Supporting Information

The van der Waals interactions in systems involving superheavy elements: the case of Oganession (Z=118)

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Abstract

This work presents a study involving dimers composed of He, Ne, Ar, Kr, Xe, Rn, and Og noble gases with the Oganesson, a super-heavy closed-shell element (Z=118).

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The He-Og, Ne-Og, Ar-Og, Kr-Og, Xe-Og, Rn-Og, and Og-Og ground state electronic potential energy curves were calculated based on the 4-component (4c) Dirac-Coulomb Hamiltonian and were counterpoise corrected. For the 4c calculations, the electron correlation was taken into account using the same methodology (MP2-srLDA) and basis set quality (Dyall´s acv3z and Dunning´s aug-cc-PVTZ). All calculations included quantum electrodynamics effects at the Gaunt interaction level. For all aforementioned dimers vibration energies, spectroscopic constants (ω_e, $\omega_e x_e$, $\omega_e y_e$, α_e, and γ_e), and lifetime as a function of the temperature (which ranged from 200 to 500K) were also calculated. Obtained results suggest that the inclusion of quantum electrodynamics effects reduces the value of the dissociation energy of all hetero-nuclear molecules with a percentage contribution ranging from 0.48% (for the He-Og dimer) to 9.63% (for the Rn-Og dimer). The lifetime calculations indicate that the Og-He dimer is close to the edge of instability and that Ng-Og dimers are relatively less stable when Gaunt correction is considered. Exploiting scaling laws, that adopt the polarizability of involved partners as scaling factors, it has been also demonstrated that in such systems the interaction is of van der Waals nature (size repulsion plus dispersion attraction) and this permitted an estimation of dissociation energy and equilibrium distance in Og-Og dimer. This further information has been exploited to evaluate the rovibrational levels in this symmetric dimer and to cast light on macroscopic properties of condensed phases concerning the complete noble gas family, emphasizing some anomalies of Og.

This Supporting Information includes the He-Og, Ne-Og, Ar-Og, Kr-Og, Xe-Og, Rn-Og, and Og-Og *ab initio* electronic energies (Section S1); He-Og, Ne-Og, Ar-Og, Kr-Og, Xe-Og, Rn-Og, and Og-Og pure vibrational ($j = 0$) and rovibrational ($j = 1$) energies calculated through Rydberg potential energy curves with Gaunt+BSSE correction (Section S2); Plots of *Ab initio* and adjusted potential energy curves (with ILJ and Rydberg forms) for the He-Og, Ne-Og, Ar-Og, Kr-Og, Xe-Og, Rn-Og, and Og-Og systems (Section S3).

S1. He-Og, Ne-Og, Ar-Og, Kr-Og, Xe-Og, Rn-Og, and Og-Og *Ab initio* electronic energies

He-Og, Ne-Og, Ar-Og, Kr-Og, Xe-Og, and Rn-Og *ab initio* electronic energies calculated with and without the inclusion of quantum electrodynamics effects (at the Gaunt interaction) and with Gaunt+BSSE (Basis Set Superposition Error) corrections (Tables S1-S6). Table S7 shows the Og-Og *ab initio* electronic energies calculated with Gaunt+BSSE corrections.

Table S1: He-Og electronic energies calculated at $CAMB3LYP + MP2/He = aug - cc - pVTZ/Og = dyall.acv3z$ level with and without inclusion of quantum electrodynamics effects at the Gaunt interaction level. The He-Og Gaunt+BSSE electronic energies were performed at MP2-srLDA/He=aug-cc-PVTZ/Og=dyall.acv3z level.

He-Og		He-Og-Gaunt		He-Og-Gaunt+BSSE	
R(Å)	Energy (hartree)	R(Å)	Energy (hartree)	R(Å)	Energy (hartree)
3.40	-54864.6023410742	3.40	-54754.7514705928	3.00	-54754.7487195103
3.50	-54864.6026213667	3.50	-54754.7517528342	3.10	-54754.7497226718
3.60	-54864.6028249878	3.60	-54754.751957931	3.20	-54754.7504557216
3.70	-54864.6029822819	3.70	-54754.7521163546	3.30	-54754.75099741
3.80	-54864.6030908389	3.80	-54754.752225766	3.40	-54754.7514007072
3.90	-54864.6031583736	3.90	-54754.7522939587	3.50	-54754.7516880018
4.00	-54864.6032084915	4.00	-54754.7523445697	3.60	-54754.7518966734
4.10	-54864.6032445578	4.10	-54754.7523810111	3.70	-54754.7520532617

4.20	-54864.603273997	4.20	-54754.7524107417	3.80	-54754.7521611737
4.30	-54864.6032830708	4.30	-54754.7524200278	3.90	-54754.7522334742
4.40	-54864.6032877662	4.40	-54754.7524248959	4.00	-54754.7522882529
4.50	-54864.6032945942	4.50	-54754.7524318544	4.10	-54754.7523273466
4.51	-54864.6032952722	4.51	-54754.7524325403	4.20	-54754.7523489514
4.52	-54864.6032959004	4.52	-54754.7524331721	4.30	-54754.7523612019
4.53	-54864.6032964785	4.53	-54754.7524337647	4.40	-54754.7523717564
4.54	-54864.6032970355	4.54	-54754.7524343285	4.45	-54754.7523758893
4.55	-54864.6032975371	4.55	-54754.7524348441	4.50	-54754.7523787201
4.56	-54864.6032979973	4.56	-54754.7524353133	**4.55**	**-54754.7523791654**
4.57	-54864.6032983967	4.57	-54754.7524357196	4.60	-54754.7523783887
4.58	-54864.6032987231	4.58	-54754.7524360585	4.70	-54754.7523751697
4.59	-54864.6032989729	4.59	-54754.7524363195	4.80	-54754.7523736019
4.60	-54864.6032991368	4.60	-54754.7524364908	4.90	-54754.7523730373
4.61	-54864.6032992143	4.61	-54754.7524365822	5.00	-54754.7523701321
4.62	**-54864.6032992843**	**4.62**	**-54754.7524366578**	5.10	-54754.7523645543
4.63	-54864.6032992418	4.63	-54754.7524366174	5.20	-54754.7523595376
4.64	-54864.603299092	4.64	-54754.7524364786	5.30	-54754.7523570746
4.65	-54864.6032988551	4.65	-54754.7524362528	5.40	-54754.7523556018
4.66	-54864.603298548	4.66	-54754.7524359543	5.50	-54754.7523525841
4.67	-54864.6032981657	4.67	-54754.7524355783	5.60	-54754.7523478556
4.68	-54864.6032977333	4.68	-54754.7524351493	5.70	-54754.7523438344
4.69	-54864.6032972472	4.69	-54754.7524346724	5.80	-54754.7523420151
4.70	-54864.6032966886	4.70	-54754.7524341175	5.90	-54754.7523414006
4.80	-54864.6032897408	4.80	-54754.7524272273	6.00	-54754.752339991
4.90	-54864.6032849568	4.90	-54754.7524224932	6.10	-54754.752337091
5.00	-54864.6032841637	5.00	-54754.752421733	6.20	-54754.7523338918

5.10	-54864.6032833746	5.10	-54754.7524209655	6.30	-54754.7523320678
5.20	-54864.6032788508	5.20	-54754.7524164687	6.40	-54754.7523317559
5.30	-54864.6032715674	5.30	-54754.7524091902	6.50	-54754.7523317426
5.40	-54864.6032659011	5.40	-54754.7524035462	6.60	-54754.7523308424
5.50	-54864.6032641319	5.50	-54754.7524017841	6.70	-54754.7523289
5.60	-54864.6032642095	5.60	-54754.7524018654	6.80	-54754.7523268728
5.70	-54864.6032627231	5.70	-54754.7524003847	6.90	-54754.7523257982
5.80	-54864.6032580688	5.80	-54754.7523957401	7.00	-54754.7523258167
5.90	-54864.6032529407	5.90	-54754.7523906145	7.10	-54754.7523261354
6.00	-54864.6032500665	6.00	-54754.752387732	7.20	-54754.7523259504
6.10	-54864.6032499727	6.10	-54754.7523876468	7.30	-54754.7523249649
6.20	-54864.6032507095	6.20	-54754.7523883816	7.40	-54754.7523236148
6.30	-54864.6032499453	6.30	-54754.7523876251	7.50	-54754.7523226114
6.40	-54864.6032471679	6.40	-54754.7523848443	7.60	-54754.7523223628
6.50	-54864.6032437135	6.50	-54754.7523813865	7.70	-54754.7523226363
6.60	-54864.603241395	6.60	-54754.7523790724	7.80	-54754.7523229462
6.70	-54864.6032410069	6.70	-54754.7523786873	7.90	-54754.7523228368
6.80	-54864.6032417232	6.80	-54754.752379407	8.00	-54754.7523222599
6.90	-54864.60324209	6.90	-54754.7523797652	8.10	-54754.7523214432
7.00	-54864.6032413548	7.00	-54754.7523790347	8.20	-54754.7523208004
7.10	-54864.6032392569	7.10	-54754.7523769367	8.30	-54754.7523206012
7.20	-54864.603237266	7.20	-54754.752374948	8.40	-54754.752320747
7.30	-54864.6032361786	7.30	-54754.7523738622	8.50	-54754.7523200152
7.40	-54864.6032361646	7.40	-54754.7523738422		-
7.50	-54864.6032369222	7.50	-54754.7523745964		-
7.60	-54864.6032373402	7.60	-54754.752375024	-	-
7.70	-54864.6032371531	7.70	-54754.7523748372	-	-

