661100	2.77634800	H	-3.34453800	-1.21538100	4.39497600
C	-5.01326500	0.18136200	-0.76439800	C	-0.31590500	-4.13439300	3.96333800	H	-5.12953200	0.43533700	5.04950000
C	-5.98842300	-0.22132100	-1.69084800	C	0.20212900	-2.83064400	3.92766400	H	-5.67019300	2.35042700	3.51559300
C	-5.63588600	-0.48376500	-3.02423800	C	0.25093700	-2.11783500	2.71691600	H	-4.46326000	2.60497200	1.35282600
C	-4.29502300	-0.35603100	-3.41960000	C	1.38670200	-2.65137500	-0.85805100	H	-5.31516000	0.37425300	0.27539000
C	-3.31488100	0.03844700	-2.49530300	C	-2.50981200	4.62979600	-1.88537300	H	-2.26148000	0.11719800	-2.80954100
C	2.66082100	2.64302500	-0.01216300	C	2.00649300	-3.76987200	-0.25557000	H	-3.99894800	-0.57464300	-4.45907100
C	-1.99965300	3.65581400	0.69637200	C	3.05599900	-4.44092700	-0.90452700	H	-6.40460800	-0.79523300	-3.75135900
C	3.97658000	3.15982700	-0.04901600	C	3.49502200	-4.01681400	-2.16885000	H	-7.03597000	-0.32829600	-1.36211400
C	4.19846900	4.54065500	-0.14470100	C	2.89201300	-2.90170800	-2.77122100	H	-2.82246200	2.56294500	-2.45448900
C	3.10920600	5.42691500	-0.22003800	C	1.85846800	-2.21383700	-2.11602000	H	-1.77526100	3.27742400	1.70602500
C	1.80048400	4.92318800	-0.19130500	C	-2.57410900	3.25069600	-1.63247400	H	-1.70137800	5.72915100	1.26238700
C	1.57849900	3.53956100	-0.08375400	C	-3.21903600	0.83271400	1.63596100	H	-2.16361700	6.61196500	-1.04938700
C	3.63279100	0.31598700	-1.20878100	C	-4.21538400	1.75993100	2.01435800	H	-2.70632800	5.00374700	-2.90384900
C	3.43553800	0.79747600	-2.52482300	C	-4.89713400	1.61599100	3.23386500	H	0.93519900	5.60281400	-0.25392100
C	4.36122800	0.50764100	-3.53744900	P	-2.35345600	0.92921800	0.00979500	H	3.28425300	6.51254700	-0.30476700
C	5.50302400	-0.26260200	-3.25631900	P	2.38273900	0.81683300	0.06437100	H	5.23106100	4.92728000	-0.16838200
C	5.71180200	-0.73502300	-1.95179500	P	-0.06995800	-1.78542500	-0.09309600	H	4.83821800	2.47411500	-0.00596200
C	-1.94805200	5.03552800	0.44117700	Ru	-0.01638500	0.42385300	-0.08695700	H	0.54248100	3.16816600	-0.05207200
C	4.78689900	-0.44626000	-0.93372800	H	1.41137700	-1.31821500	-2.57953100	H	6.60910800	-1.33088100	-1.71441500
C	3.17005400	0.31905400	1.65416200	H	3.24079500	-2.54341200	-3.75339200	H	4.98372800	-0.81397500	0.08402600
C	3.52399800	1.26261300	2.64144400	H	4.31496000	-4.54945100	-2.67902100	H	6.23322800	-0.48641300	-4.05214200
C	4.08733900	0.84591200	3.85804400	H	3.52843600	-5.30937100	-0.41538800	H	4.18890400	0.89390700	-4.55601000
C	4.30737800	-0.51792900	4.10915900	H	1.66991900	-4.12971800	3.23804200	H	2.54412000	1.40041700	-2.75582900
C	3.94667500	-1.46622000	3.13834800	H	-1.09092600	-4.50414000	0.64650100	H	4.35155200	1.59898700	4.61906600
