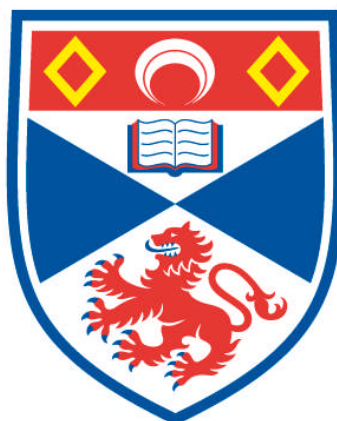


**UNDERSTANDING THE ORIGIN OF $^{35/37}\text{Cl}$ AND $^{16/18}\text{O}$
ISOTOPE EFFECTS ON ^{195}Pt AND ^{103}Rh NMR NUCLEAR
SHIELDING IN SELECTED Pt(IV) AND Rh(III)
COMPLEXES : A DFT STUDY**

Appendix B

John Christopher Davis

**A Thesis Submitted for the Degree of PhD
at the
University of St Andrews**



2013

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Appendix B

This appendix includes further raw data pertinent to the thesis. This data was used to generate the data in the Tables A.1-A.18 in Appendix A and the labelling of the isotopomers correspond to that shown in Figures 4.3 and 5.3-5.8.

Table B.1: Vibrationally averaged geometries at 0K for the $^{35/37}\text{Cl}$ isotopologues and isotopomers^a of $[\text{PtCl}_5(\text{H}_2^{16}\text{O})]^-$ calculated at the PBE0/SDD/6-31G* level [in Å].

Ref.Geom.	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009338	-0.000005	-0.053750
O	-0.585025	0.000289	-2.126413
H	-1.179878	0.778807	-2.076094
H	-1.180863	-0.777472	-2.076012
Cl	-1.662237	1.674202	0.130041
Cl	1.603329	1.655378	-0.471874
Cl	-1.664415	-1.672053	0.130125
Cl	1.601185	-1.657486	-0.471770
Cl	0.493469	-0.000233	2.175002

Vib.Av.Geom.A	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009340	-0.000006	-0.053518
O	-0.584125	0.000289	-2.137486
H	-1.169335	0.772629	-2.096492
H	-1.170304	-0.771312	-2.096394
Cl	-1.665294	1.676015	0.132277
Cl	1.605896	1.657825	-0.473057
Cl	-1.667472	-1.673858	0.132360
Cl	1.603748	-1.659935	-0.472953
Cl	0.493420	-0.000232	2.177846

Vib.Av.Geom.B1	Coordinates (Angstroms)		
	X	Y	Z

Pt	0.009286	-0.000044	-0.053593
O	-0.583944	-0.000277	-2.137618
H	-1.169835	0.771533	-2.096777
H	-1.169439	-0.772391	-2.096618
Cl	-1.665013	1.676127	0.132569
Cl	1.605762	1.657956	-0.472586
Cl	-1.667483	-1.673932	0.132410
Cl	1.603680	-1.660053	-0.473090
Cl	0.493418	0.000101	2.177702

Vib.Av.Geom.B2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009300	0.000095	-0.053523
O	-0.583863	0.000717	-2.137564
H	-1.169515	0.772702	-2.096430
H	-1.169616	-0.771220	-2.096907
Cl	-1.665606	1.675890	0.132636
Cl	1.606121	1.657629	-0.473228
Cl	-1.666764	-1.674025	0.131950
Cl	1.603284	-1.660407	-0.472728
Cl	0.493487	0.000074	2.177814

Vib.Av.Geom.C

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009348	-0.000006	-0.053601
O	-0.584153	0.000289	-2.137592
H	-1.169356	0.772624	-2.096590
H	-1.170325	-0.771307	-2.096491
Cl	-1.665274	1.675971	0.132434
Cl	1.605895	1.657900	-0.472933
Cl	-1.667452	-1.673814	0.132518
Cl	1.603747	-1.660010	-0.472829
Cl	0.493357	-0.000232	2.177648

Vib.Av.Geom.D1

	Coordinates (Angstroms)		
	X	Y	Z

Pt	0.009303	-0.000006	-0.053573
O	-0.584307	0.000290	-2.137488
H	-1.169511	0.772622	-2.096417
H	-1.170479	-0.771305	-2.096319
Cl	-1.665174	1.676195	0.132211
Cl	1.606058	1.657725	-0.472915
Cl	-1.667352	-1.674038	0.132295
Cl	1.603910	-1.659835	-0.472811
Cl	0.493492	-0.000232	2.177743

Vib.Av.Geom.D2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009430	-0.000009	-0.053513
O	-0.582560	0.000288	-2.137788
H	-1.167796	0.772609	-2.097457
H	-1.168754	-0.771304	-2.097368
Cl	-1.665685	1.675300	0.132675
Cl	1.605626	1.658194	-0.473314
Cl	-1.667858	-1.673137	0.132757
Cl	1.603469	-1.660294	-0.473208
Cl	0.493174	-0.000231	2.177892

Vib.Av.Geom.D3

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009294	-0.000166	-0.053611
O	-0.583930	-0.000697	-2.137648
H	-1.169155	0.771634	-2.097218
H	-1.170024	-0.772337	-2.096286
Cl	-1.664355	1.676342	0.132143
Cl	1.605314	1.658479	-0.472341
Cl	-1.667728	-1.673811	0.132747
Cl	1.603834	-1.659927	-0.473249
Cl	0.493393	-0.000164	2.177686

Vib.Av.Geom.E

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009252	-0.000017	-0.053529
O	-0.584021	0.000141	-2.137547

H	-1.169493	0.772270	-2.096715
H	-1.169946	-0.771653	-2.096522
Cl	-1.665357	1.675987	0.132678
Cl	1.605979	1.657535	-0.472813
Cl	-1.667184	-1.673847	0.131930
Cl	1.603767	-1.660104	-0.473022
Cl	0.493535	0.000372	2.177749

Vib.Av.Geom.F1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009276	0.000089	-0.053617
O	-0.583893	0.000679	-2.137674
H	-1.168584	0.773404	-2.096888
H	-1.170580	-0.770519	-2.096675
Cl	-1.665362	1.676068	0.132404
Cl	1.605910	1.657918	-0.473222
Cl	-1.667118	-1.674019	0.132646
Cl	1.603538	-1.660097	-0.472427
Cl	0.493435	-0.000639	2.177617

Vib.Av.Geom.F2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009288	0.000102	-0.053539
O	-0.583824	0.000766	-2.137602
H	-1.169466	0.772753	-2.096471
H	-1.169576	-0.771168	-2.096991
Cl	-1.665609	1.675910	0.132657
Cl	1.606130	1.657627	-0.473244
Cl	-1.666725	-1.674055	0.131984
Cl	1.603270	-1.660415	-0.472671
Cl	0.493496	0.000017	2.177672

Vib.Av.Geom.G1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009289	-0.000130	-0.053590

O	-0.583759	-0.000115	-2.137668
H	-1.168489	0.772589	-2.097204
H	-1.170394	-0.771342	-2.096498
Cl	-1.664647	1.676150	0.132036
Cl	1.605415	1.658355	-0.472715
Cl	-1.667793	-1.673652	0.132898
Cl	1.603867	-1.659783	-0.472968
Cl	0.493415	-0.000532	2.177728

Vib.Av.Geom.G2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009192	-0.000070	-0.053670
O	-0.584995	-0.000013	-2.137528
H	-1.170342	0.772202	-2.096272
H	-1.170975	-0.771739	-2.096060
Cl	-1.664933	1.676265	0.132347
Cl	1.606213	1.657460	-0.472329
Cl	-1.667323	-1.674099	0.132238
Cl	1.604152	-1.659550	-0.472717
Cl	0.493611	0.000140	2.177555

Vib.Av.Geom.H1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009281	-0.000134	-0.053613
O	-0.583688	-0.000154	-2.137727
H	-1.168423	0.772543	-2.097316
H	-1.170309	-0.771389	-2.096578
Cl	-1.664634	1.676152	0.132083
Cl	1.605410	1.658359	-0.472672
Cl	-1.667807	-1.673657	0.132923
Cl	1.603867	-1.659789	-0.472995
Cl	0.493432	-0.000465	2.177647

Vib.Av.Geom.H2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009286	-0.000182	-0.053635

O	-0.583868	-0.000739	-2.137708
H	-1.169074	0.771604	-2.097325
H	-1.169973	-0.772368	-2.096356
Cl	-1.664319	1.676360	0.132174
Cl	1.605290	1.658494	-0.472286
Cl	-1.667765	-1.673798	0.132799
Cl	1.603865	-1.659910	-0.473287
Cl	0.493402	-0.000129	2.177599

Vib.Av.Geom.H3

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009282	-0.000006	-0.053603
O	-0.584324	0.000290	-2.137541
H	-1.169523	0.772621	-2.096473
H	-1.170491	-0.771304	-2.096375
Cl	-1.665154	1.676231	0.132246
Cl	1.606095	1.657686	-0.472889
Cl	-1.667332	-1.674074	0.132330
Cl	1.603948	-1.659796	-0.472785
Cl	0.493499	-0.000232	2.177666

Vib.Av.Geom.I

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009243	0.000019	-0.053553
O	-0.583949	0.000426	-2.137607
H	-1.168915	0.772948	-2.096711
H	-1.170374	-0.770975	-2.096723
Cl	-1.665029	1.675991	0.131872
Cl	1.605924	1.657999	-0.473125
Cl	-1.667528	-1.673833	0.132799
Cl	1.603818	-1.659666	-0.472676
Cl	0.493565	-0.000841	2.177660

Vib.Av.Geom.J

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009296	-0.000006	-0.053610
O	-0.583948	0.000289	-2.137645

H	-1.169149	0.772621	-2.096761
H	-1.170117	-0.771304	-2.096664
Cl	-1.665068	1.676046	0.132364
Cl	1.605786	1.657953	-0.472858
Cl	-1.667245	-1.673889	0.132448
Cl	1.603638	-1.660062	-0.472753
Cl	0.493380	-0.000232	2.177716

Vib.Av.Geom.K1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009424	-0.000009	-0.053538
O	-0.582504	0.000288	-2.137844
H	-1.167737	0.772607	-2.097544
H	-1.168696	-0.771302	-2.097455
Cl	-1.665706	1.675286	0.132706
Cl	1.605632	1.658192	-0.473298
Cl	-1.667879	-1.673123	0.132788
Cl	1.603476	-1.660292	-0.473192
Cl	0.493225	-0.000231	2.177807

Vib.Av.Geom.K2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009187	-0.000099	-0.053688
O	-0.584852	-0.000096	-2.137596
H	-1.170191	0.772130	-2.096446
H	-1.170867	-0.771792	-2.096163
Cl	-1.664766	1.676388	0.132353
Cl	1.606052	1.657610	-0.472258
Cl	-1.667293	-1.674160	0.132290
Cl	1.604089	-1.659633	-0.472811
Cl	0.493585	0.000176	2.177507

Vib.Av.Geom.L

	Coordinates (Angstroms)		
	X	Y	Z

Pt	0.009288	-0.000006	-0.053636
O	-0.583874	0.000289	-2.137710
H	-1.169070	0.772621	-2.096864
H	-1.170038	-0.771304	-2.096767
Cl	-1.665062	1.676053	0.132406
Cl	1.605784	1.657959	-0.472858
Cl	-1.667240	-1.673897	0.132490
Cl	1.603636	-1.660069	-0.472754
Cl	0.493383	-0.000232	2.177657

^aSee Figure 4.3 for an explanation of the labelling scheme.

Table B.2: Vibrationally averaged geometries at 0K for the ^{35/37}Cl isotopologues and isotopomers^a of [PtCl₅(H₂¹⁸O)]⁻ calculated at the PBE0/SDD/6-31G* level [in Å].

Ref.Geom.			
	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009338	-0.000005	-0.053750
O	-0.585025	0.000289	-2.126413
H	-1.179878	0.778807	-2.076094
H	-1.180863	-0.777472	-2.076012
Cl	-1.662237	1.674202	0.130041
Cl	1.603329	1.655378	-0.471874
Cl	-1.664415	-1.672053	0.130125
Cl	1.601185	-1.657486	-0.471770
Cl	0.493469	-0.000233	2.175002

Vib.Av.Geom.A			
	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009291	-0.000006	-0.053452
O	-0.583883	0.000289	-2.136829
H	-1.169166	0.772685	-2.096285
H	-1.170135	-0.771369	-2.096187
Cl	-1.665232	1.676129	0.132176
Cl	1.605763	1.657943	-0.473191
Cl	-1.667411	-1.673972	0.132260
Cl	1.603616	-1.660053	-0.473087
Cl	0.493649	-0.000232	2.178232

Vib.Av.Geom.B1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009278	-0.000046	-0.053525
O	-0.584018	-0.000350	-2.136936
H	-1.169643	0.771778	-2.096491
H	-1.169910	-0.772256	-2.095989
Cl	-1.665100	1.676097	0.132483
Cl	1.605818	1.657975	-0.472665
Cl	-1.667522	-1.673931	0.132248
Cl	1.603603	-1.660044	-0.473262
Cl	0.493593	0.000173	2.178094

Vib.Av.Geom.B2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009282	0.000046	-0.053477
O	-0.583995	0.001353	-2.136862
H	-1.169546	0.773512	-2.095567
H	-1.169963	-0.770530	-2.096788
Cl	-1.665909	1.675713	0.132420
Cl	1.606300	1.657450	-0.473421
Cl	-1.666853	-1.673933	0.131981
Cl	1.603411	-1.660325	-0.472762
Cl	0.493688	0.000131	2.178219

Vib.Av.Geom.C

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009281	-0.000006	-0.053431
O	-0.583838	0.000289	-2.136890
H	-1.169120	0.772679	-2.096360
H	-1.170089	-0.771364	-2.096263
Cl	-1.665231	1.676148	0.132186
Cl	1.605780	1.657914	-0.473200
Cl	-1.667410	-1.673991	0.132270
Cl	1.603633	-1.660023	-0.473096
Cl	0.493634	-0.000232	2.177978

Vib.Av.Geom.D1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009314	-0.000006	-0.053453
O	-0.583921	0.000289	-2.136847
H	-1.169184	0.772689	-2.096263
H	-1.170153	-0.771373	-2.096166
Cl	-1.664990	1.676184	0.132051
Cl	1.605641	1.658133	-0.473168
Cl	-1.667168	-1.674028	0.132135
Cl	1.603493	-1.660243	-0.473063
Cl	0.493617	-0.000232	2.178215

Vib.Av.Geom.D2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009272	-0.000010	-0.053497
O	-0.583629	0.000287	-2.136988
H	-1.168938	0.772648	-2.096541
H	-1.169892	-0.771347	-2.096458
Cl	-1.665556	1.675708	0.132418
Cl	1.605952	1.657821	-0.473133
Cl	-1.667728	-1.673543	0.132499
Cl	1.603792	-1.659917	-0.473026
Cl	0.493587	-0.000231	2.178121