7.80	-54864.603236068	7.80	-54754.7523737497	-	-
7.90	-54864.6032348459	7.90	-54754.7523725244	-	-
8.00	-54864.6032339105	8.00	-54754.752371598	-	-
8.10	-54864.6032334479	8.10	-54754.7523711305	-	-
8.20	-54864.6032337065	8.20	-54754.7523713867	-	-
8.30	-54864.6032341711	8.30	-54754.7523718502	-	-
8.40	-54864.6032343651	8.40	-54754.7523720489	-	-
8.50	-54864.6032342699	8.50	-54754.7523719563	-	-

Table S2: Ne-Og electronic energies calculated at $CAMB3LYP + MP2/He = aug - cc - pVTZ/Og = dyall.acv3z$ level with and without inclusion of quantum electrodynamics effects at the Gaunt interaction level. The Ne-Og Gaunt+BSSE electronic energies were performed at MP2-srLDA/Ne=aug-cc-PVTZ/Og=dyall.acv3z level.

Ne-Og		Ne-Og-Gaunt		Ne-Og-Gaunt+BSSE	
R(Å)	Energy (hartree)	R(Å)	Energy (hartree)	R(Å)	Energy (hartree)
3.50	-54889.2696782482	3.50	-54882.590072872	2.40	54880.24834124630
3.60	-54889.2699875566	3.60	-54882.5903817458	2.50	-54880.25994892560
3.70	-54889.2701970342	3.70	-54882.5905908259	2.60	-54880.26834491500
3.80	-54889.2703352244	3.80	-54882.5907286563	2.70	-54880.27440762500
3.90	-54889.2704229254	3.90	-54882.5908160507	2.80	-54880.27878517040
4.00	-54889.2704752151	4.00	-54882.5908680905	2.90	-54880.28193900550
4.10	-54889.2705029729	4.10	-54882.5908956353	3.00	-54880.28420238310
4.20	**-54889.2705139855**	**4.20**	**-54882.5909064763**	3.10	-54880.28582941170
4.30	-54889.2705138227	4.30	-54882.5909061793	3.20	-54880.28698744940
4.40	-54889.2705064657	4.40	-54882.5908987146	3.30	-54880.28780890890
4.50	-54889.2704947164	4.50	-54882.5908868848	3.40	-54880.28839001590
4.60	-54889.2704805591	4.60	-54882.5908726636	3.50	-54880.28879236500
4.70	-54889.270465351	4.70	-54882.5908574089	3.60	-54880.28906823210
4.80	-54889.270450007	4.80	-54882.5908420308	3.70	-54880.28925604980
4.90	-54889.2704351182	4.90	-54882.5908271138	3.80	-54880.28937948290
5.00	-54889.2704210317	5.00	-54882.5908130108	3.90	-54880.28945701080
5.20	-54889.2703958868	5.20	-54882.5907878453	4.00	-54880.28950402030
5.40	-54889.2703748887	5.40	-54882.590766839	4.10	-54880.28953104580
5.60	-54889.2703575862	5.60	-54882.5907495356	4.20	-54880.28954349090
6.00	-54889.2703316134	6.00	-54882.5907235705	**4.30**	**-54880.28954459220**
7.00	-54889.2702983313	7.00	-54882.5906903002	4.40	-54880.28954002650

8.00	-54889.2702865808	8.00	-54882.5906785553	4.50	-54880.28953326940
9.00	-54889.2702818539	9.00	-54882.5906738329	4.60	-54880.28952418020
10.00	-54889.2702796023	10.00	-54882.5906715826	4.70	-54880.28951149730
-	-	-	-	4.80	-54880.28949862320
-	-	-	-	4.90	-54880.28948810630
-	-	-	-	5.00	-54880.28947850670
-	-	-	-	5.10	-54880.28946706310
-	-	-	-	5.20	-54880.28945532830
-	-	-	-	5.30	-54880.28944621770
-	-	-	-	5.40	-54880.28943966530
-	-	-	-	5.50	-54880.28943293460
-	-	-	-	5.60	-54880.28942476670
-	-	-	-	5.70	-54880.28941695470
-	-	-	-	5.80	-54880.28941164170
-	-	-	-	5.90	-54880.28940823590
-	-	-	-	6.00	-54880.28940461470
-	-	-	-	6.10	-54880.28939972420
-	-	-	-	6.20	-54880.28939469530
-	-	-	-	6.30	-54880.28939112600
-	-	-	-	6.40	-54880.28938917910
-	-	-	-	6.50	-54880.28938767370
-	-	-	-	6.60	-54880.28938545290
-	-	-	-	6.70	-54880.28938253160
-	-	-	-	6.80	-54880.28937980270
-	-	-	-	6.90	-54880.28937802980
-	-	-	-	7.00	-54880.28937708140
-	-	-	-	7.10	-54880.28937630280

				7.20	-54880.28937526860
-	-	-	-	7.30	-54880.28937381360
-	-	-	-	7.40	-54880.28937225740
-	-	-	-	7.50	-54880.28937115350
-	-	-	-	7.60	-54880.28937035660
-	-	-	-	7.70	-54880.28936993000
-	-	-	-	7.80	-54880.28936945850
-	-	-	-	7.90	-54880.28936911090
-	-	-	-	8.00	-54880.28936817880
-	-	-	-	8.10	-54880.28936749340
-	-	-	-	8.20	-54880.28936686920
-	-	-	-	8.30	-54880.28936640220
-	-	-	-	8.40	-54880.28936615100
-	-	-	-	8.50	-54880.28936580020

Table S3: Ar-Og electronic energies calculated at $CAMB3LYP + MP2/Ar = aug - cc - pVTZ/Og = dyall.acv3z$ level with and without inclusion of quantum electrodynamics effects at the Gaunt interaction level. level. The Ar-Og Gaunt+BSSE electronic energies were performed at MP2-srLDA/Ar=aug-cc-PVTZ/Og=dyall.acv3z level.

Ar-Og		Ar-Og-Gaunt		Ar-Og-Gaunt+BSSE	
R(Å)	Energy (hartree)	R(Å)	Energy (hartree)	R(Å)	Energy (hartree)
3.40	-55389.5676845601	3.40	-55279.5758847709	2.50	-55279.4873847739
3.50	-55389.5691809015	3.50	-55279.5773928159	2.60	-55279.5121426477
3.60	-55389.5702382361	3.60	-55279.5784591849	2.70	-55279.5304771094
3.70	-55389.570936121	3.70	-55279.5791640491	2.80	-55279.5440059455
3.80	-55389.5714261727	3.80	-55279.5796594764	2.90	-55279.5540433017
3.90	-55389.5717773439	3.90	-55279.5800147897	3.00	-55279.5614314924

4.00	-55389.5719768837	4.00	-55279.5802175126	3.10	-55279.5668382163
4.10	-55389.5720707877	4.10	-55279.5803138614	3.20	-55279.5708386749
4.20	-55389.5721355812	4.20	-55279.5803805325	3.30	-55279.5737335385
4.21	-55389.5721413178	4.21	-55279.5803864263	3.40	-55279.5757979574
4.22	-55389.5721468003	4.22	-55279.5803920702	3.50	-55279.5773139869
4.23	-55389.5721520141	4.23	-55279.5803974333	3.60	-55279.5783873707
4.24	-55389.5721568918	4.24	-55279.5804024588	3.70	-55279.579098166
4.25	-55389.5721613852	4.25	-55279.5804070932	3.80	-55279.5795986381
4.26	-55389.572165429	4.26	-55279.5804112802	3.90	-55279.5799581121
4.27	-55389.5721689933	4.27	-55279.5804149869	4.00	-55279.5801641434
4.28	-55389.5721720444	4.28	-55279.5804181669	4.10	-55279.5802631519
4.29	-55389.5721745504	4.29	-55279.5804208048	4.20	-55279.5803316275
4.30	-55389.5721765122	4.30	-55279.5804228898	**4.30**	**-55279.5803749783**
4.31	-55389.5721778881	4.31	-55279.5804243921	4.40	-55279.5803640232
4.32	-55389.5721786439	4.32	-55279.5804252814	4.50	-55279.5803170492
4.33	**-55389.5721787792**	**4.33**	**-55279.5804255213**	4.60	-55279.5802792511
4.34	-55389.5721783397	4.34	-55279.5804251941	4.70	-55279.580255906
4.35	-55389.5721772908	4.35	-55279.5804242527	4.80	-55279.5802193646
4.36	-55389.5721756706	4.36	-55279.5804227445	4.90	-55279.5801609926
4.37	-55389.5721735166	4.37	-55279.5804207004	5.00	-55279.5801038517
4.38	-55389.5721708514	4.38	-55279.580418137	5.10	-55279.5800678254
4.39	-55389.5721676623	4.39	-55279.5804150475	5.20	-55279.5800442371
4.40	-55389.572164005	4.40	-55279.5804114925	5.30	-55279.5800137002
4.50	-55389.5721163036	4.50	-55279.5803646312	5.40	-55279.5799712554
4.60	-55389.5720780659	4.60	-55279.5803270327	5.50	-55279.5799300909
4.70	-55389.5720545873	4.70	-55279.5803040549	5.60	-55279.579903557
4.80	-55389.5720179245	4.80	-55279.5802677788	5.70	-55279.5798896849