C	3.37427900	-1.05203200	1.92488300	H	0.63366200	-1.08604100	2.70697500	H	3.34742900	2.33408300	2.46574100
C	-1.46710100	-2.55560000	-1.04218600	H	0.57237900	-2.35168600	4.84921100	H	3.08128900	-1.81214300	1.18358500
C	-1.31066000	-3.03634700	-2.35935300	H	-0.35933600	-4.69117900	4.91451700	H	4.10184000	-2.54174300	3.32610700
C	-2.38447100	-3.63667200	-3.03650000	H	-1.18702300	-5.75197100	2.78937300	H	4.75304400	-0.84244500	5.06430800

PBE

Cl	0.03624500	1.20812100	2.21815100	C	-1.99753300	5.47959600	-0.76908000	H	-0.38178700	-2.79279300	-2.92586200
Cl	0.03522500	0.73188400	-2.47399000	C	-3.66475200	-3.53584200	-2.47165900	H	-2.30553200	-3.71347000	-4.14269600
C	-2.31336600	2.73246900	-0.28616500	C	-3.80659900	-3.12794400	-1.14680900	H	-4.52009800	-3.94854900	-3.01388600
C	-4.54088100	0.39883900	4.07013700	C	-2.71882200	-2.59642200	-0.46125600	H	-4.77351600	-3.20986600	-0.64372500
C	-3.54338000	-0.48991300	3.67257100	C	-0.21927200	-2.67391400	1.46440400	H	-2.85728900	-2.28625000	0.57695300
C	-2.88157200	-0.29671500	2.46227000	C	-0.72562400	-3.98428400	1.50060700	H	-2.07168900	-0.97207000	2.18469300
C	-3.65181500	0.33999300	-1.16162900	C	-0.78557600	-4.68977400	2.69903800	H	-3.25976400	-1.32972100	4.31293500
C	-4.99275100	0.17605200	-0.78704400	C	-0.33229400	-4.10206500	3.88240300	H	-5.05509500	0.25725400	5.02523200
C	-5.94527900	-0.23829000	-1.71633100	C	0.18302200	-2.80873900	3.85456400	H	-5.64658400	2.18663900	3.56036900
C	-5.57633500	-0.49419300	-3.03586800	C	0.23850200	-2.09986800	2.65345000	H	-4.48333000	2.51355400	1.40300100
C	-4.24330000	-0.34781300	-3.41393600	C	1.38554500	-2.60312400	-0.88528700	H	-5.30903900	0.35802700	0.24107500
C	-3.28738700	0.05659200	-2.48477000	C	-2.29722500	4.61244700	-1.81908500	H	-2.24190000	0.14448000	-2.78776400
C	2.64691100	2.60304700	-0.02666200	C	2.03980400	-3.67837800	-0.26740400	H	-3.93409800	-0.56294500	-4.44055900
C	-1.99701300	3.60921700	0.76243000	C	3.11300200	-4.31237600	-0.89302900	H	-6.32537700	-0.81681600	-3.76506000
C	3.95194700	3.11753000	-0.05997200	C	3.53612000	-3.89735400	-2.15419100	H	-6.98591700	-0.36116000	-1.40196400
C	4.17198700	4.48607800	-0.17733800	C	2.89414200	-2.82905400	-2.77672100	H	-2.68640500	2.58485900	-2.41567100
C	3.08812300	5.36179200	-0.27719200	C	1.84205500	-2.17559800	-2.14032200	H	-1.84960000	3.22022500	1.77238300
C	1.78927600	4.86094300	-0.25413400	C	-2.45557500	3.24860800	-1.58023600	H	-1.60311100	5.64233500	1.35229900
C	1.57076800	3.48863400	-0.12629600	C	-3.21391700	0.77224500	1.62608600	H	-1.87499200	6.55022500	-0.95824500
C	3.60077900	0.24602000	-1.16143400	C	-4.21360700	1.66407000	2.03651300	H	-2.40993900	4.99808400	-2.83608700
C	3.44691100	0.73277700	-2.46900900	C	-4.87174700	1.47925000	3.25131700	H	0.93100600	5.53241500	-0.33740100