Vib.Av.Geom.D3

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009297	-0.000055	-0.053576
O	-0.584088	-0.000398	-2.137001
H	-1.169166	0.772149	-2.096723
H	-1.170542	-0.771858	-2.095788
Cl	-1.665348	1.675630	0.132094
Cl	1.606116	1.657755	-0.472646
Cl	-1.668113	-1.673241	0.132856
Cl	1.604256	-1.659462	-0.473275
Cl	0.493577	-0.000430	2.178065

Vib.Av.Geom.E

	Coordinates			(Angstroms)		
	X	Y	Z	X	Y	Z
Pt	0.009268	-0.000072	-0.053457			
O	-0.584001	0.000424	-2.136879			
H	-1.169374	0.772728	-2.096164			
H	-1.170158	-0.771319	-2.096280			
Cl	-1.665278	1.676117	0.132470			
Cl	1.605705	1.657642	-0.472914			
Cl	-1.667151	-1.673921	0.131842			
Cl	1.603617	-1.660217	-0.473173			
Cl	0.493705	0.000466	2.178177			

Vib.Av.Geom.F1

	Coordinates			(Angstroms)		
	X	Y	Z	X	Y	Z
Pt	0.009280	0.000043	-0.053516			
O	-0.583891	0.000408	-2.137014			
H	-1.168952	0.772952	-2.096467			
H	-1.170368	-0.771057	-2.096226			
Cl	-1.665526	1.675844	0.132363			
Cl	1.605956	1.657731	-0.473349			
Cl	-1.667690	-1.673601	0.132510			
Cl	1.603931	-1.659768	-0.472673			
Cl	0.493614	-0.000593	2.177882			

Vib.Av.Geom.F2

	Coordinates			(Angstroms)		
	X	Y	Z	X	Y	Z
Pt	0.009272	0.000039	-0.053471			
O	-0.584046	0.001210	-2.136939			
H	-1.169549	0.773397	-2.095712			
H	-1.170066	-0.770622	-2.096706			
Cl	-1.665956	1.675591	0.132528			
Cl	1.606402	1.657237	-0.473329			
Cl	-1.667088	-1.673798	0.131977			
Cl	1.603695	-1.660134	-0.472830			
Cl	0.493671	0.000226	2.177931			

Vib.Av.Geom.G1

	Coordinates			(Angstroms)		
	X	Y	Z	X	Y	Z
Pt	0.009262	-0.000064	-0.053517			
O	-0.583876	0.000021	-2.136970			
H	-1.168796	0.772680	-2.096649			
H	-1.170416	-0.771387	-2.096129			
Cl	-1.664800	1.676193	0.131902			
Cl	1.605508	1.658335	-0.472878			
Cl	-1.667545	-1.673836	0.132739			
Cl	1.603666	-1.659972	-0.473028			
Cl	0.493593	-0.000583	2.178119			

Vib.Av.Geom.G2

	Coordinates			(Angstroms)		
	X	Y	Z	X	Y	Z
Pt	0.009303	-0.000131	-0.053547			
O	-0.584095	-0.000391	-2.136944			
H	-1.169454	0.771943	-2.096547			
H	-1.170197	-0.772126	-2.095927			
Cl	-1.664610	1.676297	0.132319			
Cl	1.605465	1.658279	-0.472545			
Cl	-1.667446	-1.673947	0.132164			
Cl	1.603662	-1.660152	-0.473286			
Cl	0.493554	0.000246	2.178115			

Vib.Av.Geom.H1

	Coordinates			(Angstroms)		
	X	Y	Z	X	Y	Z
Pt	0.009274	-0.000010	-0.053486			
O	-0.583534	0.000287	-2.137055			
H	-1.168845	0.772641	-2.096635			
H	-1.169800	-0.771340	-2.096550			
Cl	-1.665615	1.675671	0.132445			
Cl	1.605975	1.657739	-0.473153			
Cl	-1.667788	-1.673506	0.132526			
Cl	1.603815	-1.659835	-0.473045			
Cl	0.493585	-0.000231	2.177920			

Vib.Av.Geom.H2

	Coordinates			(Angstroms)		
	X	Y	Z	X	Y	Z
Pt	0.009277	-0.000053	-0.053563			
O	-0.584054	-0.000358	-2.137061			
H	-1.169133	0.772183	-2.096769			
H	-1.170508	-0.771813	-2.095889			
Cl	-1.665373	1.675570	0.132092			
Cl	1.606228	1.657717	-0.472642			
Cl	-1.668130	-1.673255	0.132897			
Cl	1.604266	-1.659397	-0.473293			
Cl	0.493574	-0.000403	2.177841			

Vib.Av.Geom.H3

	Coordinates			(Angstroms)		
	X	Y	Z	X	Y	Z
Pt	0.009304	-0.000006	-0.053432			
O	-0.583823	0.000289	-2.136899			
H	-1.169083	0.772686	-2.096361			
H	-1.170052	-0.771370	-2.096264			
Cl	-1.664908	1.676282	0.132046			
Cl	1.605556	1.658204	-0.473181			
Cl	-1.667086	-1.674126	0.132130			
Cl	1.603408	-1.660314	-0.473077			
Cl	0.493604	-0.000232	2.177999			

Vib.Av.Geom.I

	Coordinates			(Angstroms)		
	X	Y	Z	X	Y	Z
Pt	0.009256	0.000072	-0.053445			
O	-0.583958	0.000158	-2.136937			
H	-1.169130	0.772645	-2.096462			
H	-1.170316	-0.771396	-2.096133			
Cl	-1.664978	1.676106	0.131725			
Cl	1.605756	1.658105	-0.473308			
Cl	-1.667455	-1.673971	0.132587			
Cl	1.603573	-1.659728	-0.472752			
Cl	0.493733	-0.001001	2.177949			

Vib.Av.Geom.J

	Coordinates	(Angstroms)	
	X	Y	Z
Pt	0.009307	-0.000006	-0.053541
O	-0.583946	0.000289	-2.136981
H	-1.169220	0.772676	-2.096371
H	-1.170188	-0.771361	-2.096274
Cl	-1.665124	1.676030	0.132257
Cl	1.605714	1.657978	-0.472994
Cl	-1.667302	-1.673873	0.132341
Cl	1.603566	-1.660088	-0.472889
Cl	0.493537	-0.000232	2.178124

Vib.Av.Geom.K1

	Coordinates	(Angstroms)	
	X	Y	Z
Pt	0.009262	-0.000066	-0.053506
O	-0.583816	0.000026	-2.137042
H	-1.168703	0.772704	-2.096730
H	-1.170385	-0.771354	-2.096204
Cl	-1.664772	1.676188	0.131876
Cl	1.605501	1.658326	-0.472896
Cl	-1.667575	-1.673854	0.132789
Cl	1.603627	-1.659873	-0.473002
Cl	0.493599	-0.000629	2.177902

Vib.Av.Geom.K2

	Coordinates	(Angstroms)	
	X	Y	Z
Pt	0.009298	-0.000160	-0.053530
O	-0.584016	-0.000526	-2.137000
H	-1.169321	0.771845	-2.096716
H	-1.170159	-0.772226	-2.095927
Cl	-1.664398	1.676451	0.132342
Cl	1.605269	1.658384	-0.472436
Cl	-1.667442	-1.674054	0.132116
Cl	1.603613	-1.660218	-0.473381
Cl	0.493558	0.000358	2.177894

Vib.Av.Geom.L			
	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.009296	-0.000006	-0.053530
O	-0.583901	0.000289	-2.137042
H	-1.169173	0.772672	-2.096450
H	-1.170141	-0.771356	-2.096353
Cl	-1.665114	1.676056	0.132276
Cl	1.605724	1.657957	-0.472997
Cl	-1.667292	-1.673900	0.132360
Cl	1.603576	-1.660067	-0.472892
Cl	0.493524	-0.000232	2.177900

^aSee Figure 4.3 for an explanation of the labelling scheme.

Table B.3: Vibrationally averaged geometries at 0K for the ^{35/37}Cl isotopologues and isotopomers^a of *cis*-PtCl₄(H₂¹⁶O)₂ calculated at the PBE0/SDD/6-31G* level [in Å].

Ref.Geom.			
	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000000	0.000000	0.110409
Cl	0.243887	-1.651336	-1.436112
Cl	-2.311950	-0.309799	0.260916
Cl	-0.243880	1.651341	-1.436108
Cl	2.311949	0.309798	0.260925
O	0.284392	-1.496071	1.603178
H	1.261402	-1.544002	1.660629
O	-0.284403	1.496063	1.603182
H	-1.261415	1.543988	1.660623
H	0.009372	2.329092	1.186228
H	-0.009385	-2.329094	1.186214

Vib.Av.Geom.A			
	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000000	0.000001	0.109591
Cl	0.244538	-1.651558	-1.440091
Cl	-2.314451	-0.313891	0.261245
Cl	-0.244533	1.651561	-1.440085

Cl	2.314450	0.313891	0.261256
O	0.280004	-1.500327	1.613066
H	1.238825	-1.589941	1.657419
O	-0.280010	1.500312	1.613062
H	-1.238861	1.589916	1.657423
H	0.061115	2.312963	1.238272
H	-0.061126	-2.312964	1.238247

Vib.Av.Geom.B

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000018	-0.000031	0.109633
Cl	0.244108	-1.651629	-1.440023
Cl	-2.314325	-0.313354	0.260613
Cl	-0.245087	1.651300	-1.440261
Cl	2.314553	0.314170	0.261735
O	0.280600	-1.500478	1.612814
H	1.239466	-1.588482	1.658198
O	-0.279312	1.500090	1.613398
H	-1.238119	1.591460	1.656561
H	0.064004	2.312522	1.239740
H	-0.058558	-2.313298	1.236957

Vib.Av.Geom.C

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000174	0.000114	0.109755
Cl	0.243443	-1.651194	-1.440321
Cl	-2.314078	-0.314504	0.260329
Cl	-0.245594	1.651193	-1.440216
Cl	2.314780	0.313355	0.262164
O	0.280455	-1.500325	1.613140
H	1.239331	-1.589945	1.657014
O	-0.279488	1.501294	1.612459
H	-1.238268	1.591408	1.656874
H	0.061952	2.313516	1.237032
H	-0.060874	-2.312795	1.238132

Vib.Av.Geom.D

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000000	0.000001	0.109706
Cl	0.244618	-1.651583	-1.439896
Cl	-2.314453	-0.313619	0.260714
Cl	-0.244612	1.651586	-1.439891
Cl	2.314452	0.313619	0.260725
O	0.280080	-1.500490	1.613133
H	1.238907	-1.590001	1.657383
O	-0.280086	1.500476	1.613129
H	-1.238944	1.589975	1.657387
H	0.060942	2.313087	1.238188
H	-0.060953	-2.313088	1.238163

Vib.Av.Geom.E

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.000180	-0.000045	0.109806
Cl	0.246028	-1.650838	-1.440424
Cl	-2.314734	-0.313763	0.262350
Cl	-0.243383	1.651241	-1.440272
Cl	2.314105	0.313647	0.259902
O	0.278894	-1.500887	1.612959
H	1.237656	-1.592764	1.656045
O	-0.280920	1.500571	1.612969
H	-1.239809	1.588833	1.657849
H	0.058669	2.313170	1.236986
H	-0.064822	-2.312955	1.238860

Vib.Av.Geom.F

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000000	0.000001	0.109805
Cl	0.244203	-1.651235	-1.440149
Cl	-2.314368	-0.314208	0.261140
Cl	-0.244198	1.651238	-1.440144
Cl	2.314367	0.314208	0.261152

O	0.279875	-1.500950	1.612723
H	1.238682	-1.591478	1.656283
O	-0.279880	1.500935	1.612718
H	-1.238714	1.591452	1.656286
H	0.062355	2.313117	1.237797
H	-0.062366	-2.313120	1.237772

Vib.Av.Geom.G

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.000146	-0.000135	0.109716
Cl	0.245548	-1.651415	-1.440012
Cl	-2.314808	-0.313018	0.261998
Cl	-0.243305	1.651392	-1.440132
Cl	2.314016	0.314314	0.260154
O	0.279654	-1.501157	1.612583
H	1.238449	-1.590605	1.657325
O	-0.280839	1.500020	1.613253
H	-1.239745	1.588666	1.657632
H	0.059462	2.312867	1.238272
H	-0.061028	-2.313552	1.236951

Vib.Av.Geom.H

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000033	0.000123	0.109852
Cl	0.244266	-1.651284	-1.439901
Cl	-2.314322	-0.314991	0.260680
Cl	-0.244268	1.651795	-1.439632
Cl	2.314455	0.313124	0.260468
O	0.279496	-1.500394	1.613272
H	1.238321	-1.591161	1.656663
O	-0.280183	1.501417	1.612341
H	-1.239009	1.589418	1.658048
H	0.058692	2.313844	1.235499
H	-0.063075	-2.312708	1.238829

Vib.Av.Geom.I

	Coordinates (Angstroms)		
	X	Y	Z

Pt	0.000000	0.000001	0.109914
Cl	0.244308	-1.651329	-1.439901
Cl	-2.314370	-0.313896	0.260548
Cl	-0.244302	1.651332	-1.439896
Cl	2.314370	0.313896	0.260559
O	0.279809	-1.501017	1.612804
H	1.238621	-1.590536	1.657192
O	-0.279815	1.501001	1.612799
H	-1.238655	1.590509	1.657195
H	0.061083	2.313328	1.237202
H	-0.061095	-2.313331	1.237177

^aSee Figure 4.3 for an explanation of the labelling scheme.

Table B.4: Vibrationally averaged geometries at 0K for the ^{35/37}Cl isotopologues and isotopomers^a of *cis*-PtCl₄(H₂¹⁸O)₂ calculated at the PBE0/SDD/6-31G* level [in Å].