4.90	-55389.5719593627	4.90	-55279.5802095203	5.80	-55279.5798764564
5.00	-55389.5719019626	5.00	-55279.5801523568	5.90	-55279.5798552132
5.10	-55389.5718653447	5.10	-55279.5801159238	6.00	-55279.5798283808
5.20	-55389.5718411473	5.20	-55279.5800918759	6.10	-55279.5798054351
5.30	-55389.5718098129	5.30	-55279.5800606672	6.20	-55279.5797928576
5.40	-55389.5717664721	5.40	-55279.5800174145	6.30	-55279.5797882534
5.50	-55389.5717243053	5.50	-55279.579975343	6.40	-55279.5797838318
5.60	-55389.5716966313	5.60	-55279.5799477457	6.50	-55279.5797738351
5.70	-55389.5716817979	5.70	-55279.5799329716	6.60	-55279.5797585632
5.80	-55389.5716671575	5.80	-55279.5799183893	6.70	-55279.5797434296
5.90	-55389.5716447419	5.90	-55279.5798960284	6.80	-55279.5797341502
6.00	-55389.5716167989	6.00	-55279.5798681347	6.90	-55279.5797318277
6.10	-55389.5715928133	6.10	-55279.5798442025	7.00	-55279.579732624
6.20	-55389.5715792602	6.20	-55279.579830688	7.10	-55279.579731466
6.30	-55389.571573734	6.30	-55279.5798252115	7.20	-55279.5797256122
6.40	-55389.5715684818	6.40	-55279.5798200006	7.30	-55279.5797162195
6.50	-55389.57155774	6.50	-55279.5798092984	7.40	-55279.5797071091
6.60	-55389.5715417673	6.60	-55279.579793363	7.50	-55279.579701827
6.70	-55389.5715259934	6.70	-55279.5797776261	7.60	-55279.5797013724
6.80	-55389.571516191	6.80	-55279.5797678501	7.70	-55279.5797035301
6.90	-55389.5715134069	6.90	-55279.5797651005	7.80	-55279.579704958
7.00	-55389.5715139411	7.00	-55279.5797656721	7.90	-55279.5797034353
7.10	-55389.5715122368	7.10	-55279.579764001	8.00	-55279.5796987453
7.20	-55389.5715060931	7.20	-55279.5797578857	8.10	-55279.5796926919
7.30	-55389.5714964706	7.30	-55279.5797482923	8.20	-55279.5796877923
7.40	-55389.5714870196	7.40	-55279.579738873	8.30	-55279.5796857631
7.50	-55389.5714815991	7.50	-55279.5797334744	8.40	-55279.579686547

7.60	-55389.5714807069	7.60	-55279.5797326157	8.50	-55279.5796888353
7.70	-55389.5714826947	7.70	-55279.5797346282	8.75	-55279.5796891117
7.80	-55389.5714836661	7.80	-55279.5797356308	9.00	-55279.5796809685
7.90	-55389.5714818282	7.90	-55279.5797338154	9.25	-55279.579679295
8.00	-55389.5714769403	8.00	-55279.5797289618	9.50	-55279.579682779
8.10	-55389.5714705754	8.10	-55279.5797226189	10.00	-55279.5796763134
8.20	-55389.5714655173	8.20	-55279.5797175854	12.50	-55279.5796756215
8.30	-55389.5714632741	8.30	-55279.5797153635	15.00	-55279.5796765914
8.40	-55389.5714638579	8.40	-55279.5797159761	-	-
8.50	-55389.5714659362	8.50	-55279.5797180735	-	-

Table S4: Kr-Og electronic energies calculated at $CAMB3LYP + MP2/Kr = dyall.acv3z/Og = dyall.acv3z$ level with and without inclusion of quantum electrodynamics effects at the Gaunt interaction level. The Kr-Og Gaunt+BSSE electronic energies were performed at MP2-srLDA/Kr=aug-cc-PVTZ/Og=dyall.acv3z level.

Kr-Og		Kr-Og-Gaunt		Kr-Og-Gaunt+BSSE	
R(Å)	Energy (hartree)	R(Å)	Energy (hartree)	R(Å)	Energy (hartree)
3.50	-57648.8554139482	3.50	-57537.4274015089	2.50	-57537.3005424645
3.60	-57648.857010416	3.60	-57537.4290134988	2.60	-57537.3348558743
3.70	-57648.8581204207	3.70	-57537.4301357445	2.70	-57537.3605434433
3.80	-57648.8588686459	3.80	-57537.4308936562	2.80	-57537.379564124
3.90	-57648.8593896075	3.90	-57537.4314222679	2.90	-57537.393752308
4.00	-57648.8597417706	4.00	-57537.431780534	3.00	-57537.4043187374
4.10	-57648.8599419881	4.10	-57537.431985628	3.10	-57537.4120732953
4.20	-57648.8600415959	4.20	-57537.4320891413	3.20	-57537.4178225983
4.30	-57648.8600944952	4.30	-57537.4321452078	3.30	-57537.4220682262
4.31	-57648.8600980391	4.31	-57537.4321490343	3.40	-57537.4251232608
4.32	-57648.8601012259	4.32	-57537.4321524949	3.50	-57537.4273355699
4.33	-57648.8601040796	4.33	-57537.4321556239	3.60	-57537.4289513962
4.34	-57648.8601065035	4.34	-57537.4321583189	3.70	-57537.4300771903
4.35	-57648.8601085167	4.35	-57537.4321605854	3.80	-57537.4308384069
4.36	-57648.8601101843	4.36	-57537.4321625157	3.90	-57537.4313701814
4.37	-57648.8601113758	4.37	-57537.4321639434	4.00	-57537.4317313023
4.38	-57648.8601121267	4.38	-57537.4321649477	4.10	-57537.4319392499
4.39	**-57648.8601123469**	4.39	-57537.4321654009	4.20	-57537.4320455043
4.40	-57648.8601121441	**4.40**	**-57537.4321654369**	4.30	-57537.4321039939
4.41	-57648.8601113574	4.41	-57537.4321648893	**4.40**	**-57537.4321264825**
4.42	-57648.8601102183	4.42	-57537.4321639677	4.50	-57537.4321039145
4.43	-57648.8601085892	4.43	-57537.4321625657	4.60	-57537.4320527531

4.44	-57648.8601064984	4.44	-57537.4321606988	4.70	-57537.432000874
4.45	-57648.8601039698	4.45	-57537.4321583718	4.80	-57537.4319548573
4.46	-57648.8601009633	4.46	-57537.4321555857	4.90	-57537.4319009349
4.47	-57648.8600975724	4.47	-57537.4321523978	5.00	-57537.4318340669
4.48	-57648.8600938376	4.48	-57537.4321488633	5.10	-57537.431768883
4.49	-57648.8600897423	4.49	-57537.4321449715	5.20	-57537.4317180261
4.50	-57648.8600853142	4.50	-57537.4321407433	5.30	-57537.4316772768
4.60	-57648.8600304215	4.60	-57537.4320876161	5.40	-57537.4316338931
4.70	-57648.8599752964	4.70	-57537.4320339872	5.50	-57537.4315840158
4.80	-57648.8599263962	4.80	-57537.4319863593	5.60	-57537.4315374041
4.90	-57648.8598699725	4.90	-57537.4319310482	5.70	-57537.4315030503
5.00	-57648.859800846	5.00	-57537.4318628678	5.80	-57537.431479069
5.10	-57648.8597336824	5.10	-57537.4317965626	5.90	-57537.431456173
5.20	-57648.8596810373	5.20	-57537.4317446913	6.00	-57537.4314279526
5.30	-57648.8596386943	5.30	-57537.4317030458	6.10	-57537.4313972589
5.40	-57648.8595938038	5.40	-57537.4316587816	6.20	-57537.4313720131
5.50	-57648.8595425854	5.50	-57537.4316081401	6.30	-57537.4313561297
5.60	-57648.8594946097	5.60	-57537.4315607159	6.40	-57537.4313460868
5.70	-57648.8594592476	5.70	-57537.4315258601	6.50	-57537.4313353941
5.80	-57648.859434015	5.80	-57537.4315011143	6.60	-57537.4313203664
5.90	-57648.8594101336	5.90	-57537.4314776914	6.70	-57537.431302614
6.00	-57648.8593810519	6.00	-57537.4314490483	6.80	-57537.4312872287
6.10	-57648.8593495913	6.10	-57537.4314180102	6.90	-57537.4312776785
6.20	-57648.859323671	6.20	-57537.4313924809	7.00	-57537.4312732602
6.30	-57648.8593070816	6.30	-57537.4313762657	7.10	-57537.4312700707
6.40	-57648.859296418	6.40	-57537.4313659797	7.20	-57537.4312646292
6.50	-57648.8592851182	6.50	-57537.4313550365	7.30	-57537.4312559993