C	4.36077000	0.39683100	-3.46286700	P	-2.37049800	0.92518700	0.01538800	H	3.26029200	6.43724000	-0.37946000
C	5.44789300	-0.42818400	-3.16823400	P	2.36820600	0.79757300	0.08056300	H	5.19501200	4.87251800	-0.19957400
C	5.61357300	-0.90757500	-1.87178600	P	-0.06420900	-1.76486500	-0.12405200	H	4.80667000	2.43756400	0.00181400
C	-1.84810000	4.97355000	0.52230300	Ru	-0.01339500	0.45444500	-0.07496100	H	0.53883800	3.12917400	-0.10527500
C	4.69882600	-0.57017500	-0.87316000	H	1.37621500	-1.31050600	-2.61889100	H	6.46463000	-1.54912800	-1.62547000
C	3.11470000	0.30747800	1.67229700	H	3.23196200	-2.47406000	-3.75366400	H	4.86234700	-0.94855200	0.13678300
C	3.49318100	1.23809000	2.64541600	H	4.37526000	-4.39817500	-2.64578900	H	6.16834200	-0.69091600	-3.94854600
C	4.00290300	0.81100100	3.87074500	H	3.61449900	-5.14393500	-0.38939200	H	4.22353900	0.78839200	-4.47487800
C	4.14140900	-0.54967600	4.14154900	H	1.72278400	-4.03037900	0.71600900	H	2.60088400	1.37975000	-2.71066600
C	3.75748400	-1.48508800	3.18152400	H	-1.07274200	-4.46623500	0.58379700	H	4.28675000	1.55207300	4.62317200
C	3.24211300	-1.05675500	1.96050900	H	0.61777200	-1.07730400	2.65325600	H	3.37052700	2.30680700	2.45966800
C	-1.46624600	-2.47141800	-1.07769600	H	0.54465800	-2.33398400	4.77077500	H	2.93016500	-1.80217500	1.22575500
C	-1.33898400	-2.87575600	-2.41071700	H	-0.38335700	-4.65555500	4.82481000	H	3.84781900	-2.55613600	3.38368600
C	-2.42944500	-3.40310500	-3.10132400	H	-1.18953600	-5.70617500	2.70842200	H	4.54253200	-0.88138800	5.10377700

WB97X-D

Cl	0.03949900	1.22274200	2.20655100	C	-1.99487800	5.48791400	-0.79871800	H	-0.39574700	-2.82038200	-2.91469000
Cl	0.04161300	0.76644400	-2.45072600	C	-3.67788400	-3.55639400	-2.44516300	H	-2.32222300	-3.75394800	-4.11671100
C	-2.30771100	2.74338800	-0.29654700	C	-3.81616800	-3.13418100	-1.12430800	H	-4.53460300	-3.97503900	-2.98066400
C	-4.53427600	0.42349400	4.06815100	C	-2.76423000	-2.59633500	-0.44697000	H	-4.78172400	-3.21098700	-0.61776800
C	-3.53939800	-0.46927900	3.67288100	C	-0.22196100	-2.67527800	1.46593600	H	-2.86186300	-2.27670600	0.58881900
C	-2.87580300	-0.27999500	2.46302000	C	-0.71497000	-3.99089700	1.49720500	H	-2.06815900	-0.95859600	2.18687000
C	-3.63489100	0.34183400	-1.16080000	C	-0.77601400	-4.69901600	2.69400000	H	-3.25940500	-1.30930100	4.31458000
C	-4.97702000	0.18512400	-0.78755900	C	-0.33810900	-4.10826700	3.88166300	H	-5.05002500	0.28501600	5.02286700
C	-5.92915800	-0.23392100	-1.71515900	C	0.16256300	-2.80912700	3.85955100	H	-5.63323300	2.21426100	3.55459000
C	-5.55851800	-0.50197800	-3.03172000	C	-0.21958100	-2.09815600	2.65959500	H	-4.46662500	2.53420200	1.39800200