Vib.Av.Geom.A

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000000	0.000000	0.109300
Cl	0.243976	-1.651677	-1.440228
Cl	-2.314392	-0.314222	0.261809
Cl	-0.243970	1.651681	-1.440224
Cl	2.314391	0.314222	0.261820
O	0.280214	-1.499608	1.612677
H	1.239110	-1.586720	1.659159
O	-0.280221	1.499600	1.612682
H	-1.239149	1.586699	1.659163
H	0.057799	2.313039	1.237067
H	-0.057810	-2.313034	1.237046

Vib.Av.Geom.B

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000042	0.000045	0.109306
Cl	0.243207	-1.651654	-1.440151
Cl	-2.314161	-0.313936	0.260807
Cl	-0.245135	1.651489	-1.440435
Cl	2.314644	0.313955	0.262912
O	0.281387	-1.499554	1.612578
H	1.240386	-1.585026	1.659316
O	-0.279325	1.499592	1.612838

H	-1.238182	1.589665	1.657391
H	0.062278	2.312536	1.238828
H	-0.055025	-2.313285	1.236399

Vib.Av.Geom.C

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000008	-0.000021	0.109395
Cl	0.244090	-1.651551	-1.440149
Cl	-2.314333	-0.314101	0.261304
Cl	-0.244679	1.651603	-1.440209
Cl	2.314494	0.313984	0.261948
O	0.280431	-1.499562	1.612841
H	1.239374	-1.587802	1.657918
O	-0.279826	1.499867	1.612544
H	-1.238691	1.588966	1.657724
H	0.060623	2.312873	1.237818
H	-0.059177	-2.312754	1.237906

Vib.Av.Geom.D

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000000	0.000000	0.109204
Cl	0.244683	-1.651700	-1.440205
Cl	-2.314413	-0.313559	0.262150
Cl	-0.244677	1.651703	-1.440201
Cl	2.314412	0.313559	0.262161
O	0.280247	-1.499771	1.612406
H	1.239160	-1.587444	1.658188
O	-0.280254	1.499763	1.612411
H	-1.239199	1.587421	1.658192
H	0.058566	2.313043	1.237051
H	-0.058578	-2.313038	1.237031

Vib.Av.Geom.E

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.000157	-0.000010	0.109269
Cl	0.245981	-1.651553	-1.440291
Cl	-2.314833	-0.313750	0.263434

Cl	-0.243486	1.651932	-1.439961
Cl	2.314070	0.313270	0.261110
O	0.279840	-1.500092	1.612189
H	1.238733	-1.588922	1.657318
O	-0.281407	1.500091	1.611976
H	-1.240425	1.585826	1.658443
H	0.055266	2.313455	1.235245
H	-0.060320	-2.313084	1.237232

Vib.Av.Geom.F

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000000	0.000000	0.109510
Cl	0.244566	-1.651431	-1.440193
Cl	-2.314461	-0.313809	0.261429
Cl	-0.244561	1.651435	-1.440189
Cl	2.314460	0.313808	0.261441
O	0.280344	-1.499810	1.612701
H	1.239243	-1.588505	1.657645
O	-0.280351	1.499803	1.612705
H	-1.239278	1.588484	1.657648
H	0.059768	2.312863	1.237873
H	-0.059779	-2.312860	1.237852

Vib.Av.Geom.G

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.000147	-0.000103	0.109254
Cl	0.245754	-1.651865	-1.440123
Cl	-2.314794	-0.312906	0.263209
Cl	-0.243399	1.651650	-1.440118
Cl	2.314006	0.314230	0.261251
O	0.279913	-1.500613	1.611763
H	1.238788	-1.588828	1.657527
O	-0.281159	1.499537	1.612455
H	-1.240168	1.586828	1.657685
H	0.057588	2.312827	1.237067
H	-0.059285	-2.313518	1.235918

Vib.Av.Geom.H			
	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000033	0.000107	0.109326
Cl	0.244708	-1.651593	-1.440229
Cl	-2.314317	-0.314723	0.261827
Cl	-0.244724	1.652017	-1.439751
Cl	2.314488	0.312903	0.261576
O	0.279601	-1.499032	1.613136
H	1.238493	-1.589529	1.656925
O	-0.280249	1.500215	1.612303
H	-1.239134	1.587914	1.658412
H	0.058354	2.313289	1.236401
H	-0.062811	-2.312023	1.239817

Vib.Av.Geom.I			
	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000000	0.000000	0.109346
Cl	0.244726	-1.651532	-1.440249
Cl	-2.314366	-0.313742	0.261817
Cl	-0.244720	1.651536	-1.440244
Cl	2.314365	0.313742	0.261829
O	0.279733	-1.499601	1.612823
H	1.238583	-1.589258	1.657556
O	-0.279740	1.499593	1.612826
H	-1.238618	1.589235	1.657560
H	0.061368	2.312530	1.238456
H	-0.061381	-2.312527	1.238435

^aSee Figure 4.3 for an explanation of the labelling scheme.

Table B.5: Vibrationally averaged geometries at 0K for the ^{35/37}Cl isotopologues and isotopomers^a of *cis*-PtCl₄(H₂¹⁸O) (H₂¹⁶O) calculated at the PBE0/SDD/6-31G* level [in Å].

Vib.Av.Geom.A			
	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.000114	-0.00019	0.109445
Cl	0.244811	-1.651674	-1.440134

Cl	-2.314551	-0.313363	0.261564
Cl	-0.2445	1.651736	-1.440013
Cl	2.314362	0.314215	0.261648
O	0.280318	-1.500218	1.613069
H	1.239191	-1.587354	1.659228
O	-0.28002	1.49993	1.612156
H	-1.238918	1.58998	1.656244
H	0.061738	2.312659	1.237816
H	-0.057668	-2.31338	1.237066

Vib.Av.Geom.B

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000029	-0.00017	0.109462
Cl	0.244292	-1.651779	-1.440091
Cl	-2.314419	-0.313048	0.261016
Cl	-0.245122	1.651561	-1.440074
Cl	2.314462	0.314356	0.262051
O	0.280516	-1.50028	1.613
H	1.239377	-1.587926	1.658774
O	-0.279734	1.499823	1.612343
H	-1.238626	1.590108	1.656266
H	0.062295	2.312428	1.237933
H	-0.058163	-2.313366	1.237344

Vib.Av.Geom.C

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000119	-0.000044	0.109515
Cl	0.243708	-1.651614	-1.440081
Cl	-2.314117	-0.314034	0.260561
Cl	-0.245715	1.651624	-1.439814
Cl	2.31476	0.31359	0.262375
O	0.280324	-1.499983	1.613184
H	1.239205	-1.586651	1.65981
O	-0.279731	1.500658	1.611837
H	-1.238591	1.591158	1.655841
H	0.062306	2.312953	1.236822

H	-0.057044	-2.313226	1.236898
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Vib.Av.Geom.D

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.000112	-0.000195	0.109563
Cl	0.24469	-1.65141	-1.440293
Cl	-2.314483	-0.313324	0.26121
Cl	-0.244502	1.651566	-1.44005
Cl	2.314374	0.313927	0.261394
O	0.280349	-1.500143	1.613291
H	1.239234	-1.587417	1.659088
O	-0.279993	1.500116	1.612152
H	-1.238864	1.590581	1.656098
H	0.062203	2.31264	1.237714
H	-0.057937	-2.313332	1.237562

Vib.Av.Geom.E

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.000161	-0.000358	0.10955
Cl	0.246144	-1.651146	-1.4406
Cl	-2.315033	-0.312416	0.262925
Cl	-0.243287	1.65107	-1.440147
Cl	2.313835	0.314727	0.260436
O	0.279048	-1.500946	1.613064
H	1.237817	-1.590071	1.658511
O	-0.28109	1.499638	1.612396
H	-1.240074	1.587226	1.657682
H	0.057781	2.312652	1.236556
H	-0.060988	-2.313647	1.237611

Vib.Av.Geom.F

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.000038	-0.000244	0.109677
Cl	0.244533	-1.651464	-1.44008
Cl	-2.31451	-0.313378	0.261265
Cl	-0.244252	1.651399	-1.439966

Cl	2.31426	0.314849	0.261164
O	0.279723	-1.500868	1.612903
H	1.238524	-1.589984	1.658031
O	-0.279987	1.50026	1.612092
H	-1.238874	1.590471	1.656053
H	0.061865	2.312714	1.237278
H	-0.060413	-2.313342	1.237062

Vib.Av.Geom.G

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.000168	-0.000282	0.109602
Cl	0.245228	-1.651186	-1.440507
Cl	-2.314639	-0.312896	0.261758
Cl	-0.244043	1.651129	-1.440106
Cl	2.314126	0.314534	0.261173
O	0.279763	-1.500815	1.613034
H	1.238574	-1.589069	1.65875
O	-0.279827	1.5001	1.612292
H	-1.238707	1.590351	1.65642
H	0.061887	2.312553	1.237362
H	-0.059375	-2.313623	1.237159

Vib.Av.Geom.H

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.00012	-0.000224	0.109683
Cl	0.244639	-1.651204	-1.440279
Cl	-2.314415	-0.31394	0.261492
Cl	-0.244	1.651593	-1.439849
Cl	2.314285	0.314114	0.261002
O	0.279535	-1.500479	1.613262
H	1.238357	-1.588744	1.658951
O	-0.280187	1.500691	1.611735
H	-1.239063	1.591067	1.655524
H	0.061901	2.312931	1.236654
H	-0.059607	-2.313263	1.23732

Vib.Av.Geom.I

	Coordinates (Angstroms)		
	X	Y	Z

Pt	-0.000119	-0.000236	0.109625
Cl	0.244496	-1.651435	-1.440215
Cl	-2.314499	-0.31338	0.261244
Cl	-0.244129	1.65143	-1.439977
Cl	2.314192	0.314453	0.261334
O	0.280086	-1.500425	1.613171
H	1.238935	-1.588155	1.658888
O	-0.27967	1.500183	1.612251
H	-1.23852	1.591069	1.656049
H	0.062947	2.312556	1.237831
H	-0.058623	-2.313412	1.237353

^aSee Figure 4.3 for an explanation of the labelling scheme.

Table B.6: Vibrationally averaged geometries at 0K for the ^{35/37}Cl isotopologues^a and isotopomers of *fac*-[PtCl₃(H₂¹⁶O)₃]⁺ and *fac*-[PtCl₃(H₂¹⁶O)₂(H₂¹⁸O)]⁺ calculated at the PBE0/SDD/6-31G* level [in Å].

Ref.Geom.	Coordinates (Angstroms)		
	X	Y	Z
	Pt	0.000000	0.000000
Cl	1.437775	1.247668	-1.061685
Cl	-1.799399	0.621316	-1.061685
Cl	0.361624	-1.868984	-1.061685
O	1.622156	-0.650882	1.396165
H	2.197578	0.088314	1.670298
O	-0.247398	1.730270	1.396165
H	-1.175271	1.859001	1.670298
O	-1.374759	-1.079388	1.396165
H	-1.022307	-1.947315	1.670298
H	0.000000	2.513786	0.864219
H	2.177003	-1.256893	0.864219
H	-2.177003	-1.256893	0.864219

Vib.Av.Geom.A	Coordinates (Angstroms)		
	X	Y	Z
	Pt	0.000032	-0.000001
Cl	1.440160	1.249363	-1.063035

Cl	-1.801996	0.622477	-1.062969
Cl	0.361894	-1.871930	-1.062893
O	1.630891	-0.649625	1.401229
H	2.205760	0.060048	1.667246
O	-0.253446	1.736703	1.401731
H	-1.156113	1.880187	1.665429
O	-1.377778	-1.087059	1.401776
H	-1.052412	-1.942249	1.662344
H	0.017355	2.513270	0.906249
H	2.168959	-1.270504	0.904503
H	-2.186557	-1.237649	0.906453

Vib.Av.Geom.B

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.000003	0.000036	0.165942
Cl	1.439896	1.249421	-1.062853
Cl	-1.801838	0.622090	-1.063509
Cl	0.361383	-1.871927	-1.062893
O	1.630804	-0.648968	1.401586
H	2.205328	0.061039	1.667430
O	-0.251988	1.736836	1.401935
H	-1.153568	1.879273	1.669749
O	-1.377652	-1.087834	1.401538
H	-1.052584	-1.943766	1.660127
H	0.015830	2.513649	0.905454
H	2.169232	-1.269763	0.905164
H	-2.186861	-1.236999	0.906388

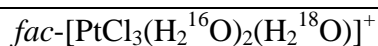
Vib.Av.Geom.C

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000044	-0.000025	0.165980
Cl	1.439720	1.249462	-1.063093
Cl	-1.801614	0.622259	-1.063184
Cl	0.361463	-1.871840	-1.063086
O	1.630627	-0.649228	1.401996
H	2.204966	0.060721	1.668333

O	-0.252347	1.737018	1.401569
H	-1.154336	1.880002	1.667735
O	-1.377732	-1.087749	1.401465
H	-1.052131	-1.942852	1.662014
H	0.016633	2.513500	0.905137
H	2.169300	-1.269817	0.905595
H	-2.186139	-1.238561	0.905687

Vib.Av.Geom.D

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000114	0.000012	0.165982
Cl	1.439879	1.249219	-1.063187
Cl	-1.801738	0.622341	-1.062997
Cl	0.361778	-1.871670	-1.063058
O	1.630936	-0.649809	1.401344
H	2.205716	0.059850	1.667543
O	-0.253764	1.736604	1.401794
H	-1.156544	1.879596	1.665316
O	-1.378156	-1.086816	1.401845
H	-1.052235	-1.941186	1.664230
H	0.016626	2.513214	0.906206
H	2.169052	-1.270422	0.904386
H	-2.186008	-1.239050	0.905705



Vib.Av.Geom.A

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.000042	0.000055	0.165925
Cl	1.440158	1.249460	-1.063113
Cl	-1.802261	0.622223	-1.062754
Cl	0.361551	-1.872182	-1.062589
O	1.629878	-0.648562	1.401545
H	2.202437	0.061611	1.671255
O	-0.251051	1.737072	1.401486

H	-1.152688	1.880990	1.668454
O	-1.377817	-1.088909	1.400073
H	-1.054457	-1.947490	1.652643
H	0.018407	2.513420	0.905041
H	2.170671	-1.267160	0.905029
H	-2.188492	-1.233019	0.905371

Vib.Av.Geom.B

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.000093	-0.000073	0.165964
Cl	1.439653	1.249116	-1.063491
Cl	-1.801771	0.622748	-1.062816
Cl	0.362047	-1.871913	-1.062876
O	1.629855	-0.648442	1.401737
H	2.202881	0.061725	1.670448
O	-0.251357	1.736884	1.401750
H	-1.152806	1.879701	1.669860
O	-1.378085	-1.088342	1.400630
H	-1.054120	-1.945653	1.656333
H	0.016550	2.513546	0.905051
H	2.170183	-1.267877	0.905691
H	-2.187759	-1.234878	0.905276

Vib.Av.Geom.C

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000097	0.000035	0.166021
Cl	1.439999	1.249230	-1.063178
Cl	-1.802070	0.621182	-1.062815
Cl	0.361368	-1.871512	-1.063550
O	1.629670	-0.648717	1.401825
H	2.202627	0.061201	1.671323

O	-0.251206	1.736904	1.401942
H	-1.152772	1.880219	1.669403
O	-1.378610	-1.087224	1.400491
H	-1.055258	-1.944667	1.656547
H	0.017513	2.513440	0.905448
H	2.170159	-1.267846	0.905607
H	-2.188302	-1.233340	0.904997

Vib.Av.Geom.D

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.000067	0.000014	0.166017
Cl	1.439835	1.249018	-1.063471
Cl	-1.801832	0.622239	-1.062905
Cl	0.361799	-1.871720	-1.062879
O	1.629820	-0.648296	1.401724
H	2.202601	0.061971	1.670682
O	-0.250912	1.736890	1.401923
H	-1.151673	1.878516	1.672839
O	-1.378148	-1.088457	1.400266
H	-1.054615	-1.946498	1.654236
H	0.014529	2.513868	0.904580
H	2.170321	-1.267381	0.905477
H	-2.188276	-1.233589	0.905118

^aSee Figure 4.3 for an explanation of the labelling scheme.