6.60	-57648.8592695256	6.60	-57537.431339797	7.40	-57537.4312459701
6.70	-57648.8592512233	6.70	-57537.4313218171	7.50	-57537.4312375231
6.80	-57648.8592352953	6.80	-57537.431306216	7.60	-57537.431232706
6.90	-57648.8592252691	6.90	-57537.4312964947	7.80	-57537.4312307359
7.00	-57648.859220569	7.00	-57537.4312921012	7.90	-57537.4312292788
7.10	-57648.8592167945	7.10	-57537.4312886129	8.00	-57537.4312256464
7.20	-57648.8592109633	7.20	-57537.4312830658	8.10	-57537.4312203385
7.30	-57648.8592019851	7.30	-57537.4312743669	8.20	-57537.4312147891
7.40	-57648.8591916271	7.40	-57537.4312642797	8.30	-57537.4312105184
7.50	-57648.8591829542	7.50	-57537.4312558594	8.40	-57537.4312085539
7.60	-57648.8591777144	7.60	-57537.4312508783	-	-
7.70	-57648.859175838	7.70	-57537.4312492543	-	-
7.80	-57648.8591749457	7.80	-57537.4312486028	-	-
7.90	-57648.859173096	7.90	-57537.4312469932	-	-
8.00	-57648.859169225	8.00	-57537.4312433492	-	-
8.10	-57648.8591635117	8.10	-57537.4312378629	-	-
8.20	-57648.8591577659	8.20	-57537.4312323365	-	-
8.30	-57648.8591532846	8.30	-57537.4312280639	-	-
8.40	-57648.8591508895	8.40	-57537.4312258868	-	-
8.50	-57648.8591505	8.50	-57537.4312256918	-	-

Table S5: Xe-Og electronic energies calculated at $CAMB3LYP + MP2/Xe = dyall.acv3z/Og = dyall.acv3z$ level with and without inclusion of quantum electrodynamics effects at the Gaunt interaction level. The Xe-Og Gaunt+BSSE electronic energies were performed at MP2-srLDA/Xe=dyall.acv3z/Og=dyall.acv3z level.

Xe-Og		Xe-Og-Gaunt		Xe-Og-Gaunt+BSSE	
R(Å)	Energy (hartree)	R(Å)	Energy (hartree)	R(Å)	Energy (hartree)
3.50	-62306.1585157583	3.50	-62189.8728576908	3.00	-62189.8352712549
3.60	-62306.1612353271	3.60	-62189.8756053701	3.10	-62189.8477173838
3.70	-62306.1632113887	3.70	-62189.8776041286	3.20	-62189.8569832655
3.80	-62306.1646082519	3.80	-62189.8790193736	3.30	-62189.8639081223
3.90	-62306.1655735257	3.90	-62189.8799995637	3.40	-62189.8690523731
4.00	-62306.1662403753	4.00	-62189.8806785803	3.50	-62189.8728110911
4.10	-62306.1666851096	4.10	-62189.8811332959	3.60	-62189.8755629599
4.20	-62306.1669538065	4.20	-62189.8814102121	3.70	-62189.877565705
4.30	-62306.1670987733	4.30	-62189.8815620303	3.80	-62189.8789847848
4.35	-62306.1671404557	4.35	-62189.881606705	3.90	-62189.8799683648
4.40	-62306.167167221	4.40	-62189.8816362281	4.00	-62189.880650638
4.45	-62306.1671810561	4.45	-62189.8816525876	4.10	-62189.8811086713
4.46	-62306.1671824797	4.46	-62189.8816544957	4.20	-62189.881388695
4.47	-62306.1671831949	4.47	-62189.8816557027	4.30	-62189.8815435493
4.48	**-62306.1671835665**	4.48	-62189.8816565286	4.40	-62189.8816205378
4.49	-62306.167183481	**4.49**	**-62189.8816569113**	**4.50**	**-62189.8816437484**
4.50	-62306.1671829536	4.50	-62189.8816568451	4.60	-62189.8816222508
4.51	-62306.1671819667	4.51	-62189.8816562996	4.70	-62189.8815699206
4.52	-62306.1671805222	4.52	-62189.8816552943	4.80	-62189.881503901
4.53	-62306.1671786638	4.53	-62189.8816538697	4.90	-62189.8814343174
4.54	-62306.1671763504	4.54	-62189.8816519763	5.00	-62189.8813613038
4.55	-62306.1671736942	4.55	-62189.8816497412	5.10	-62189.881283941

4.60	-62306.167154851	4.60	-62189.8816329255	5.20	-62189.8812064698
4.65	-62306.167128462	4.65	-62189.881608393	5.30	-62189.8811346545
4.70	-62306.1670968125	4.70	-62189.8815784773	5.40	-62189.8810702223
4.80	-62306.1670257032	4.80	-62189.8815105592	5.50	-62189.8810105281
4.90	-62306.1669516197	4.90	-62189.8814392727	5.60	-62189.8809528751
5.00	-62306.1668744926	5.00	-62189.8813646647	5.70	-62189.8808982931
5.10	-62306.1667932957	5.10	-62189.881285735	5.80	-62189.8808497514
5.20	-62306.1667124839	5.20	-62189.8812070036	5.90	-62189.8808078394
5.30	-62306.1666374922	5.30	-62189.881133929	6.00	-62189.880770948
5.40	-62306.1665700866	5.40	-62189.8810682869	6.10	-62189.8807363778
5.50	-62306.1665075603	5.50	-62189.8810074261	6.20	-62189.8807033188
5.60	-62306.166447326	5.60	-62189.8809487504	6.30	-62189.8806731049
5.70	-62306.1663905248	5.70	-62189.880893429	6.40	-62189.8806472041
5.80	-62306.166339524	5.80	-62189.8808438258	6.50	-62189.8806254607
5.90	-62306.1662955596	5.90	-62189.8808012079	6.60	-62189.8806062987
6.00	-62306.1662567202	6.00	-62189.8807636409	6.70	-62189.8805881397
6.10	-62306.1662204628	6.10	-62189.8807286084	6.80	-62189.8805703866
6.20	-62306.1661856993	6.20	-62189.8806950259	6.90	-62189.8805538491
6.30	-62306.1661539227	6.30	-62189.8806643796	7.00	-62189.8805397189
6.40	-62306.1661264478	6.40	-62189.8806380031	7.10	-62189.880528197
6.50	-62306.1661033621	6.50	-62189.8806159692	7.20	-62189.8805184391
6.60	-62306.1660828603	6.60	-62189.880596482	7.30	-62189.8805094003
6.70	-62306.1660634347	6.70	-62189.880578052	7.40	-62189.8805003296
6.80	-62306.1660444939	6.80	-62189.8805600657	7.50	-62189.8804912119
6.90	-62306.1660268779	6.90	-62189.8805433686	7.60	-62189.8804827349
7.00	-62306.1660118343	7.00	-62189.8805292326	7.70	-62189.8804756137
7.10	-62306.1659991245	7.10	-62189.8805174043	7.80	-62189.8804699847

7.20	-62306.1659884775	7.20	-62189.8805075957	7.90	-62189.880465425
7.30	-62306.1659785706	7.30	-62189.8804985177	8.00	-62189.880461211
7.40	-62306.1659686011	7.40	-62189.8804893516	8.10	-62189.8804568302
7.50	-62306.1659587572	7.50	-62189.8804802876	8.20	-62189.8804521829
7.60	-62306.1659493339	7.60	-62189.8804716244	8.30	-62189.8804475178
7.70	-62306.1659414081	7.70	-62189.8804644383	8.40	-62189.8804433293
7.80	-62306.165934794	7.80	-62189.8804585412	8.50	-62189.8804399502
7.90	-62306.1659293997	7.90	-62189.8804538535	-	-
8.00	-62306.165924426	8.00	-62189.8804495636	-	-
8.10	-62306.1659192015	8.10	-62189.8804450026	-	-
8.20	-62306.1659138785	8.20	-62189.8804403376	-	-
8.30	-62306.1659085232	8.30	-62189.8804356215	-	-
8.40	-62306.1659035401	8.40	-62189.8804312616	-	-
8.50	-62306.1658995132	8.50	-62189.8804278294	-	-

Table S6: Rn-Og electronic energies calculated at $CAMB3LYP + MP2/Rn = dyall.acv3z/Og = dyall.acv3z$ level with and without inclusion of quantum electrodynamics effects at the Gaunt interaction level. The Rn-Og Gaunt+BSSE electronic energies were performed at MP2-srLDA/Rn=dyall.acv3z/Og=dyall.acv3z level.