C	-4.22439900	-0.36231900	-3.40862300	C	1.37408600	-2.60098800	-0.89146000	H	-5.29477400	0.37635500	0.23840200
C	-3.26918200	0.04750700	-2.48117000	C	-2.30791800	4.61500100	-1.84003600	H	-2.22349700	0.13315500	-2.78364500
C	2.65427900	2.59534400	-0.03142100	C	2.03450800	-3.67568700	-0.27974900	H	-3.91404900	-0.58634000	-4.43298200
C	-1.97996100	3.62632900	0.74333200	C	3.10038600	-4.31150900	-0.91641600	H	-6.30707100	-0.82865200	-3.75960700
C	3.96465900	3.09616500	-0.06537800	C	3.50933100	-3.89899400	-2.18291300	H	-6.97069300	-0.35122800	-1.40167000
C	4.19939500	4.46170700	-0.18908300	C	2.86221400	-2.82996500	-2.79909700	H	-2.70568000	2.58464600	-2.42075200
C	3.12526400	5.34862500	-0.29495600	C	1.81835000	-2.17459500	-2.15143300	H	-1.82214100	3.24371800	1.75414900
C	1.82111400	4.86166400	-0.27159000	C	-2.46486200	3.25271200	-1.59164400	H	-1.57836100	5.66255500	1.31746600
C	1.58820900	3.49230900	-0.13733200	C	-3.20340200	0.78888700	1.62491600	H	-1.87295000	6.55724000	-0.99545200
C	3.58724200	0.22652000	-1.15599000	C	-4.20033500	1.68475500	2.03299400	H	-2.43160600	4.99484800	-2.85794300
C	3.44926500	0.72328500	-2.46161500	C	-4.86046900	1.50380900	3.24740300	H	0.96983500	5.54150900	-0.35984000
C	4.36259200	0.37759800	-3.45256800	P	-2.35613900	0.93633200	0.01502300	H	3.30902000	6.42166100	-0.40226100
C	5.43415500	-0.46709900	-3.15714900	P	2.35831900	0.79212500	0.08471700	H	5.22659100	4.83692500	-0.21166800
C	5.58435600	-0.95680300	-1.86274000	P	-0.07074700	-1.76029800	-0.12138900	H	4.81214500	2.40766900	0.00103700
C	-1.83246600	4.98923400	0.49391100	Ru	-0.01298100	0.45936700	-0.06753300	H	0.55211700	3.14478900	-0.11753500
C	4.66973300	-0.61008500	-0.86721800	H	1.34911500	-1.30893200	-2.62560500	H	6.42255900	-1.61463200	-1.61549100
C	3.10605300	0.30486300	1.67779400	H	3.18960500	-2.47652700	-3.78013700	H	4.82199300	-0.99747400	0.14098700
C	3.50077100	1.23753700	2.64250600	H	4.34205400	-4.40168300	-2.68347700	H	6.15442800	-0.93721800	-3.93508000
C	4.01171600	0.81312200	3.86830700	H	3.60666200	-5.14289300	-0.41726500	H	4.23747600	0.77769300	-4.46282200
C	4.13524000	-0.54713000	4.14822900	H	1.72751300	-4.02690500	0.70716800	H	2.61758800	1.38805600	-2.70409900
C	3.73474400	-1.48453100	3.19700100	H	-1.05114800	-4.47470700	0.57721400	H	4.30836700	1.55606200	4.61392400
C	3.21827500	-1.05858300	1.97564200	H	0.58806900	-1.07160800	2.66370500	H	3.39023000	2.30639800	2.45009100
C	-1.47528900	-2.47692600	-1.06761500	H	0.51160300	-2.33170300	4.77928400	H	2.89383700	-1.80551300	1.24795100
C	-1.35185500	-2.89638800	-2.39631700	H	-0.39010800	-4.66369200	4.82288300	H	3.81279600	-2.55517000	3.40631600
C	-2.44400500	-3.43113500	-3.07883900	H	-1.16903600	-5.71975900	2.69887100	H	4.53736100	-0.87681900	5.11072200