Table B.7: Vibrationally averaged geometries at 0K for the ^{35/37}Cl isotopologues^a of *fac*-[PtCl₃(H₂¹⁸O)₂(H₂¹⁶O)]⁺ calculated at the PBE0/SDD/6-31G* level [in Å].

Vib.Av.Geom.A

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000084	-0.000095	0.165916
Cl	1.440034	1.249293	-1.063194

Cl	-1.801867	0.621883	-1.06307
Cl	0.361404	-1.871801	-1.062958
O	1.630894	-0.647754	1.401162
H	2.205755	0.062738	1.665227
O	-0.251526	1.735721	1.402222
H	-1.152705	1.87725	1.672085
O	-1.379509	-1.086887	1.400533
H	-1.056357	-1.943712	1.658809
H	0.014796	2.513289	0.906066
H	2.168872	-1.269588	0.905362
H	-2.188566	-1.234165	0.904457

Vib.Av.Geom.B

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000024	-0.000175	0.165997
Cl	1.439444	1.24905	-1.063723
Cl	-1.801744	0.622885	-1.062871
Cl	0.362316	-1.871907	-1.062562
O	1.631098	-0.647865	1.401145
H	2.207346	0.062409	1.662905
O	-0.2516	1.73567	1.402118
H	-1.152632	1.876748	1.672688
O	-1.380031	-1.08712	1.39997
H	-1.056903	-1.943729	1.658906
H	0.013847	2.513231	0.905552
H	2.167524	-1.271441	0.905695
H	-2.18869	-1.234771	0.90343

Vib.Av.Geom.C

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000128	-0.000247	0.165994
Cl	1.439222	1.250151	-1.063174
Cl	-1.801277	0.622588	-1.063572
Cl	0.361257	-1.87249	-1.062194

O	1.631604	-0.647889	1.400565
H	2.208111	0.062397	1.661748
O	-0.251602	1.735477	1.402197
H	-1.152606	1.876244	1.672981
O	-1.379913	-1.086744	1.40025
H	-1.056704	-1.942976	1.660269
H	0.013634	2.513192	0.905764
H	2.167704	-1.271683	0.90503
H	-2.188262	-1.235111	0.903489

Vib.Av.Geom.D

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000075	-0.000143	0.165982
Cl	1.439899	1.249432	-1.063104
Cl	-1.801833	0.622324	-1.062891
Cl	0.361684	-1.871997	-1.062579
O	1.631545	-0.647884	1.400708
H	2.208225	0.062395	1.661537
O	-0.251873	1.735829	1.401793
H	-1.152809	1.876473	1.672852
O	-1.380026	-1.086857	1.400017
H	-1.056802	-1.943258	1.659479
H	0.013018	2.513486	0.905132
H	2.167472	-1.27196	0.905317
H	-2.188514	-1.234877	0.903354

^aSee Figure 4.3 for an explanation of the labelling scheme.

Table B.8: Vibrationally averaged geometries at 0K for the ^{35/37}Cl isotopologues of *fac*-[PtCl₃(H₂¹⁸O)₃]⁺ calculated at the PBE0/SDD/6-31G* level [in Å].

Vib.Av.Geom.A

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000051	0.000013	0.165877

Cl	1.439831	1.249159	-1.063315
Cl	-1.801788	0.622318	-1.063237
Cl	0.361819	-1.871569	-1.063179
O	1.630108	-0.649925	1.401506
H	2.205104	0.05955	1.668063
O	-0.252534	1.736443	1.401617
H	-1.154886	1.87951	1.666835
O	-1.377741	-1.086569	1.401532
H	-1.051877	-1.94099	1.664136
H	0.017149	2.513174	0.905759
H	2.168275	-1.270858	0.904844
H	-2.185865	-1.238777	0.905674

Vib.Av.Geom.B

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000027	-0.000061	0.165923
Cl	1.439568	1.249389	-1.063125
Cl	-1.801622	0.622605	-1.06332
Cl	0.361848	-1.871813	-1.063027
O	1.630375	-0.649758	1.401169
H	2.20559	0.059805	1.666986
O	-0.252375	1.736535	1.401284
H	-1.154677	1.879962	1.666544
O	-1.378	-1.086752	1.40151
H	-1.052257	-1.941311	1.663808
H	0.017536	2.513046	0.905196
H	2.168199	-1.27106	0.904581
H	-2.186095	-1.238696	0.905527

Vib.Av.Geom.C

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000134	-0.000041	0.165973
Cl	1.439593	1.249617	-1.063164
Cl	-1.801589	0.622314	-1.063146

Cl	0.36143	-1.871896	-1.063108
O	1.630243	-0.650023	1.401361
H	2.204389	0.059599	1.669206
O	-0.252558	1.736829	1.401006
H	-1.155141	1.881049	1.664899
O	-1.377899	-1.086968	1.401185
H	-1.052577	-1.942035	1.662468
H	0.018708	2.51301	0.905073
H	2.16928	-1.269921	0.904446
H	-2.186313	-1.237915	0.905349

Vib.Av.Geom.D

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.00002	-0.000034	0.165995
Cl	1.43989	1.249262	-1.063072
Cl	-1.801752	0.622397	-1.06302
Cl	0.361864	-1.871571	-1.063028
O	1.630513	-0.649802	1.400943
H	2.206069	0.059721	1.666172
O	-0.252509	1.736893	1.400915
H	-1.154969	1.880634	1.665421
O	-1.378129	-1.087002	1.401141
H	-1.052471	-1.941691	1.663119
H	0.017957	2.513174	0.904761
H	2.167955	-1.271496	0.904398
H	-2.186225	-1.238674	0.905075

^bSee Figure 5.3 for an explanation of the labelling scheme.

Table B.9: Vibrationally averaged geometries at 0K for the ^{35/37}Cl isotopologues and isotopomers of [PtCl₅(¹⁶OH)]²⁻ calculated at the PBE0/SDD/6-31G* level [in Å].

Ref.Geom.	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001691	0.000000	-0.111757

Cl	0.180857	-0.000007	2.290148
Cl	-2.379549	0.000154	-0.036535
Cl	-0.012958	2.370436	-0.141361
Cl	2.347235	-0.000154	-0.334426
Cl	-0.013267	-2.370435	-0.141353
O	-0.138348	0.000005	-2.111740
H	-1.104508	0.000048	-2.209119

Vib.Av.Geom.A

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001218	0.000000	-0.112757
Cl	0.180189	-0.000006	2.292580
Cl	-2.383233	0.000154	-0.028284
Cl	-0.013108	2.374476	-0.144473
Cl	2.352735	-0.000154	-0.329601
Cl	-0.013417	-2.374475	-0.144466
O	-0.136990	0.000005	-2.118717
H	-1.064022	0.000045	-2.226911

Vib.Av.Geom.B

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001204	0.000000	-0.112788
Cl	0.179829	-0.000006	2.292599
Cl	-2.383169	0.000154	-0.028091
Cl	-0.012885	2.374452	-0.144416
Cl	2.352679	-0.000154	-0.329880
Cl	-0.013194	-2.374452	-0.144408
O	-0.136904	0.000005	-2.118753
H	-1.063935	0.000044	-2.226980

Vib.Av.Geom.C1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001193	0.000026	-0.112726
Cl	0.180380	-0.000786	2.292583
Cl	-2.383282	0.000427	-0.028537
Cl	-0.013130	2.374377	-0.144590
Cl	2.352650	0.000112	-0.329715

Cl	-0.013375	-2.374488	-0.143973
O	-0.136846	-0.000052	-2.118714
H	-1.063863	0.000409	-2.226925

Vib.Av.Geom.C2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001132	0.000000	-0.112767
Cl	0.181099	-0.000006	2.292650
Cl	-2.383270	0.000154	-0.028642
Cl	-0.013415	2.374529	-0.144491
Cl	2.352472	-0.000154	-0.329483
Cl	-0.013725	-2.374527	-0.144484
O	-0.136606	0.000005	-2.118741
H	-1.063607	0.000044	-2.227243

Vib.Av.Geom.C3

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001192	0.000000	-0.112859
Cl	0.179637	-0.000006	2.292725
Cl	-2.383027	0.000154	-0.028241
Cl	-0.012796	2.374458	-0.144394
Cl	2.352650	-0.000154	-0.329788
Cl	-0.013106	-2.374458	-0.144387
O	-0.136682	0.000005	-2.118837
H	-1.063695	0.000044	-2.227251

Vib.Av.Geom.D1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001147	0.000022	-0.112745
Cl	0.180177	-0.000619	2.292741
Cl	-2.383277	0.000380	-0.029430
Cl	-0.012764	2.374282	-0.143964
Cl	2.352464	0.000059	-0.330490
Cl	-0.012983	-2.374536	-0.143409
O	-0.136690	0.000175	-2.118735
H	-1.063692	-0.000024	-2.227165

Vib.Av.Geom.D2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001099	-0.000061	-0.112750
Cl	0.181161	0.000751	2.292521
Cl	-2.383194	-0.000143	-0.028751
Cl	-0.013208	2.374553	-0.144104
Cl	2.352392	-0.000370	-0.329377
Cl	-0.013622	-2.374277	-0.144644
O	-0.136943	0.000110	-2.118772
H	-1.063954	0.000166	-2.227055

Vib.Av.Geom.E1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001145	0.000000	-0.112863
Cl	0.180392	-0.000006	2.292503
Cl	-2.383085	0.000155	-0.028456
Cl	-0.013153	2.374392	-0.144441
Cl	2.352667	-0.000154	-0.329498
Cl	-0.013463	-2.374391	-0.144434
O	-0.136771	0.000005	-2.118844
H	-1.063781	0.000043	-2.227271

Vib.Av.Geom.E2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001192	0.000000	-0.112675
Cl	0.180363	-0.000006	2.292630
Cl	-2.383239	0.000154	-0.028361
Cl	-0.013081	2.374395	-0.144570
Cl	2.352663	-0.000154	-0.329508
Cl	-0.013390	-2.374394	-0.144563
O	-0.136969	0.000005	-2.118634
H	-1.063987	0.000045	-2.226840

Vib.Av.Geom.F1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001192	-0.000033	-0.112766
Cl	0.180074	0.000922	2.292674
Cl	-2.383163	-0.000201	-0.028441
Cl	-0.012867	2.374464	-0.143833
Cl	2.352639	-0.000493	-0.329889
Cl	-0.013278	-2.374339	-0.144656
O	-0.137095	0.000032	-2.118736
H	-1.064128	-0.000473	-2.226796

Vib.Av.Geom.F2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001135	0.000000	-0.112814
Cl	0.180992	-0.000006	2.292514
Cl	-2.383183	0.000154	-0.028592
Cl	-0.013389	2.374495	-0.144416
Cl	2.352555	-0.000154	-0.329412
Cl	-0.013698	-2.374493	-0.144408
O	-0.136916	0.000005	-2.118780
H	-1.063932	0.000044	-2.227070

Vib.Av.Geom.F3

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001352	0.000000	-0.112812
Cl	0.178990	-0.000006	2.292455
Cl	-2.383038	0.000154	-0.028049
Cl	-0.012947	2.374435	-0.144310
Cl	2.352867	-0.000154	-0.330316
Cl	-0.013256	-2.374434	-0.144303
O	-0.136771	0.000005	-2.118786
H	-1.063807	0.000044	-2.226971

Vib.Av.Geom.G1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001107	-0.000004	-0.112830
Cl	0.180790	-0.000614	2.292464
Cl	-2.383382	0.000420	-0.029460
Cl	-0.012925	2.374366	-0.143818
Cl	2.352209	0.000033	-0.330117
Cl	-0.013108	-2.374427	-0.143334
O	-0.136711	0.000022	-2.118872
H	-1.063711	-0.000645	-2.227297

Vib.Av.Geom.G2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001137	0.000000	-0.112723
Cl	0.181055	-0.000006	2.292618
Cl	-2.383140	0.000154	-0.028627
Cl	-0.013382	2.374397	-0.144508
Cl	2.352515	-0.000154	-0.329360
Cl	-0.013692	-2.374396	-0.144501
O	-0.136974	0.000005	-2.118684
H	-1.063990	0.000045	-2.226925

Vib.Av.Geom.G3

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001241	0.000000	-0.112777
Cl	0.179756	-0.000006	2.292614
Cl	-2.383102	0.000154	-0.028230
Cl	-0.012945	2.374348	-0.144483
Cl	2.352621	-0.000154	-0.329652
Cl	-0.013254	-2.374347	-0.144475
O	-0.136657	0.000005	-2.118758
H	-1.063673	0.000045	-2.227118

Vib.Av.Geom.H1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001266	-0.000032	-0.112857
Cl	0.179653	0.000617	2.292328
Cl	-2.383246	-0.000028	-0.029065
Cl	-0.012827	2.374483	-0.143066
Cl	2.352706	-0.000405	-0.330596
Cl	-0.013140	-2.374263	-0.143644
O	-0.136937	-0.000078	-2.118851
H	-1.063967	0.000060	-2.226989

Vib.Av.Geom.H2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001111	0.000004	-0.112795
Cl	0.181135	0.000768	2.292567
Cl	-2.383289	-0.000468	-0.028761
Cl	-0.013071	2.374616	-0.144062
Cl	2.352321	-0.000582	-0.329361
Cl	-0.013593	-2.374264	-0.144632
O	-0.137057	0.000216	-2.118767
H	-1.064073	0.000191	-2.226956

Vib.Av.Geom.II

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001175	0.000000	-0.112736
Cl	0.180118	-0.000006	2.292561
Cl	-2.383134	0.000154	-0.028195
Cl	-0.012905	2.374398	-0.144473
Cl	2.352634	-0.000154	-0.329582
Cl	-0.013215	-2.374397	-0.144466
O	-0.137103	0.000005	-2.118692
H	-1.064128	0.000045	-2.226846

Vib.Av.Geom.I2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001252	0.000000	-0.112830
Cl	0.179889	-0.000007	2.292335
Cl	-2.382999	0.000153	-0.028215
Cl	-0.013299	2.374466	-0.144452
Cl	2.352726	-0.000155	-0.329867
Cl	-0.013609	-2.374463	-0.144443
O	-0.136571	0.000006	-2.118818
H	-1.063579	0.000045	-2.227262

Vib.Av.Geom.J

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001197	0.000000	-0.112810
Cl	0.180432	-0.000006	2.292544
Cl	-2.383189	0.000154	-0.028411
Cl	-0.013242	2.374363	-0.144486
Cl	2.352598	-0.000154	-0.329463
Cl	-0.013552	-2.374362	-0.144479
O	-0.136641	0.000005	-2.118791
H	-1.063650	0.000045	-2.227198

Vib.Av.Geom.K1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001116	0.000000	-0.112771
Cl	0.181033	-0.000006	2.292534
Cl	-2.383124	0.000154	-0.028567
Cl	-0.013330	2.374485	-0.144452
Cl	2.352536	-0.000154	-0.329307
Cl	-0.013639	-2.374484	-0.144444
O	-0.137014	0.000005	-2.118730
H	-1.064027	0.000045	-2.226940

 Vib.Av.Geom.K2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001230	0.000000	-0.112796
Cl	0.179396	-0.000006	2.292497
Cl	-2.383053	0.000154	-0.028103
Cl	-0.012717	2.374339	-0.144387
Cl	2.352692	-0.000154	-0.329895
Cl	-0.013026	-2.374338	-0.144379
O	-0.136859	0.000005	-2.118772
H	-1.063889	0.000045	-2.226999

Vib.Av.Geom.K3

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001199	-0.000003	-0.112813
Cl	0.180435	0.000675	2.292336
Cl	-2.383344	-0.000208	-0.029346
Cl	-0.012921	2.374425	-0.143306
Cl	2.352288	-0.000456	-0.330349
Cl	-0.013341	-2.374281	-0.143843
O	-0.136757	0.000135	-2.118815
H	-1.063779	0.000515	-2.227074

^bSee Figure 5.3 for an explanation of the labelling scheme.