Rn-Og		Rn-Og-Gaunt		Rn-Og-Gaunt+BSSE	
R(Å)	Energy (hartree)	R(Å)	Energy (hartree)	R(Å)	Energy (hartree)
3.40	-78466.8567102563	3.40	-78324.1635048617	3.40	-78324.1634323175
3.50	-78466.8609823644	3.50	-78324.1678339947	3.50	-78324.167766665
3.60	-78466.8640592708	3.60	-78324.1709582991	3.60	-78324.1708955721
3.70	-78466.8662658945	3.70	-78324.1732043003	3.70	-78324.1731461186
3.80	-78466.8678138562	3.80	-78324.1747854375	3.80	-78324.1747312762
3.90	-78466.8688601203	3.90	-78324.1758594615	3.90	-78324.1758091335
4.00	-78466.8695486617	4.00	-78324.1765717072	4.00	-78324.1765249081
4.10	-78466.8699858418	4.10	-78324.1770292195	4.10	-78324.1769860154
4.20	-78466.8702326101	4.20	-78324.1772788976	4.20	-78324.1772392942
4.30	-78466.8703387881	4.30	-78324.1774151149	4.30	-78324.1773788205
4.40	**-78466.870354124**	**4.40**	**-78324.1774439798**	**4.40**	**-78324.1774108703**
4.50	-78466.8703137569	4.50	-78324.1774157038	4.50	-78324.1773855844
4.60	-78466.870233257	4.60	-78324.1773459983	4.60	-78324.1773186059
4.70	-78466.8701241018	4.70	-78324.1772466744	4.70	-78324.1772218848
4.80	-78466.8700009774	4.80	-78324.1771325083	4.80	-78324.1771099623
4.90	-78466.8698761686	4.90	-78324.1770158134	4.90	-78324.1769952343
5.00	-78466.8697535058	5.00	-78324.1769010343	5.00	-78324.1768821147
5.10	-78466.8696329041	5.10	-78324.1767876109	5.10	-78324.1767704139
5.20	-78466.8695158264	5.20	-78324.1766773626	5.20	-78324.1766616369
5.30	-78466.8694059828	5.30	-78324.1765738101	5.30	-78324.1765594812
5.40	-78466.8693055327	5.40	-78324.176479443	5.40	-78324.1764663516
5.50	-78466.8692137786	5.50	-78324.1763934731	5.50	-78324.1763817035

5.60	-78466.8691290026	5.60	-78324.176314046	5.60	-78324.176303432
5.70	-78466.8690504635	5.70	-78324.1762408864	5.70	-78324.1762312966
5.80	-78466.868978483	5.80	-78324.1761739597	5.80	-78324.1761655471
5.90	-78466.8689140783	5.90	-78324.1761143706	5.90	-78324.1761067947
6.00	-78466.8688565919	6.00	-78324.1760615467	6.00	-78324.1760548297
6.10	-78466.8688045618	6.10	-78324.1759995875	6.10	-78324.1759935808
6.20	-78466.868756649	6.20	-78324.1759560144	6.20	-78324.1759506231
6.30	-78466.86871289	6.30	-78324.1759164562	6.30	-78324.1759116522
6.40	-78466.86867336	6.40	-78324.1758809932	6.40	-78324.1758766902
6.50	-78466.8686381758	6.50	-78324.175849688	6.50	-78324.1758457821
6.60	-78466.868606826	6.60	-78324.1758221702	6.60	-78324.1758187214
6.70	-78466.868578218	6.70	-78324.1757972768	6.70	-78324.1757941626
6.80	-78466.8685518905	6.80	-78324.1757745043	6.80	-78324.1757717336
6.90	-78466.8685273714	6.90	-78324.1757534314	6.90	-78324.1757508627
7.00	-78466.8685054152	7.00	-78324.1757347187	7.00	-78324.1757321366
7.10	-78466.8684854029	7.10	-78324.1757180631	7.10	-78324.1757157708
7.20	-78466.8684677254	7.20	-78324.1757036692	7.20	-78324.1757015014
7.30	-78466.8684520952	7.30	-78324.1756908086	7.30	-78324.1756886699
7.40	-78466.8684369565	7.40	-78324.175678899	7.40	-78324.1756768271
7.50	-78466.8684228632	7.50	-78324.1756677776	7.50	-78324.1756656231
7.60	-78466.8684094052	7.60	-78324.1756570392	7.60	-78324.1756548635
7.70	-78466.8683971783	7.70	-78324.1756477293	7.70	-78324.1756456894
7.80	-78466.8683860347	7.80	-78324.1756392484	7.80	-78324.1756375607
7.90	-78466.868376197	7.90	-78324.1756323066	7.90	-78324.1756307495
8.00	-78466.868367246	8.00	-78324.1756257695	8.00	-78324.1756242699
8.10	-78466.8683586845	8.10	-78324.1756196505	8.10	-78324.1756183425
8.20	-78466.8683504293	8.20	-78324.1756138024	8.20	-78324.1756124987

R	Energy	R	Energy	R	Energy
8.30	-78466.8683422485	8.30	-78324.1756081642	8.30	-78324.1756069195
8.40	-78466.8683347211	8.40	-78324.1756027945	8.40	-78324.1756018016
8.50	-78466.8683276874	8.50	-78324.175598148	8.50	-78324.1755971544
-	-	8.75	-78324.1756038668	8.75	-78324,1756029411
-	-	9.00	-78324.1755964265	9.00	-78324,1755956126
-	-	9.25	-78324.1755889596	9.25	-78324,1755884164
-	-	9.50	-78324.1755838242	9.50	-78324,1755834131
-	-	10.00	-78324.1755763292	10.00	-78324,1755760079
-	-	11.00	-78324.1755664207	11.00	-78324,175566419
-	-	12.00	-78324.1755612608	12.00	-78324,1755612914
-	-	13.00	-78324.1755581567	13.00	-78324,175558153
-	-	14.00	-78324.1755563147	14.00	-78324,1755561355
-	-	15.00	-78324.1755551397	15.00	-78324,1755551142

Table S7: Og-Og Gaunt+BSSE electronic energies calculated at MP2-srLDA/Og=dyall.acv3z level.

Og-Og-Gaunt+BSSE	
R(Å)	Energy (hartree)
2.80	-109503.665190701
2.90	-109503.694952964
3.00	-109503.717308395
3.10	-109503.734021998
3.20	-109503.746451589
3.30	-109503.755621899
3.40	-109503.762324954
3.50	-109503.767171565
3.60	-109503.770619478

3.70	-109503.773023336
3.80	-109503.774657333
3.90	-109503.775723316
4.00	-109503.776372705
4.10	-109503.77672543
4.15	-109503.776819789
4.20	-109503.776871021
4.25	**-109503.776885929**
4.30	-109503.77687068
4.35	-109503.776830775
4.40	-109503.776771124
4.50	-109503.77660991
4.60	-109503.776414443
4.70	-109503.776200576
4.80	-109503.77597962
4.90	-109503.775760644
5.00	-109503.775550559
5.10	-109503.775352869
5.20	-109503.775168353
5.30	-109503.774996901
5.40	-109503.774839395
5.50	-109503.774695422
5.60	-109503.774564622
5.70	-109503.774446528
5.80	-109503.774339376
5.90	-109503.774241802
6.00	-109503.774153241

6.10	-109503.774073165
6.20	-109503.774001269
6.30	-109503.77393617
6.40	-109503.773877255
6.50	-109503.773823406
6.60	-109503.773774382
6.70	-109503.773729919
6.80	-109503.773689565
6.90	-109503.773653327
7.00	-109503.773618981
7.10	-109503.773588286
7.20	-109503.773559663
7.30	-109503.773537591
7.40	-109503.773509256
7.50	-109503.773486782
7.60	-109503.773466194
7.70	-109503.773447019
7.80	-109503.773429231
7.90	-109503.773412823
8.00	-109503.773397353
8.10	-109503.77338284
8.20	-109503.773369009
8.30	-109503.773356109
8.40	-109503.773344075
8.50	-109503.773332596
9.00	-109503.773284039
10.00	-109503.773214936

11.00	-109503.773167065
12.00	-109503.773131228
13.00	-109503.773102721
14.00	-109503.77307914
15.00	-109503.773059546
16.00	-109503.773042671

S2. He-Og, Ne-Og, Ar-Og, Kr-Og, Xe-Og, Rn-Og, and Og-Og pure vibrational ($j = 0$) and rovibrational ($j = 1$) energies calculated through Rydberg potential energy curves with Gaunt+BSSE correction

Tables 8 and 9 show the He-Og, Ne-Og, Ar-Og, Kr-Og, Xe-Og, and Rn-Og pure vibrational ($j = 0$) and rovibrational ($j = 1$) energies, respectively, calculated through Rydberg potential energy curves with Gaunt+BSSE correction. The Og-Og pure vibrational ($j = 0$) and rovibrational ($j = 1$) energies calculated through Rydberg potential energy curves with Gaunt+BSSE correction are shown in Table 10.