Table B.10: Vibrationally averaged geometries at 0K for the ^{35/37}Cl isotopologues and isotopomers of [PtCl₅(¹⁸OH)]²⁻ calculated at the PBE0/SDD/6-31G* level [in Å].

Vib.Av.Geom.A

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001199	0	-0.112696
Cl	0.180136	-0.000006	2.292674
Cl	-2.383168	0.000154	-0.028022

Cl	-0.013096	2.37445	-0.144751
Cl	2.352717	-0.000154	-0.329484
Cl	-0.013405	-2.374449	-0.144743
O	-0.136967	0.000005	-2.118447
H	-1.064072	0.000044	-2.226741

Vib.Av.Geom.B

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001204	0	-0.112716
Cl	0.179717	-0.000006	2.292644
Cl	-2.383094	0.000154	-0.027845
Cl	-0.012872	2.374416	-0.144703
Cl	2.352716	-0.000154	-0.329757
Cl	-0.013182	-2.374415	-0.144695
O	-0.137081	0.000005	-2.118463
H	-1.064201	0.000044	-2.226656

Vib.Av.Geom.C1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001175	0.000026	-0.11266
Cl	0.180329	-0.000806	2.292615
Cl	-2.383229	0.000435	-0.028259
Cl	-0.013117	2.37437	-0.144862
Cl	2.352628	0.000137	-0.329593
Cl	-0.013375	-2.374497	-0.144233
O	-0.136801	-0.000044	-2.118443
H	-1.063897	0.000567	-2.226773

Vib.Av.Geom.C2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001139	0	-0.112787
Cl	0.181066	-0.000006	2.292682
Cl	-2.383272	0.000154	-0.028271
Cl	-0.013426	2.374575	-0.144629
Cl	2.352439	-0.000154	-0.329217
Cl	-0.013736	-2.374575	-0.144622
O	-0.136687	0.000005	-2.118551

H	-1.063777	0.000045	-2.227061
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Vib.Av.Geom.C3

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001196	0	-0.112784
Cl	0.179542	-0.000006	2.292723
Cl	-2.383123	0.000154	-0.027951
Cl	-0.012785	2.374351	-0.144684
Cl	2.352712	-0.000154	-0.329678
Cl	-0.013095	-2.374351	-0.144676
O	-0.136681	0.000005	-2.118558
H	-1.063789	0.000044	-2.226947

Vib.Av.Geom.D1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001132	0.000023	-0.112667
Cl	0.180098	-0.000638	2.292732
Cl	-2.383245	0.000394	-0.029162
Cl	-0.012749	2.374225	-0.144247
Cl	2.352477	0.000085	-0.330375
Cl	-0.012976	-2.374507	-0.143686
O	-0.136694	0.000153	-2.118454
H	-1.063788	0.000051	-2.226878

Vib.Av.Geom.D2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.00114	-0.000067	-0.112713
Cl	0.18111	0.000772	2.292698
Cl	-2.383272	-0.000154	-0.028472
Cl	-0.013279	2.374637	-0.144366
Cl	2.352333	-0.000393	-0.329258
Cl	-0.013679	-2.374329	-0.144897
O	-0.136911	0.000142	-2.118502
H	-1.06401	0.000077	-2.226833

Vib.Av.Geom.E1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001156	0	-0.112813
Cl	0.180344	-0.000006	2.292618
Cl	-2.383123	0.000155	-0.02817
Cl	-0.01316	2.374435	-0.144739
Cl	2.352626	-0.000154	-0.329342
Cl	-0.013469	-2.374436	-0.144731
O	-0.136781	0.000004	-2.118579
H	-1.063877	0.000045	-2.227058

Vib.Av.Geom.E2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001179	0	-0.112611
Cl	0.180317	-0.000006	2.292717
Cl	-2.383246	0.000154	-0.028112
Cl	-0.013068	2.374329	-0.144829
Cl	2.352658	-0.000154	-0.32941
Cl	-0.013378	-2.374328	-0.144821
O	-0.136926	0.000005	-2.118361
H	-1.064029	0.000045	-2.226673

Vib.Av.Geom.F1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001177	-0.000038	-0.112701
Cl	0.180026	0.000859	2.292742
Cl	-2.383112	-0.00015	-0.028165
Cl	-0.012888	2.374437	-0.144159
Cl	2.352631	-0.000481	-0.329757
Cl	-0.013255	-2.374287	-0.144898
O	-0.137058	0.000035	-2.118467
H	-1.064175	-0.000484	-2.22663

Vib.Av.Geom.F2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001143	0	-0.112765
Cl	0.18097	-0.000006	2.292622
Cl	-2.383237	0.000154	-0.028316
Cl	-0.013392	2.374533	-0.144696
Cl	2.352507	-0.000154	-0.329265
Cl	-0.013701	-2.374529	-0.144688
O	-0.136894	0.000006	-2.118517
H	-1.063987	0.000042	-2.22687

Vib.Av.Geom.F3

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001334	0	-0.112755
Cl	0.178888	-0.000006	2.292557
Cl	-2.382962	0.000154	-0.027737
Cl	-0.012915	2.374442	-0.144613
Cl	2.352833	-0.000154	-0.330199
Cl	-0.013225	-2.374441	-0.144605
O	-0.136747	0.000005	-2.118517
H	-1.063859	0.000044	-2.226849

Vib.Av.Geom.G1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001107	0.000031	-0.112704
Cl	0.180712	-0.000611	2.292713
Cl	-2.383328	0.000459	-0.029348
Cl	-0.012983	2.37423	-0.144232
Cl	2.352339	0.000068	-0.330119
Cl	-0.013167	-2.37458	-0.143757
O	-0.136876	0.000071	-2.118496
H	-1.063969	-0.000755	-2.226905

Vib.Av.Geom.G2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001138	0	-0.112673
Cl	0.181045	-0.000006	2.292766
Cl	-2.383179	0.000154	-0.028382
Cl	-0.013387	2.37442	-0.144767
Cl	2.352476	-0.000154	-0.329238
Cl	-0.013697	-2.374419	-0.14476
O	-0.136935	0.000005	-2.118421
H	-1.064033	0.000045	-2.226746

Vib.Av.Geom.G3

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001226	0	-0.11269
Cl	0.179677	-0.000006	2.292582
Cl	-2.383076	0.000154	-0.027972
Cl	-0.012927	2.374334	-0.144758
Cl	2.352621	-0.000154	-0.329548
Cl	-0.013236	-2.374333	-0.144751
O	-0.136655	0.000005	-2.118468
H	-1.063759	0.000044	-2.226821

Vib.Av.Geom.H1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001253	-0.00006	-0.112797
Cl	0.179557	0.000641	2.292427
Cl	-2.383151	-0.000036	-0.028778
Cl	-0.012811	2.374618	-0.143354
Cl	2.352642	-0.000431	-0.330483
Cl	-0.01311	-2.374246	-0.14393
O	-0.136921	-0.000032	-2.118579
H	-1.064026	-0.000115	-2.226856

Vib.Av.Geom.H2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001139	-0.000085	-0.112728
Cl	0.18106	0.000928	2.292637
Cl	-2.383218	-0.000249	-0.028486
Cl	-0.013204	2.374572	-0.144246
Cl	2.352268	-0.00046	-0.329266
Cl	-0.013646	-2.37422	-0.144981
O	-0.137005	0.000164	-2.118521
H	-1.064107	-0.000019	-2.22677

Vib.Av.Geom.I1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001163	0	-0.112667
Cl	0.180049	-0.000006	2.292646
Cl	-2.38311	0.000154	-0.02794
Cl	-0.012886	2.374341	-0.144743
Cl	2.352624	-0.000154	-0.32949
Cl	-0.013196	-2.37434	-0.144735
O	-0.137077	0.000005	-2.118415
H	-1.064187	0.000044	-2.226662

Vib.Av.Geom.I2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001231	0	-0.112791
Cl	0.179837	-0.000007	2.292505
Cl	-2.382948	0.000152	-0.027904
Cl	-0.013282	2.374422	-0.144758
Cl	2.35271	-0.000155	-0.329718
Cl	-0.013592	-2.374417	-0.144748
O	-0.136562	0.000007	-2.118566
H	-1.063657	0.000044	-2.227098

Vib.Av.Geom.J

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001202	0	-0.112728
Cl	0.180356	-0.000006	2.292539
Cl	-2.383157	0.000154	-0.028196
Cl	-0.013254	2.374369	-0.144766
Cl	2.352645	-0.000154	-0.329322
Cl	-0.013563	-2.374368	-0.144758
O	-0.136839	0.000005	-2.118489
H	-1.063948	0.000045	-2.22685

Vib.Av.Geom.K1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001104	0	-0.112703
Cl	0.18101	-0.000006	2.292609
Cl	-2.383107	0.000154	-0.028325
Cl	-0.013332	2.374424	-0.144722
Cl	2.352529	-0.000154	-0.329189
Cl	-0.013641	-2.374424	-0.144715
O	-0.136988	0.000005	-2.118455
H	-1.064083	0.000045	-2.226752

Vib.Av.Geom.K2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001227	0	-0.112724
Cl	0.179272	-0.000006	2.292587
Cl	-2.382937	0.000154	-0.027876
Cl	-0.012703	2.374258	-0.144675
Cl	2.352714	-0.000154	-0.329785
Cl	-0.013013	-2.374258	-0.144667
O	-0.137055	0.000005	-2.11848
H	-1.064171	0.000044	-2.226671

 Vib.Av.Geom.K3

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.001156	-0.000048	-0.112755
Cl	0.180366	0.000689	2.292454
Cl	-2.383167	-0.000253	-0.029062
Cl	-0.012953	2.374574	-0.143591
Cl	2.35238	-0.000496	-0.330241
Cl	-0.013375	-2.374113	-0.144125
O	-0.136739	0.000114	-2.118573
H	-1.063838	0.000609	-2.226947

^bSee Figure 5.3 for an explanation of the labelling scheme.

Table B.11: Vibrationally averaged geometries at 0K for the ^{35/37}Cl isotopologues and isotopomers of *cis*-[PtCl₄(¹⁶OH)₂]²⁻ calculated at the PBE0/SDD/6-31G* level [in Å].

 Ref.Geom.

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.005234	-0.041070	-0.159770
Cl	0.186333	2.135828	0.824409
Cl	-2.377710	0.050104	-0.197412
Cl	2.350484	-0.264412	-0.239681
Cl	-0.073385	-1.107281	2.012893
O	-0.143552	-1.798755	-1.122356
H	-1.066167	-2.020990	-0.919124
O	0.041164	0.736065	-1.996956
H	0.019736	-0.116096	-2.467877

 Vib.Av.Geom.A

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004734	-0.042053	-0.161099
Cl	0.185723	2.139933	0.823306
Cl	-2.381646	0.057518	-0.194221
Cl	2.355965	-0.261474	-0.238662
Cl	-0.075064	-1.114097	2.013676
O	-0.139922	-1.811392	-1.114297

H	-1.015336	-2.076273	-0.854821
O	0.041694	0.745287	-2.000511
H	0.025461	-0.081578	-2.481487

Vib.Av.Geom.B1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004758	-0.042205	-0.161119
Cl	0.185110	2.139635	0.823403
Cl	-2.381342	0.058017	-0.194367
Cl	2.356090	-0.261247	-0.238548
Cl	-0.074740	-1.113945	2.013656
O	-0.139885	-1.811514	-1.114411
H	-1.015283	-2.076440	-0.854926
O	0.041530	0.745039	-2.000623
H	0.025104	-0.081878	-2.481498

Vib.Av.Geom.B2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004682	-0.042160	-0.161312
Cl	0.185466	2.139581	0.823635
Cl	-2.381418	0.057903	-0.193830
Cl	2.355859	-0.261453	-0.237963
Cl	-0.074625	-1.113618	2.013513
O	-0.140499	-1.811581	-1.114428
H	-1.015997	-2.076101	-0.854959
O	0.041647	0.745246	-2.000732
H	0.024927	-0.081646	-2.481640

Vib.Av.Geom.C1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004789	-0.041999	-0.161117
Cl	0.185734	2.139457	0.823524
Cl	-2.381889	0.057221	-0.194357
Cl	2.356060	-0.261706	-0.238845
Cl	-0.075118	-1.113758	2.013880
O	-0.140047	-1.811421	-1.114244
H	-1.015863	-2.075501	-0.855701

O	0.041637	0.745586	-2.000411
H	0.026056	-0.081198	-2.481553

Vib.Av.Geom.C2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004757	-0.041991	-0.161123
Cl	0.185471	2.139994	0.823100
Cl	-2.381367	0.057557	-0.194097
Cl	2.356110	-0.261686	-0.238549
Cl	-0.075054	-1.113990	2.013563
O	-0.139987	-1.811583	-1.113930
H	-1.015521	-2.076197	-0.854689
O	0.041297	0.745550	-2.000502
H	0.025499	-0.081288	-2.481529

Vib.Av.Geom.D

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004729	-0.042224	-0.161156
Cl	0.185663	2.139400	0.823917
Cl	-2.381571	0.057636	-0.194605
Cl	2.355947	-0.261174	-0.238827
Cl	-0.074960	-1.113435	2.013848
O	-0.139995	-1.811599	-1.114310
H	-1.015959	-2.075505	-0.856253
O	0.041405	0.745008	-2.000677
H	0.026026	-0.081928	-2.481560