Table S8: He-Og, Ne-Og, Ar-Og, Kr-Og, Xe-Og and Rn-Og pure vibrational energies calculated through Rydberg potential energy curves with Gaunt+BSSE correction.

υ	j	**He-Og**	**Ne-Og**	**Ar-Og**	**Kr-Og**	**Xe-Og**	**Rn-Og**
0		8.476142	7.549907	12.002413	9.598012	9.081379	9.520494
1		–	20.279274	34.209154	28.228960	26.796158	28.191263
2		–	29.514297	54.058530	45.911021	43.904832	46.367219
3		–	35.504440	71.708113	62.562878	60.371820	64.049436
4		–	38.906579	87.330368	78.125114	76.168439	81.239268

5	–	–	101.080703	92.581221	91.274410	97.938347
6	–	–	113.071850	105.964432	105.678854	114.148592
7	–	–	123.364295	118.344462	119.380535	129.872206
8	–	–	131.976917	129.799619	132.387104	145.111676
9	–	–	138.925710	140.390083	144.713270	159.869762
10	–	–	144.300359	150.144157	156.378096	174.149489
11	–	–	148.318395	159.057902	167.401900	187.954130
12	–	–	151.190693	167.104113	177.803356	201.287188
13	–	–	152.877167	174.250155	187.597276	214.152372
14	–	–	–	180.487316	196.793365	226.553571
15	–	–	–	185.864074	205.396010	238.494819
16	–	–	–	190.487497	213.405117	249.980265
17	–	–	–	194.466123	220.818032	261.014136
18	–	–	–	197.840574	227.632673	271.600700
19	–	–	–	200.533085	233.851882	281.744229
20	–	–	–	–	239.488304	291.448968
21	–	–	–	–	244.567740	300.719101
22	0	–	–	–	249.127675	309.558729
23	–	–	–	–	253.209029	317.971853
24	–	–	–	–	256.843291	325.962370
25	–	–	–	–	260.039028	333.534071
26	–	–	–	–	262.765514	340.690671
27	–	–	–	–	–	347.435836
28	–	–	–	–	–	353.773239
29	–	–	–	–	–	359.706623
30	–	–	–	–	–	365.239882
31	–	–	–	–	–	370.377135

32	–	–	–	–	–	375.122792
33	–	–	–	–	–	379.481585
34	–	–	–	–	–	383.458524
35	–	–	–	–	–	387.058746
36	–	–	–	–	–	390.287236
37	–	–	–	–	–	393.148421
38	–	–	–	–	–	395.645829
39	–	–	–	–	–	397.782424
40	–	–	–	–	–	399.563564
41	–	–	–	–	–	401.007279
42	–	–	–	–	–	402.164564
43	–	–	–	–	–	403.123656
44	–	–	–	–	–	403.965954
45	–	–	–	–	–	404.732934
46	–	–	–	–	–	405.437737
47	–	–	–	–	–	406.079932
48	–	–	–	–	–	406.650616
49	–	–	–	–	–	407.130147

Table S9: He-Og, Ne-Og, Ar-Og, Kr-Og, Xe-Og and Rn-Og Rovibrational energies ($j = 1$) calculated through Rydberg potential energy curves with Gaunt+BSSE correction.

υ	j	**He-Og**	**Ne-Og**	**Ar-Og**	**Kr-Og**	**Xe-Og**	**Rn-Og**
0		8.787948	7.642203	12.052616	9.624528	9.081379	9.534188
1		–	20.361864	34.257409	8.255046	26.796158	28.204807
2		–	29.584779	54.104734	5.936591	43.904832	46.380611
3		–	35.561482	71.752187	2.587853	60.371820	64.062675

4		–	38.949757	87.372247	8.149431	76.168439	81.252350
5		–	–	101.120320	2.604834	91.274410	97.951270
6		–	–	113.109106	5.987315	105.678854	114.161353
7		–	–	123.399034	18.366605	119.380535	129.884804
8		–	–	132.008910	29.821020	132.387104	145.124108
9		–	–	138.954687	40.410730	144.713270	159.882025
10		–	–	144.326134	50.164026	156.378096	174.161581
11		–	–	148.340934	59.076949	167.401900	187.966048
12		–	–	151.209660	67.122275	177.803356	201.298929
13		–	–	152.890964	74.267361	187.597276	214.163935
14		–	–	–	80.503513	196.793365	226.564952
15		–	–	–	85.879254	205.396010	238.506016
16		–	–	–	90.501699	213.405117	249.991275
17		–	–	–	94.479364	220.818032	261.024956
18		–	–	–	97.852769	227.632673	271.611326
19		–	–	–	200.543869	233.851882	281.754659
20		–	–	–	–	239.488304	291.459198
21		–	–	–	–	244.567740	300.729127
22	1	–	–	–	–	249.127675	309.568547
23		–	–	–	–	253.209029	317.981461
24		–	–	–	–	256.843291	325.971761
25		–	–	–	–	260.039028	333.543242
26		–	–	–	–	262.765514	340.699616
27		–	–	–	–	–	347.444549
28		–	–	–	–	–	353.781714
29		–	–	–	–	–	359.714855
30		–	–	–	–	–	365.247862

31	–	–	–	–	–	370.384855
32	–	–	–	–	–	375.130245
33	–	–	–	–	–	379.488761
34	–	–	–	–	–	383.465412
35	–	–	–	–	–	387.065335
36	–	–	–	–	–	390.293511
37	–	–	–	–	–	393.154366
38	–	–	–	–	–	395.651422
39	–	–	–	–	–	397.787639
40	–	–	–	–	–	399.568373
41	–	–	–	–	–	401.011667
42	–	–	–	–	–	402.168568
43	–	–	–	–	–	403.127364
44	–	–	–	–	–	403.969442
45	–	–	–	–	–	404.736238
46	–	–	–	–	–	405.440865
47	–	–	–	–	–	406.082873
48	–	–	–	–	–	406.653340
49	–	–	–	–	–	407.132576

Table S10: Og-Og pure vibrational ($j = 0$) and rovibrational energies ($j = 1$) calculated through Rydberg potential energy curves with Gaunt+BSSE correction.

v	j	**Og-Og**	v	j	**Og-Og**	v	j	**Og-Og**	v	j	**Og-Og**
0		12.170905	54		749.444922	0		12.183558	54		749.450903
1		36.211813	55		753.980830	1		36.224374	55		753.986670
2		59.847558	56		758.301889	2		59.860027	56		758.307590
3		83.076717	57		762.419446	3		83.089091	57		762.425010

4		105.897942	58		766.344728	4		105.910222	58		766.350159
5		128.309976	59		770.088574	5		128.322159	59		770.093875
6		150.311656	60		773.661183	6		150.323743	60		773.666357
7		171.901931	61		777.071925	7		171.913919	61		777.076974
8		193.079867	62		780.329208	8		193.091756	62		780.334135
9		213.844663	63		783.440434	9		213.856450	63		783.445241
10		234.195659	64		786.412008	10		234.207345	64		786.416697
11		254.132357	65		789.249422	11		254.143939	65		789.253994
12		273.654426	66		791.957380	12		273.665904	66		791.961836
13		292.761720	67		794.539981	13		292.773092	67		794.544322
14		311.454294	68		797.000934	14		311.465559	68		797.005161
15	0	329.732415	69	0	799.343819	15	1	329.743571	69	1	799.347933
16		347.596576	70		801.572369	16		347.607622	70		801.576370
17		365.047515	71		803.690767	17		365.058450	71		803.694657
18		382.086224	72		805.703925	18		382.097046	72		805.707705
19		398.713966	73		807.617684	19		398.724674	73		807.621359
20		414.932284	74		809.438883	20		414.942877	74		809.442456
21		430.743016	75		811.175233	21		430.753493	75		811.178710
22		446.148302	76		812.834999	22		446.158660	76		812.838385
23		461.150589	77		814.426547	23		461.160828	77		814.429850
24		475.752641	78		815.957866	24		475.762759	78		815.961092
25		489.957530	79		817.436175	25		489.967527	79		817.439328
26		503.768639	80		818.867680	26		503.778513	80		818.870767
27		517.189643	81		820.257497	27		517.199392	81		820.260521
28		530.224499	82		821.609680	28		530.234122	82		821.612646
29		542.877416	83		822.927332	29		542.886913	83		822.930242
30		555.152835	84		824.212731	30		555.162204	84		824.215588