Vib.Av.Geom.E1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004779	-0.042093	-0.161156
Cl	0.185231	2.139461	0.823683
Cl	-2.381627	0.057340	-0.194505
Cl	2.356085	-0.261824	-0.238712
Cl	-0.074657	-1.113593	2.013981
O	-0.140064	-1.811399	-1.114534
H	-1.016093	-2.075163	-0.856603
O	0.041781	0.745427	-2.000497

H	0.026487	-0.081410	-2.481562
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Vib.Av.Geom.E2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004793	-0.042097	-0.161112
Cl	0.185515	2.139736	0.823129
Cl	-2.381266	0.057540	-0.194067
Cl	2.356280	-0.261010	-0.238664
Cl	-0.075372	-1.113970	2.013416
O	-0.140098	-1.811652	-1.113877
H	-1.015615	-2.076236	-0.854531
O	0.041475	0.745098	-2.000652
H	0.025373	-0.081855	-2.481458

Vib.Av.Geom.E3

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004764	-0.042143	-0.161275
Cl	0.185538	2.139195	0.823893
Cl	-2.381803	0.057867	-0.194092
Cl	2.355889	-0.261428	-0.238499
Cl	-0.074890	-1.113475	2.013900
O	-0.140227	-1.811582	-1.114392
H	-1.015959	-2.075728	-0.855559
O	0.041666	0.745155	-2.000715
H	0.024942	-0.081783	-2.481543

Vib.Av.Geom.E4

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004702	-0.042060	-0.161309
Cl	0.185365	2.139615	0.823784
Cl	-2.381389	0.057712	-0.194002
Cl	2.355879	-0.261814	-0.238236
Cl	-0.074642	-1.113314	2.013786
O	-0.140210	-1.811552	-1.114333
H	-1.016083	-2.075527	-0.855936
O	0.041379	0.745229	-2.000821

H	0.025599	-0.081701	-2.481689
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Vib.Av.Geom.F

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004755	-0.041996	-0.161137
Cl	0.185535	2.139515	0.823559
Cl	-2.381615	0.057568	-0.194434
Cl	2.355927	-0.261601	-0.238870
Cl	-0.074838	-1.113706	2.013860
O	-0.140080	-1.811632	-1.113853
H	-1.015907	-2.075677	-0.855309
O	0.041789	0.745359	-2.000518
H	0.026405	-0.081531	-2.481469

Vib.Av.Geom.G1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004732	-0.042118	-0.161156
Cl	0.185807	2.139436	0.823673
Cl	-2.381703	0.057144	-0.194522
Cl	2.355898	-0.261511	-0.238751
Cl	-0.074966	-1.113641	2.013983
O	-0.140118	-1.811426	-1.114521
H	-1.015977	-2.075435	-0.856104
O	0.041693	0.745350	-2.000514
H	0.025884	-0.081491	-2.481546

Vib.Av.Geom.G2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004803	-0.042209	-0.161299
Cl	0.185319	2.139527	0.823591
Cl	-2.381442	0.057989	-0.193857
Cl	2.356020	-0.261030	-0.238188
Cl	-0.074980	-1.113604	2.013564
O	-0.140242	-1.811664	-1.114281
H	-1.015933	-2.075860	-0.855315
O	0.041341	0.744681	-2.000985
H	0.025165	-0.082399	-2.481565

Vib.Av.Geom.H1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004801	-0.042039	-0.161154
Cl	0.185364	2.139842	0.823118
Cl	-2.381480	0.057294	-0.194039
Cl	2.356050	-0.261668	-0.238546
Cl	-0.075035	-1.113997	2.013619
O	-0.139887	-1.811479	-1.114142
H	-1.015416	-2.076115	-0.854912
O	0.041789	0.745513	-2.000459
H	0.025829	-0.081301	-2.481520

Vib.Av.Geom.H2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004760	-0.042078	-0.161277
Cl	0.185347	2.139399	0.823787
Cl	-2.381507	0.057813	-0.193984
Cl	2.355907	-0.261643	-0.238596
Cl	-0.074922	-1.113418	2.013791
O	-0.140179	-1.811712	-1.114003
H	-1.016186	-2.075354	-0.855844
O	0.041602	0.745242	-2.000702
H	0.026424	-0.081664	-2.481631

Vib.Av.Geom.I

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004791	-0.042128	-0.161294
Cl	0.185361	2.139576	0.823441
Cl	-2.381350	0.057444	-0.193751
Cl	2.355963	-0.261541	-0.238180
Cl	-0.075014	-1.113574	2.013503
O	-0.140288	-1.811561	-1.114285
H	-1.016086	-2.075566	-0.855590
O	0.041539	0.745312	-2.000690
H	0.025664	-0.081550	-2.481664

^bSee Figure 5.5 for an explanation of the labelling scheme.

Table B.12: Vibrationally averaged bond-lengths at 0K for the ^{35/37}Cl isotopologues and isotopomers of *cis*-[PtCl₄(¹⁸OH)₂]²⁻ calculated at the PBE0/SDD/6-31G* level [in Å].

Vib.Av.Geom.A

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004664	-0.042054	-0.161162
Cl	0.185824	2.139947	0.822900
Cl	-2.381469	0.057584	-0.194084
Cl	2.355939	-0.261598	-0.238304
Cl	-0.074986	-1.114316	2.013533
O	-0.139945	-1.811075	-1.114507
H	-1.014845	-2.077069	-0.853632
O	0.041429	0.745868	-2.000077
H	0.023887	-0.080779	-2.481597

Vib.Av.Geom.B1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004695	-0.042112	-0.161063
Cl	0.185944	2.139776	0.822749
Cl	-2.381574	0.057385	-0.194198
Cl	2.356117	-0.260998	-0.238583
Cl	-0.075253	-1.114439	2.013247
O	-0.140147	-1.811202	-1.114249
H	-1.015516	-2.076268	-0.854461
O	0.041827	0.745590	-2.000113
H	0.025333	-0.081173	-2.481469

Vib.Av.Geom.B2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004655	-0.042016	-0.161407
Cl	0.185473	2.139488	0.823738
Cl	-2.381595	0.057684	-0.193817
Cl	2.355830	-0.261922	-0.237816
Cl	-0.074440	-1.113659	2.013308

O	-0.140465	-1.811377	-1.114131
H	-1.016155	-2.075749	-0.855040
O	0.041521	0.745499	-2.000580
H	0.025361	-0.081362	-2.481760

Vib.Av.Geom.C1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004658	-0.042019	-0.161152
Cl	0.185873	2.139669	0.823158
Cl	-2.381577	0.057281	-0.194232
Cl	2.355938	-0.261851	-0.238542
Cl	-0.074960	-1.114014	2.013551
O	-0.139920	-1.811192	-1.114295
H	-1.015618	-2.075792	-0.855477
O	0.041528	0.746127	-1.999943
H	0.025742	-0.080460	-2.481639

Vib.Av.Geom.C2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004714	-0.041987	-0.161282
Cl	0.185525	2.139664	0.822910
Cl	-2.381667	0.057572	-0.193481
Cl	2.356062	-0.261572	-0.238041
Cl	-0.074925	-1.113910	2.013324
O	-0.140380	-1.811201	-1.114328
H	-1.015550	-2.076492	-0.853891
O	0.042092	0.745724	-2.000287
H	0.024813	-0.081029	-2.481618

Vib.Av.Geom.D

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004710	-0.042137	-0.161340
Cl	0.185642	2.139492	0.823483
Cl	-2.381505	0.057813	-0.193928
Cl	2.355999	-0.261171	-0.238031
Cl	-0.074946	-1.114100	2.013247
O	-0.140253	-1.811520	-1.113939

H	-1.015936	-2.075935	-0.854859
O	0.041273	0.745175	-2.000621
H	0.025141	-0.081728	-2.481737

Vib.Av.Geom.E1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004693	-0.042095	-0.161212
Cl	0.186099	2.139549	0.823257
Cl	-2.381718	0.056783	-0.193966
Cl	2.355786	-0.261430	-0.238324
Cl	-0.075079	-1.113707	2.013411
O	-0.140191	-1.811026	-1.114705
H	-1.016021	-2.075309	-0.856125
O	0.042202	0.745843	-2.000102
H	0.026077	-0.080838	-2.481621

Vib.Av.Geom.E2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004657	-0.041960	-0.161211
Cl	0.185500	2.139778	0.822739
Cl	-2.381341	0.057499	-0.194065
Cl	2.355780	-0.261571	-0.238007
Cl	-0.074510	-1.114365	2.013329
O	-0.140108	-1.811267	-1.114022
H	-1.015308	-2.076617	-0.853782
O	0.041939	0.745550	-2.000352
H	0.024768	-0.081301	-2.481511

Vib.Av.Geom.E3

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004684	-0.042035	-0.161320
Cl	0.185798	2.139464	0.823524
Cl	-2.381718	0.057484	-0.193873
Cl	2.355825	-0.261830	-0.238068
Cl	-0.074826	-1.113785	2.013493
O	-0.140217	-1.811162	-1.114522

H	-1.015678	-2.076021	-0.854937
O	0.041399	0.745586	-2.000362
H	0.024777	-0.081244	-2.481579

Vib.Av.Geom.E4

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004692	-0.041948	-0.161362
Cl	0.185447	2.139728	0.823653
Cl	-2.381713	0.057623	-0.193845
Cl	2.355774	-0.262021	-0.237900
Cl	-0.074424	-1.113628	2.013342
O	-0.140412	-1.811228	-1.114245
H	-1.016019	-2.075764	-0.854952
O	0.041564	0.745144	-2.000686
H	0.024966	-0.081873	-2.481580

Vib.Av.Geom.F

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004654	-0.041970	-0.161140
Cl	0.185957	2.139686	0.823074
Cl	-2.381742	0.057175	-0.194295
Cl	2.355775	-0.261754	-0.238491
Cl	-0.074707	-1.113852	2.013443
O	-0.140236	-1.811200	-1.114144
H	-1.015585	-2.076247	-0.854243
O	0.042042	0.746037	-1.999952
H	0.025082	-0.080595	-2.481507

Vib.Av.Geom.G1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004714	-0.042081	-0.161434
Cl	0.185771	2.139277	0.823763
Cl	-2.381810	0.057150	-0.193513
Cl	2.355798	-0.261574	-0.237958
Cl	-0.074975	-1.113503	2.013310
O	-0.140255	-1.811211	-1.114519
H	-1.015904	-2.075691	-0.855359

O	0.042109	0.745302	-2.000595
H	0.025679	-0.081545	-2.481796

Vib.Av.Geom.G2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004692	-0.042008	-0.161337
Cl	0.185539	2.139814	0.823192
Cl	-2.381533	0.057553	-0.193713
Cl	2.355917	-0.261590	-0.237918
Cl	-0.074798	-1.114095	2.013119
O	-0.140125	-1.811462	-1.113914
H	-1.015498	-2.076457	-0.854078
O	0.041613	0.745268	-2.000612
H	0.024974	-0.081689	-2.481600

Vib.Av.Geom.H1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004683	-0.041983	-0.161140
Cl	0.185461	2.139858	0.822647
Cl	-2.381160	0.057319	-0.193944
Cl	2.355838	-0.261775	-0.238325
Cl	-0.074888	-1.114368	2.013463
O	-0.139887	-1.811024	-1.114473
H	-1.015150	-2.076396	-0.854545
O	0.041891	0.745709	-2.000165
H	0.024746	-0.081130	-2.481354

Vib.Av.Geom.H2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004688	-0.041912	-0.161325
Cl	0.185690	2.139443	0.823448
Cl	-2.381779	0.057401	-0.193829
Cl	2.355823	-0.262049	-0.238156
Cl	-0.074771	-1.113696	2.013415
O	-0.140078	-1.811233	-1.114158
H	-1.015193	-2.076687	-0.853676
O	0.041595	0.745551	-2.000402

H	0.024382	-0.081276	-2.481598
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Vib.Av.Geom.I

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.004695	-0.041993	-0.161349
Cl	0.185709	2.139590	0.823188
Cl	-2.381357	0.057263	-0.193519
Cl	2.355736	-0.261629	-0.237969
Cl	-0.075058	-1.113986	2.013189
O	-0.140053	-1.811256	-1.114202
H	-1.014962	-2.077097	-0.853220
O	0.041811	0.745398	-2.000537
H	0.024171	-0.081501	-2.481584

^bSee Figure 5.5 for an explanation of the labelling scheme.

Table B.13: Vibrationally averaged geometries at 0K for the ^{35/37}Cl isotopologues^b and isotopomers of *fac*-[PtCl₃(¹⁶OH)₃]²⁻ and *fac*-[PtCl₃(¹⁸OH)₃]²⁻ calculated at the PBE0/SDD/6-31G* level [in Å].

Ref.Geom.