31	567.055386	85	825.467467	31	567.064625	85	825.470271
32	578.589857	86	826.692555	32	578.598965	86	826.695307
33	589.761151	87	827.888532	33	589.770127	87	827.891234
34	600.574249	88	829.055540	34	600.583092	88	829.058192
35	611.034172	89	830.193378	35	611.042881	89	830.195979
36	621.145946	90	831.301549	36	621.154519	90	831.304100
37	630.914577	91	832.379291	37	630.923013	91	832.381789
38	640.345028	92	833.425587	38	640.353326	92	833.428031
39	649.442214	93	834.439181	39	649.450372	93	834.441570
40	658.210996	94	835.418567	40	658.219015	94	835.420899
41	666.656202	95	836.361981	41	666.664078	95	836.364253
42	674.782641	96	837.267370	42	674.790376	96	837.269579
43	682.595156	97	838.132356	43	682.602747	97	838.134498
44	690.098665	98	838.954176	44	690.106111	98	838.956246
45	697.298238	99	839.729599	45	697.305539	99	839.731593
46	704.199176	100	840.454806	46	704.206331	100	840.456716
47	710.807106	101	841.125210	47	710.814113	101	841.127028
48	717.128082	102	841.735185	48	717.134941	102	841.736898
49	723.168693	103	842.277618	49	723.175405	103	842.279212
50	728.936165	104	842.743145	50	728.942729	104	842.744597
51	734.438436	105	843.118640	51	734.444853	105	843.119913
52	739.684214	106	843.384657	52	739.690485	106	843.385690
53	744.682979		-	53	744.689104	107	-

S3. Plots of *Ab initio* and adjusted potential energy curves (with ILJ and Rydberg forms) for the He-Og, Ne-Og, Ar-Og, Kr-Og, Xe-Og, Rn-Og, and Og-Og systems

Figures S1 (For He-Og, Ne-Og, and Ar-Og systems) and S2 (For Kr-Og, Xe-Og, and Rn-Og systems) show a comparison between the *Ab initio* (with and without Gaunt corrections) and ILJ adjusted potential energy curves. Figures S3 and S4 show the same comparison using the Rydberg adjusted potential energy curves. Figures S5 presents a comparison between the *Ab initio* (with Gaunt + BSSE corrections) and ILJ adjusted potential energy curves for the He-Og, Ne-Og, Ar-Og, Kr-Og, Xe-Og, and Rn-Og systems. The comparison between the *Ab initio* (with Gaunt + BSSE corrections) and Rydberg adjusted potential energy curve is presented in Figure S6. The comparison between the *Ab initio* (with Gaunt + BSSE corrections) and ILJ and Rydberg adjusted potential energy curves for the Og-Og system is depicted in Figure S7.
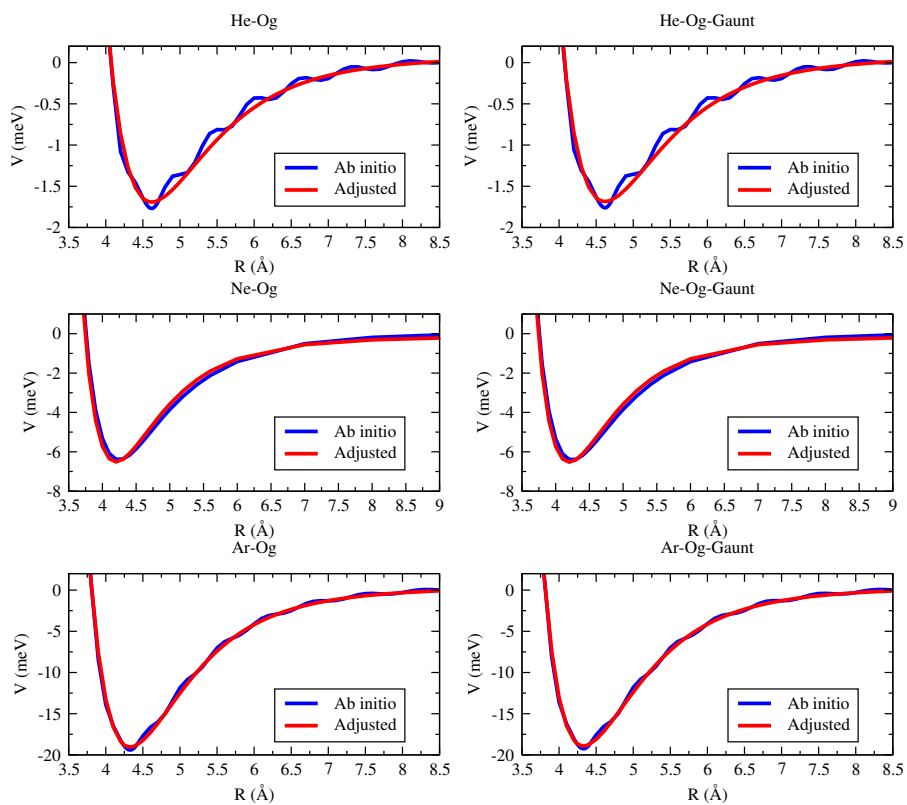
Figure S1: *Ab initio* and ILJ adjusted potential energy curves of the He-Og (Without Gaunt), He-Og (with Gaunt), Ne-Og (Without Gaunt), Ne-Og (With Gaunt), Ar-Og (Without Gaunt), and Ar-Og (With Gaunt) systems.
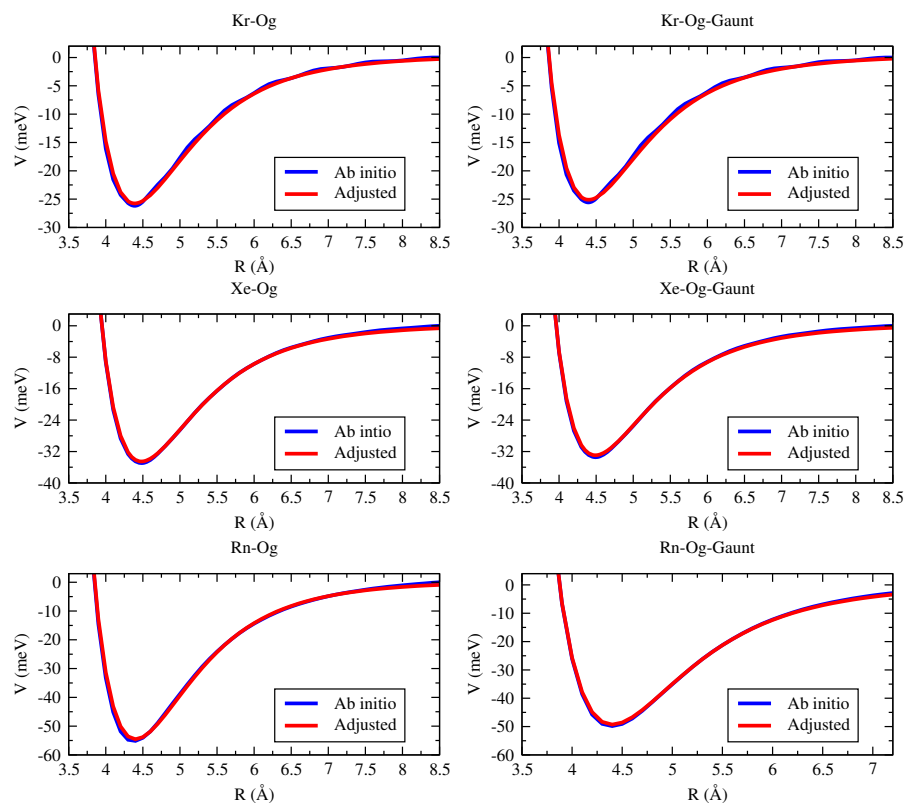
Figure S2: *Ab initio* and ILJ adjusted potential energy curves of the Kr-Og (Without Gaunt), Kr-Og (With Gaunt), Xe-Og (Without Gaunt), Xe-Og (With Gaunt), Rn-Og (Without Gaunt), and Rn-Og (With Gaunt) systems.
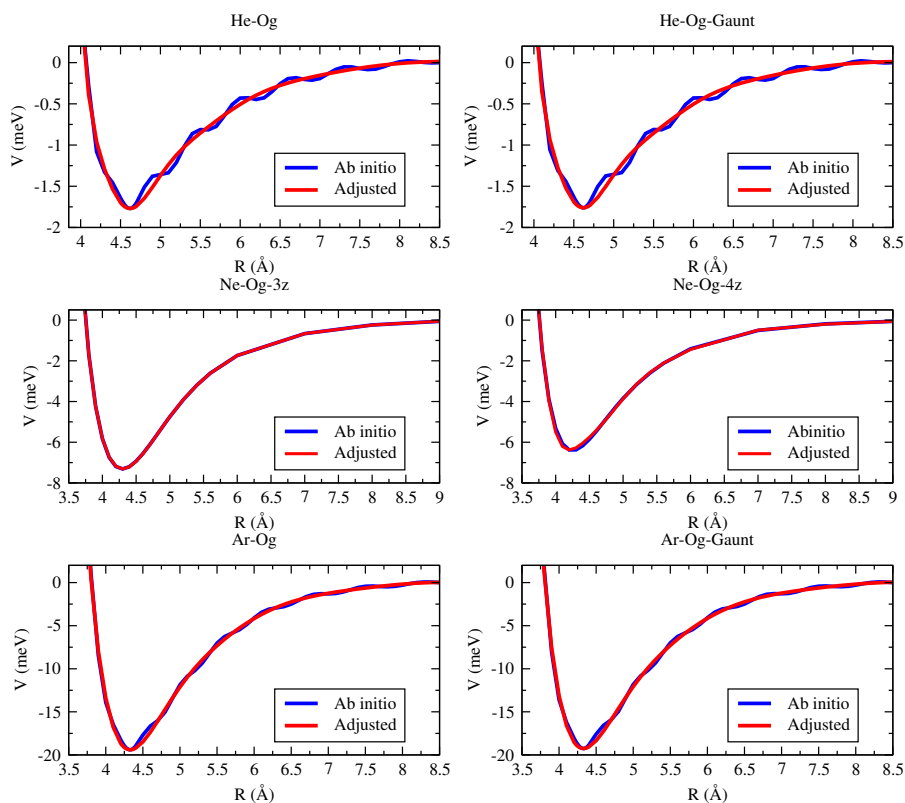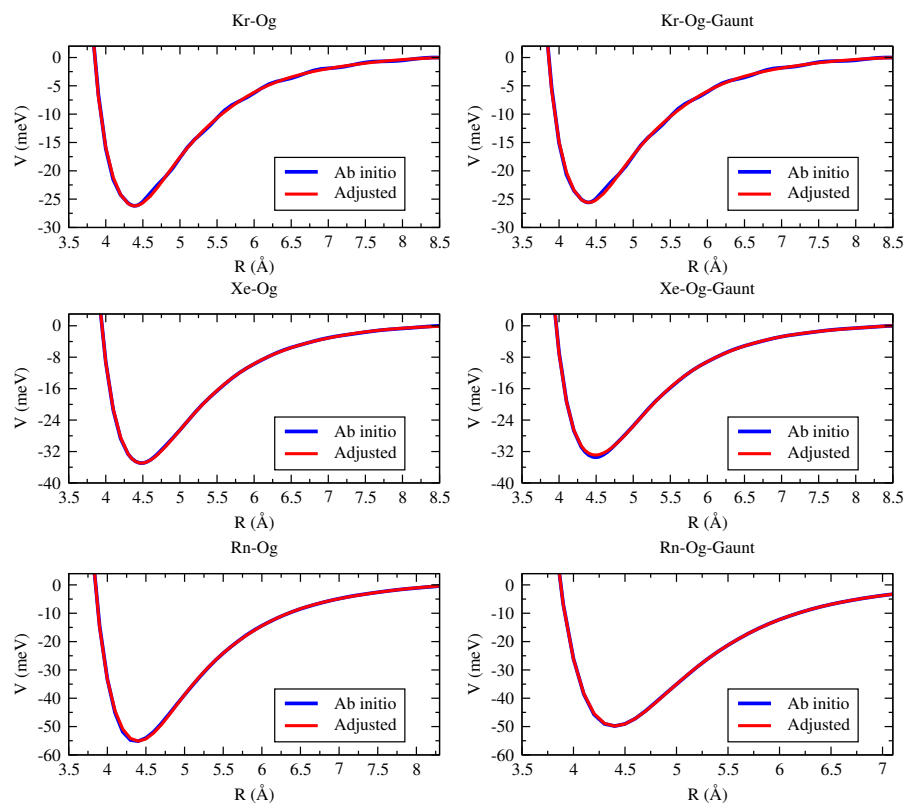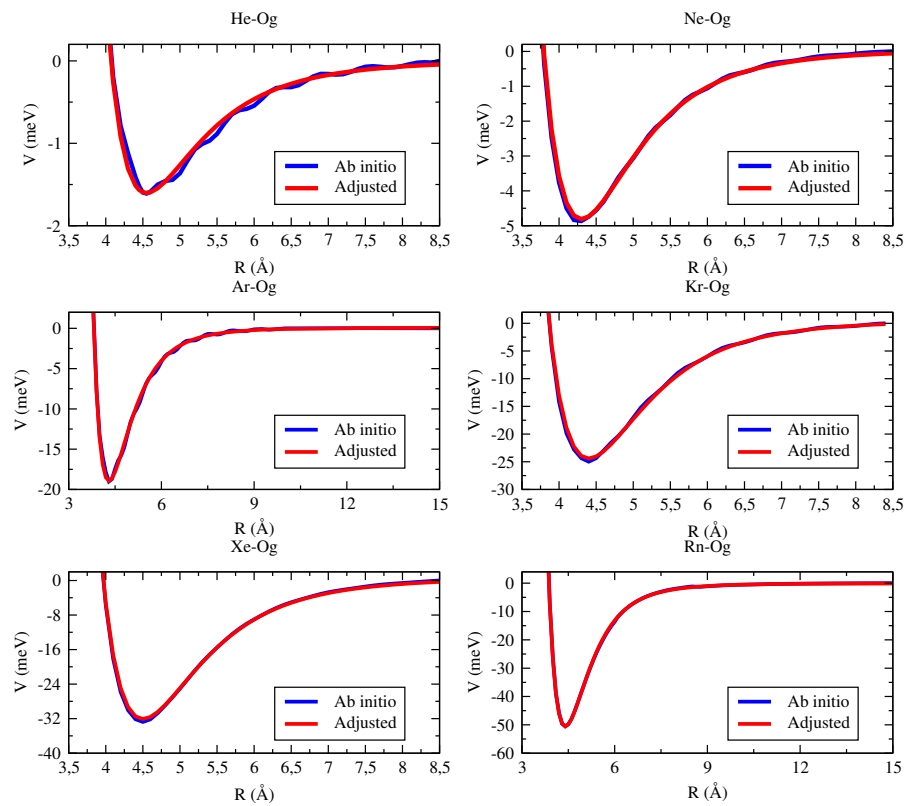
Figure S3: *Ab initio* and Rydberg adjusted potential energy curves of the He-Og (Without Gaunt), He-Og (With Gaunt), Ne-Og (Without Gaunt), Ne-Og (With Gaunt), Ar-Og (Without Gaunt), and Ar-Og (With Gaunt) systems.