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.000000	0.000000	0.240145
O	0.469464	1.542626	1.409862
O	1.101221	-1.177881	1.409862
O	-1.570685	-0.364745	1.409862
Cl	-0.662141	-1.932637	-1.085585
Cl	-1.342642	1.539749	-1.085585
Cl	2.004783	0.392888	-1.085585
H	0.000000	2.246334	0.932275
H	1.945382	-1.123167	0.932275
H	-1.945382	-1.123167	0.932275

Vib.Av.Geom.A

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.000074	0.000048	0.240737
O	0.477894	1.544681	1.414965
O	1.098426	-1.186531	1.414904

O	-1.576400	-0.358914	1.415275
Cl	-0.659267	-1.935155	-1.089672
Cl	-1.345680	1.538478	-1.090154
Cl	2.005230	0.396991	-1.089848
H	0.028956	2.235931	0.959626
H	1.921253	-1.144445	0.958926
H	-1.944418	-1.099508	0.965033

Vib.Av.Geom.B

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.000163	-0.000155	0.240720
O	0.477886	1.544143	1.415236
O	1.098088	-1.186833	1.415035
O	-1.576772	-0.359243	1.414762
Cl	-0.659709	-1.935721	-1.088348
Cl	-1.344042	1.539190	-1.090524
Cl	2.004576	0.398779	-1.090507
H	0.031979	2.236239	0.958172
H	1.920912	-1.145041	0.959033
H	-1.942144	-1.102509	0.966658

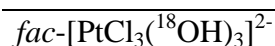
Vib.Av.Geom.C

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.000174	0.000051	0.240765
O	0.478105	1.544388	1.415186
O	1.097936	-1.186780	1.414994
O	-1.576651	-0.359158	1.414949
Cl	-0.658777	-1.935740	-1.088988
Cl	-1.344685	1.539314	-1.089944
Cl	2.004418	0.397392	-1.090451
H	0.029916	2.235985	0.959575
H	1.920451	-1.146330	0.958294
H	-1.942838	-1.101424	0.965942

Vib.Av.Geom.D

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.000088	0.000048	0.240783

O	0.478389	1.544565	1.414894
O	1.098214	-1.186580	1.414991
O	-1.576483	-0.358546	1.415281
Cl	-0.659064	-1.934789	-1.089637
Cl	-1.345886	1.538423	-1.089909
Cl	2.005234	0.396548	-1.089683
H	0.028846	2.235793	0.960112
H	1.921133	-1.144308	0.959184
H	-1.945303	-1.098421	0.964520



Vib.Av.Geom.A

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.000023	0.000051	0.240508
O	0.477468	1.544552	1.414774
O	1.098285	-1.186309	1.414743
O	-1.576195	-0.359061	1.414860
Cl	-0.659155	-1.935445	-1.089289
Cl	-1.346092	1.538502	-1.089858
Cl	2.005469	0.397317	-1.089704
H	0.028258	2.235822	0.959585
H	1.921109	-1.144786	0.958548
H	-1.944701	-1.099182	0.964098

Vib.Av.Geom.B

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.000182	-0.000089	0.240490
O	0.477765	1.543924	1.415052
O	1.098246	-1.186258	1.414932
O	-1.576586	-0.359886	1.414378
Cl	-0.659633	-1.936154	-1.088087
Cl	-1.344405	1.539404	-1.090327
Cl	2.004749	0.398963	-1.090199
H	0.034837	2.236843	0.956119
H	1.921054	-1.144751	0.958717
H	-1.940017	-1.105115	0.967718

Vib.Av.Geom.C

	Coordinates (Angstroms)		
	X	Y	Z

Pt	-0.000297	0.000084	0.240644
O	0.477625	1.544565	1.414709
O	1.098276	-1.186014	1.414815
O	-1.575970	-0.360090	1.415362
Cl	-0.658381	-1.935826	-1.089166
Cl	-1.344674	1.539576	-1.089968
Cl	2.004386	0.397137	-1.090316
H	0.029809	2.236209	0.958648
H	1.920618	-1.145715	0.957635
H	-1.941360	-1.103307	0.967094

Vib.Av.Geom.D

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.000056	0.000093	0.240565
O	0.477581	1.544508	1.414877
O	1.098481	-1.186174	1.414655
O	-1.576169	-0.358926	1.415026
Cl	-0.659167	-1.935243	-1.089402
Cl	-1.346209	1.538523	-1.089709
Cl	2.005606	0.396721	-1.089484
H	0.027958	2.235715	0.959988
H	1.921273	-1.144473	0.958404
H	-1.944985	-1.098770	0.964063

^bSee Figure 5.6 for an explanation of the labelling scheme.

Table B.14: Vibrationally averaged geometries at 0K for the ^{35/37}Cl isotopologues^b and isotopomers of *cis*-[PtCl₂(¹⁶OH)₄]²⁻ and *cis*-[PtCl₂(¹⁸OH)₄]²⁻ calculated at the PBE0/SDD/6-31G* level [in Å].

Ref.Geom.	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.015095	-0.184781	0.024015
Cl	1.821017	1.407352	-0.109379
O	-1.414088	-1.592620	0.154797
H	-1.589223	-1.652234	-0.800689
O	-0.103675	-0.501545	-1.985946
H	0.666760	-1.092004	-2.027566
Cl	-1.736858	1.500510	-0.106790

O	0.037228	-0.075302	2.049713
H	-0.600344	-0.782621	2.231758
O	1.373872	-1.628016	0.034247
H	2.122849	-1.113995	0.375746

Vib.Av.Geom.A

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.012582	-0.187135	0.022703
Cl	1.820292	1.411830	-0.113108
O	-1.423393	-1.591957	0.172126
H	-1.698913	-1.592587	-0.742129
O	-0.094040	-0.473908	-1.997246
H	0.660623	-1.060932	-2.060822
Cl	-1.744614	1.498569	-0.107702
O	0.036780	-0.077860	2.054422
H	-0.648783	-0.695943	2.236303
O	1.374123	-1.638781	0.043479
H	2.093043	-1.161827	0.443668

Vib.Av.Geom.B1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.012582	-0.187153	0.022679
Cl	1.820374	1.411789	-0.112554
O	-1.423503	-1.591783	0.172610
H	-1.699488	-1.592561	-0.741536
O	-0.094324	-0.473536	-1.997276
H	0.660267	-1.060625	-2.061158
Cl	-1.744523	1.498263	-0.108006
O	0.037128	-0.077545	2.054303
H	-0.646875	-0.696948	2.236494
O	1.373816	-1.639138	0.043297
H	2.092992	-1.162351	0.443159

Vib.Av.Geom.B2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.012559	-0.187049	0.022677
Cl	1.820589	1.411616	-0.112750

O	-1.423515	-1.591657	0.172736
H	-1.700369	-1.591665	-0.741295
O	-0.094355	-0.473733	-1.997198
H	0.659847	-1.061346	-2.060775
Cl	-1.744566	1.498347	-0.108078
O	0.037237	-0.078241	2.054448
H	-0.647717	-0.696900	2.236205
O	1.374107	-1.638671	0.043271
H	2.093010	-1.161757	0.443546

Vib.Av.Geom.C

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.012509	-0.187027	0.022705
Cl	1.820460	1.411266	-0.112761
O	-1.423493	-1.591626	0.172603
H	-1.700360	-1.591587	-0.741418
O	-0.094230	-0.473427	-1.997240
H	0.659848	-1.061192	-2.060900
Cl	-1.744516	1.498199	-0.107957
O	0.036870	-0.078054	2.054383
H	-0.648016	-0.696781	2.236077
O	1.373964	-1.638852	0.043382
H	2.093109	-1.161971	0.443159

cis-[PtCl₂(¹⁸OH)₄]²⁻

Vib.Av.Geom.A

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.012655	-0.187116	0.022668
Cl	1.820791	1.411326	-0.114306
O	-1.422942	-1.592315	0.171471
H	-1.695558	-1.595120	-0.743364
O	-0.093263	-0.474135	-1.996863
H	0.662785	-1.059481	-2.060565
Cl	-1.745396	1.498253	-0.107455
O	0.036475	-0.077832	2.054324
H	-0.647026	-0.697875	2.236370
O	1.374118	-1.638366	0.043877
H	2.093010	-1.161307	0.444148

Vib.Av.Geom.B1

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.012663	-0.187091	0.022810
Cl	1.821126	1.411191	-0.113980
O	-1.422595	-1.592620	0.171476
H	-1.695691	-1.594958	-0.743296
O	-0.093806	-0.473533	-1.996797
H	0.661984	-1.059190	-2.060878
Cl	-1.745513	1.498051	-0.108131
O	0.036653	-0.077821	2.054437
H	-0.646125	-0.698482	2.236577
O	1.373775	-1.638688	0.043450
H	2.093304	-1.161655	0.442371

Vib.Av.Geom.B2

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.012551	-0.187021	0.022595
Cl	1.821247	1.411337	-0.113937
O	-1.422740	-1.592142	0.171796
H	-1.697102	-1.593649	-0.742791
O	-0.094020	-0.474278	-1.996983
H	0.661117	-1.060796	-2.060738
Cl	-1.745179	1.497902	-0.107407
O	0.035939	-0.077710	2.054212
H	-0.647247	-0.698125	2.235898
O	1.373872	-1.638594	0.043939
H	2.093414	-1.161197	0.442300

Vib.Av.Geom.C

	Coordinates (Angstroms)		
	X	Y	Z
Pt	-0.012492	-0.187096	0.022727
Cl	1.821110	1.411000	-0.113990

O	-1.423055	-1.592050	0.171460
H	-1.697519	-1.593073	-0.743127
O	-0.093535	-0.473582	-1.996794
H	0.661576	-1.060129	-2.060653
Cl	-1.745570	1.497967	-0.107666
O	0.036363	-0.077551	2.054386
H	-0.648273	-0.696558	2.236415
O	1.373755	-1.638738	0.043609
H	2.093302	-1.161663	0.442405

^bSee Figure 5.7 for an explanation of the labelling scheme.

Table B.15: Vibrationally averaged geometries at 0K for the ^{35/37}Cl isotopologues^b and isotopomers of [PtCl(¹⁶OH)₅]²⁻ and [PtCl(¹⁸OH)₅]²⁻ calculated at the PBE0/SDD/6-31G* level [in Å].

Ref.Geom.	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.149183	0.036684	-0.009332
O	-0.047769	1.501396	-1.391190
O	0.631085	-1.422137	-1.338214
H	1.547671	-1.129709	-1.472211
H	-0.182880	2.215636	-0.745473
O	-0.250422	1.513264	1.336938
H	-1.175041	1.294567	1.530103
Cl	-2.252913	-0.414632	-0.070935
O	0.518003	-1.406584	1.391965
H	0.552484	-2.138504	0.752468
O	2.111850	0.339039	0.122823
H	2.219013	-0.254423	0.890359

Vib.Av.Geom.A	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.149948	0.037127	-0.008460
O	-0.040402	1.493960	-1.408938

O	0.616024	-1.419824	-1.354469
H	1.505966	-1.120589	-1.538094
H	-0.154147	2.217682	-0.797179
O	-0.238253	1.505652	1.358551
H	-1.132625	1.278832	1.580993
Cl	-2.255354	-0.422335	-0.076685
O	0.504254	-1.401785	1.408430
H	0.515498	-2.144602	0.798319
O	2.116298	0.356468	0.121721
H	2.239951	-0.212907	0.894783

Vib.Av.Geom.B

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.149966	0.037159	-0.008525
O	-0.040875	1.494340	-1.408623
O	0.615878	-1.419998	-1.354377
H	1.506020	-1.121232	-1.537585
H	-0.155270	2.217637	-0.796528
O	-0.237846	1.505628	1.358667
H	-1.131929	1.278368	1.581966
Cl	-2.255188	-0.422138	-0.076540
O	0.504109	-1.401307	1.408728
H	0.514981	-2.144471	0.799011
O	2.116434	0.356022	0.121880
H	2.239700	-0.213273	0.895056

[PtCl(¹⁸OH)₅]²⁻
Vib.Av.Geom.A

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.149984	0.036983	-0.008450
O	-0.041019	1.493778	-1.408690
O	0.616612	-1.419358	-1.354169
H	1.506480	-1.119739	-1.538161
H	-0.155302	2.217242	-0.796613
O	-0.238128	1.505203	1.358247
H	-1.132109	1.277772	1.582111
Cl	-2.255253	-0.422347	-0.077160
O	0.504392	-1.401285	1.408614
H	0.515568	-2.144609	0.798970
O	2.116021	0.356680	0.121646
H	2.239810	-0.212640	0.894817

Vib.Av.Geom.B

	Coordinates (Angstroms)		
	X	Y	Z
Pt	0.149916	0.037084	-0.008455
O	-0.041125	1.493965	-1.408696
O	0.616110	-1.419582	-1.354007
H	1.506357	-1.120785	-1.537215
H	-0.155060	2.217518	-0.796662
O	-0.237558	1.505095	1.358566
H	-1.131684	1.278107	1.582221
Cl	-2.254578	-0.422363	-0.077047
O	0.504030	-1.401115	1.408650
H	0.514959	-2.144522	0.799094
O	2.116044	0.356461	0.121569
H	2.239741	-0.212399	0.895087

^bSee Figure 5.8 for an explanation of the labelling scheme.

Table B.16: Vibrationally averaged geometries at 0K for the ^{35/37}Cl isotopologues and isotopomers^a of [RhCl₅(H₂¹⁶O)]²⁻ calculated at the PBE0/SDD/6-31G* level [in Å].

Ref.Geom.

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.029721	0.000000	-0.052968
Cl	1.601905	1.677378	-0.580545
Cl	1.601907	-1.677378	-0.580542
Cl	-1.695159	-1.709692	0.158107
Cl	0.621778	0.000002	2.188991
Cl	-1.695158	1.709693	0.158105
O	-0.761771	-0.000001	-2.095176
H	-1.321479	0.772051	-1.852493
H	-1.321455	-0.772074	-1.852500

Vib.Av.Geom.A

	Coordinates (Angstroms)		
	X	Y	Z

Rh	0.030042	0.000000	-0.052788
Cl	1.605707	1.680180	-0.580626
Cl	1.605708	-1.680179	-0.580624
Cl	-1.698212	-1.713472	0.159673
Cl	0.622268	0.000002	2.192148
Cl	-1.698212	1.713472	0.159671
O	-0.768347	-0.000001	-2.108480
H	-1.320111	0.769130	-1.862406
H	-1.320084	-0.769155	-1.862415

Vib.Av.Geom.B1

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.030049	0.000138	-0.052872
Cl	1.605904	1.680095	-0.580816
Cl	1.605663	-1.680265	-0.580374
Cl	-1.698065	-1.713137	0.160004
Cl	0.622194	-0.000378	2.192059
Cl	-1.698692	1.713139	0.159684
O	-0.768306	0.000588	-2.108631
H	-1.319952	0.769760	-1.862359
H	-1.320172	-0.768480	-1.862693

Vib.Av.Geom.B2

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.030026	0.000158	-0.052747
Cl	1.605360	1.680611	-0.581141
Cl	1.604937	-1.680866	-0.579827
Cl	-1.697090	-1.713739	0.159368
Cl	0.622502	-0.000668	2.192159
Cl	-1.698352	1.714048	0.159477
O	-0.768232	0.000750	-2.108450
H	-1.319981	0.769820	-1.862111
H	-1.319977	-0.768502	-1.862742

Vib.Av.Geom.C

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.029902	0.000000	-0.052983

Cl	1.606133	1.679860	-0.580013
Cl	1.606135	-1.679859	-0.580011
Cl	-1.698396	-1.713483	0.159638
Cl	0.622699	0.000002	2.191420
Cl	-1.698395	1.713484	0.159636
O	-0.769445	-0.000001	-2.108505
H	-1.321074	0.769117	-1.862064
H	-1.321047	-0.769142	-1.862073

Vib.Av.Geom.D1

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.030223	0.000000	-0.052837
Cl	1.605593	1.680574	-0.580854
Cl	1.605595	-1.680573	-0.580851
Cl	-1.698125	-1.712872	0.159854
Cl	0.621827	0.000002	2.192289
Cl	-1.698124	1.712873	0.159853
O	-0.767758	-0.000002	-2.108666
H	-1.319592	0.769109	-1.862722
H	-1.319564	-0.769135	-1.862731

Vib.Av.Geom.D2

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.030184	0.000000	-0.052779
Cl	1.605332	1.680566	-0.580920
Cl	1.605334	-1.680565	-0.580917
Cl	-1.698338	-1.712564	0.159954
Cl	0.621929	0.000002	2.192352
Cl	-1.698337	1.712565	0.159952
O	-0.767305	-0.000001	-2.108759
H	-1.319217	0.769099	-1.862987
H	-1.319190	-0.769125	-1.862996

Vib.Av.Geom.D3

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.030090	0.000200	-0.052813

Cl	1.605788	1.680302	-0.581322
Cl	1.605076	-1.680723	-0.580078
Cl	-1.697239	-1.713140	0.159595
Cl	0.622119	-0.000481	2.192200
Cl	-1.698874	1.713343	0.159881
O	-0.767986	0.000962	-2.108613
H	-1.319552	0.770172	-1.862315
H	-1.319962	-0.768108	-1.862918

Vib.Av.Geom.E

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.029924	-0.000017	-0.052803
Cl	1.605591	1.679918	-0.580465
Cl	1.605512	-1.680371	-0.580404
Cl	-1.697557	-1.713657	0.159166
Cl	0.622441	0.000309	2.192072
Cl	-1.698220	1.713989	0.159845
O	-0.768811	-0.000070	-2.108484
H	-1.320885	0.768738	-1.862079
H	-1.320083	-0.769565	-1.862447

Vib.Av.Geom.F1

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.030002	-0.000227	-0.052893
Cl	1.605243	1.680472	-0.580023
Cl	1.605860	-1.680265	-0.580937
Cl	-1.698529	-1.713181	0.159557
Cl	0.622058	0.000661	2.191756
Cl	-1.697357	1.713277	0.160040
O	-0.768552	-0.000983	-2.108545
H	-1.320411	0.768113	-1.862736
H	-1.320142	-0.770147	-1.862091

Vib.Av.Geom.F2

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.029964	0.000166	-0.052848
Cl	1.605866	1.680067	-0.580881

Cl	1.605007	-1.680740	-0.579916
Cl	-1.696719	-1.713778	0.159293
Cl	0.622168	-0.000174	2.191822
Cl	-1.698517	1.714017	0.159826
O	-0.768841	0.000729	-2.108413
H	-1.320640	0.769686	-1.861810
H	-1.320370	-0.768625	-1.862559

Vib.Av.Geom.G1

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.029972	-0.000158	-0.052806
Cl	1.604890	1.680648	-0.580109
Cl	1.605793	-1.680034	-0.580899
Cl	-1.698791	-1.713807	0.159853
Cl	0.622346	0.000105	2.192112
Cl	-1.696990	1.713623	0.159293
O	-0.768492	-0.000632	-2.108540
H	-1.320366	0.768442	-1.862582
H	-1.320033	-0.769854	-1.862240

Vib.Av.Geom.G2

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.030041	0.000083	-0.052783
Cl	1.605088	1.680785	-0.580761
Cl	1.605307	-1.680728	-0.580391
Cl	-1.697606	-1.713717	0.159686
Cl	0.622250	-0.000441	2.192199
Cl	-1.697723	1.713858	0.159335
O	-0.768274	0.000341	-2.108498
H	-1.319830	0.769636	-1.862412
H	-1.320192	-0.768668	-1.862464

Vib.Av.Geom.H1

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.030156	0.000000	-0.052848
Cl	1.605409	1.680489	-0.580765

Cl	1.605411	-1.680488	-0.580762
Cl	-1.698225	-1.712665	0.159982
Cl	0.621829	0.000002	2.191904
Cl	-1.698224	1.712665	0.159980
O	-0.767712	-0.000001	-2.108573
H	-1.319590	0.769100	-1.862723
H	-1.319563	-0.769126	-1.862733

Vib.Av.Geom.H2

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.030040	-0.000232	-0.052896
Cl	1.605217	1.680552	-0.579782
Cl	1.606098	-1.680099	-0.581315
Cl	-1.699049	-1.713307	0.159926
Cl	0.622039	0.000642	2.191762
Cl	-1.697102	1.713076	0.159678
O	-0.768412	-0.001138	-2.108480
H	-1.320411	0.767897	-1.862750
H	-1.319889	-0.770374	-1.862033

Vib.Av.Geom.H3

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.030079	0.000000	-0.052884
Cl	1.605615	1.680422	-0.580351
Cl	1.605617	-1.680421	-0.580348
Cl	-1.698056	-1.713357	0.159565
Cl	0.622440	0.000001	2.191756
Cl	-1.698056	1.713357	0.159563
O	-0.768577	-0.000001	-2.108457
H	-1.320325	0.769119	-1.862307
H	-1.320298	-0.769144	-1.862317

Vib.Av.Geom.I

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.029876	0.000008	-0.052848
Cl	1.605729	1.679784	-0.580069
Cl	1.605567	-1.680359	-0.580130

Cl	-1.697757	-1.713587	0.158999
Cl	0.622905	0.000448	2.191548
Cl	-1.698467	1.713801	0.159760
O	-0.769064	-0.000050	-2.108327
H	-1.321243	0.768665	-1.861880
H	-1.320250	-0.769628	-1.862321

Vib.Av.Geom.J

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.030087	0.000000	-0.052841
Cl	1.605418	1.680443	-0.580623
Cl	1.605420	-1.680442	-0.580621
Cl	-1.697972	-1.713421	0.159683
Cl	0.622115	0.000002	2.192167
Cl	-1.697971	1.713421	0.159681
O	-0.768281	-0.000001	-2.108601
H	-1.320007	0.769128	-1.862461
H	-1.319980	-0.769154	-1.862470

Table B.17: Vibrationally averaged geometries at 0K for the $^{35/37}\text{Cl}$ isotopologues and isotopomers^a of *cis*- $[\text{RhCl}_4(\text{H}_2^{16}\text{O})_2]^-$ calculated at the PBE0/SDD/6-31G* level [in Å].

Ref.Geom.

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.000008	-0.000005	-0.129817
Cl	0.503061	-1.670629	1.390530
Cl	2.270545	0.627392	-0.332794
Cl	-2.270557	-0.627408	-0.332764
Cl	-0.503043	1.670654	1.390521
O	-0.580470	1.477424	-1.567820
H	-0.577835	2.223394	-0.932291
H	-1.516001	1.177401	-1.585944
O	0.580423	-1.477404	-1.567812
H	1.515973	-1.177436	-1.585965
H	0.577774	-2.223422	-0.932342

Vib.Av.Geom.A

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.000014	-0.000017	-0.128604
Cl	0.503938	-1.671324	1.394422
Cl	2.274352	0.628877	-0.331621
Cl	-2.274373	-0.628893	-0.331588
Cl	-0.503923	1.671357	1.394420
O	-0.580698	1.480677	-1.580535
H	-0.566450	2.225604	-0.959468
H	-1.510414	1.187352	-1.595244
O	0.580639	-1.480606	-1.580482
H	1.510375	-1.187345	-1.595216
H	0.566377	-2.225632	-0.959496

Vib.Av.Geom.B

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.000082	0.000056	-0.128606
Cl	0.503577	-1.671321	1.394509
Cl	2.274467	0.628610	-0.331989
Cl	-2.274148	-0.629001	-0.331382
Cl	-0.504335	1.671270	1.394421
O	-0.580839	1.480816	-1.580405
H	-0.565619	2.225993	-0.959656
H	-1.510749	1.188061	-1.594269
O	0.580724	-1.480486	-1.580551
H	1.510302	-1.186766	-1.595828
H	0.567170	-2.225361	-0.959383

Vib.Av.Geom.C

	Coordinates (Angstroms)		
	X	Y	Z
Rh	-0.000008	-0.000107	-0.128625
Cl	0.504297	-1.671180	1.394128
Cl	2.274403	0.628538	-0.331593
Cl	-2.274570	-0.628574	-0.331569
Cl	-0.504288	1.671481	1.394319

O	-0.580794	1.480891	-1.580154
H	-0.566919	2.225527	-0.958692
H	-1.510425	1.187332	-1.595208
O	0.581032	-1.480707	-1.580482
H	1.510712	-1.187179	-1.594999
H	0.566863	-2.225715	-0.959506

Vib.Av.Geom.D

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.000014	-0.000017	-0.128569
Cl	0.503849	-1.671179	1.394611
Cl	2.274437	0.628563	-0.331903
Cl	-2.274456	-0.628579	-0.331871
Cl	-0.503834	1.671212	1.394609
O	-0.581564	1.480369	-1.580560
H	-0.567844	2.225317	-0.959525
H	-1.511065	1.186279	-1.595113
O	0.581504	-1.480299	-1.580507
H	1.511025	-1.186268	-1.595091
H	0.567777	-2.225342	-0.959552

Vib.Av.Geom.E

	Coordinates (Angstroms)		
	X	Y	Z
Rh	-0.000016	-0.000086	-0.128556
Cl	0.503854	-1.671155	1.394238
Cl	2.274742	0.628275	-0.332077
Cl	-2.274200	-0.628565	-0.331318
Cl	-0.504766	1.671384	1.394406
O	-0.580994	1.480713	-1.580282
H	-0.566625	2.225622	-0.959171
H	-1.510705	1.187412	-1.594811
O	0.581218	-1.480182	-1.580749
H	1.510696	-1.185959	-1.595660
H	0.567895	-2.225318	-0.959934

Vib.Av.Geom.F

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.000015	-0.000017	-0.128587
Cl	0.504237	-1.671438	1.394150
Cl	2.274513	0.628541	-0.331586
Cl	-2.274536	-0.628557	-0.331554
Cl	-0.504222	1.671469	1.394147
O	-0.581021	1.480561	-1.580523
H	-0.567242	2.225420	-0.959375
H	-1.510600	1.186782	-1.595365
O	0.580960	-1.480486	-1.580465
H	1.510564	-1.186768	-1.595344
H	0.567175	-2.225449	-0.959396

Vib.Av.Geom.G

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.000002	-0.000147	-0.128501
Cl	0.503925	-1.671167	1.394443
Cl	2.274337	0.628635	-0.331875
Cl	-2.274493	-0.628571	-0.331976
Cl	-0.503805	1.671472	1.394514
O	-0.581368	1.480295	-1.580366
H	-0.567461	2.225304	-0.959372
H	-1.510930	1.186407	-1.594904
O	0.581360	-1.480099	-1.580843
H	1.510942	-1.186225	-1.595183
H	0.567410	-2.225436	-0.960288

Vib.Av.Geom.H

	Coordinates (Angstroms)		
	X	Y	Z

Rh	0.000096	0.000064	-0.128586
Cl	0.503847	-1.671388	1.394242
Cl	2.274641	0.628269	-0.331957
Cl	-2.274292	-0.628709	-0.331317
Cl	-0.504630	1.671380	1.394186
O	-0.581120	1.480627	-1.580448
H	-0.566441	2.225768	-0.959657
H	-1.510878	1.187374	-1.594490
O	0.580986	-1.480282	-1.580643
H	1.510435	-1.186105	-1.596093
H	0.567938	-2.225145	-0.959458

Vib.Av.Geom.I

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.000014	-0.000017	-0.128554
Cl	0.503950	-1.671382	1.394366
Cl	2.274438	0.628550	-0.331857
Cl	-2.274458	-0.628566	-0.331824
Cl	-0.503934	1.671414	1.394363
O	-0.581411	1.480284	-1.580640
H	-0.567644	2.225305	-0.959701
H	-1.510933	1.186275	-1.595205
O	0.581349	-1.480211	-1.580584
H	1.510897	-1.186257	-1.595186
H	0.567580	-2.225332	-0.959722

^aSee Figure 4.3 for an explanation of the labelling scheme.

Table B.18: Vibrationally averaged geometries at 0K for the ^{35/37}Cl isotopologues and isotopomers^a of *fac*-[RhCl₃(H₂¹⁶O)₃]²⁻ calculated at the PBE0/SDD/6-31G* level [in Å].

Ref.Geom.

	Coordinates (Angstroms)		
	X	Y	Z

Rh	0.000000	0.000000	0.220087
O	0.000000	-1.801260	1.350249
O	-1.559937	0.900630	1.350249
O	1.559937	0.900630	1.350249
Cl	0.000000	1.983580	-0.942639
Cl	1.717831	-0.991790	-0.942639
Cl	-1.717831	-0.991790	-0.942639
H	0.772646	-2.258670	0.960783
H	-2.342389	0.460204	0.960783
H	1.569743	1.798466	0.960783
H	2.342389	0.460204	0.960783
H	-1.569743	1.798466	0.960783
H	-0.772646	-2.258670	0.960783

Vib.Av.Geom.A

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.000000	-0.000036	0.218933
O	0.000000	-1.807489	1.360429
O	-1.564796	0.903590	1.361009
O	1.564798	0.903591	1.361012
Cl	0.000001	1.982988	-0.948283
Cl	1.718035	-0.991338	-0.947752
Cl	-1.718035	-0.991339	-0.947752
H	0.763712	-2.265781	0.988076
H	-2.343489	0.470840	0.989078
H	1.580059	1.793831	0.987871
H	2.343480	0.470837	0.989064
H	-1.580079	1.793843	0.987902
H	-0.763713	-2.265766	0.988059

Vib.Av.Geom.B

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.000000	-0.000004	0.218980
O	0.000000	-1.807098	1.360879
O	-1.565095	0.903616	1.360743
O	1.565095	0.903616	1.360743
Cl	0.000000	1.983485	-0.947582

Cl	1.717504	-0.991748	-0.948007
Cl	-1.717504	-0.991748	-0.948007
H	0.763705	-2.265560	0.988723
H	-2.343639	0.471054	0.988318
H	1.580052	1.793961	0.987820
H	2.343639	0.471054	0.988318
H	-1.580052	1.793961	0.987820
H	-0.763705	-2.265560	0.988723

Vib.Av.Geom.C

	Coordinates (Angstroms)		
	X	Y	Z
Rh	-0.000037	-0.000019	0.219024
O	0.000150	-1.807324	1.360693
O	-1.565133	0.903790	1.360719
O	1.564977	0.903525	1.360996
Cl	0.000205	1.983215	-0.947790
Cl	1.717624	-0.991428	-0.947791
Cl	-1.717678	-0.991697	-0.947856
H	0.763404	-2.265826	0.987659
H	-2.343743	0.470978	0.988718
H	1.579802	1.794028	0.988480
H	2.343557	0.471224	0.988322
H	-1.580319	1.793959	0.987415
H	-0.764035	-2.265449	0.989123

Vib.Av.Geom.D

	Coordinates (Angstroms)		
	X	Y	Z
Rh	0.000000	-0.000010	0.219072
O	0.000000	-1.807525	1.360395
O	-1.564913	0.903644	1.361017
O	1.564913	0.903643	1.361017
Cl	0.000000	1.982830	-0.948060
Cl	1.717971	-0.991319	-0.947620
Cl	-1.717971	-0.991320	-0.947620
H	0.763708	-2.265798	0.988027
H	-2.343514	0.470842	0.988971

H	1.580163	1.793871	0.987864
H	2.343514	0.470845	0.988968
H	-1.580166	1.793870	0.987862
H	-0.763713	-2.265795	0.988033

^aSee Figure 4.3 for an explanation of the labelling scheme.