Figure S4: *Ab initio* and Rydberg adjusted potential energy curves of the Kr-Og (Without Gaunt), Kr-Og (With Gaunt), Xe-Og (Without Gaunt), Xe-Og (With Gaunt), Rn-Og (Without Gaunt), and Rn-Og (With Gaunt) systems.

Figure S5: *Ab initio* and ILJ adjusted potential energy curves of the He-Og, Ne-Og, Ar-Og, Kr-Og, Xe-Og and Rn-og systems with Gaunt+BSSE correction.
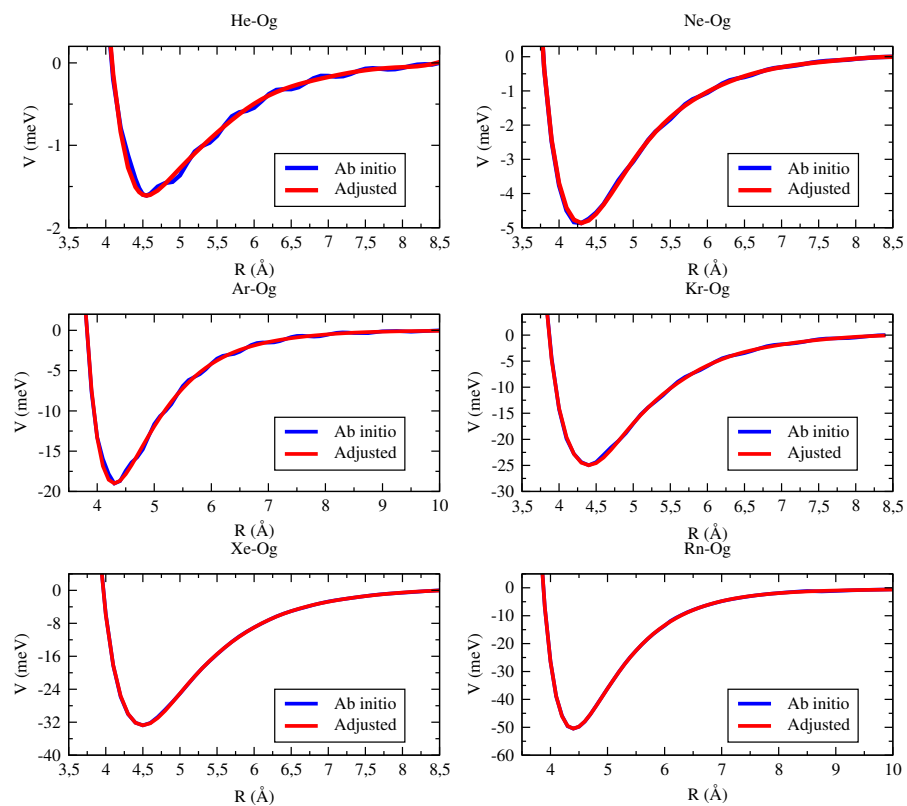
Figure S6: *Ab initio* and Rydberg adjusted potential energy curves of the He-Og, Ne-Og, Ar-Og, Kr-Og, Xe-Og and Rn-Og systems with Gaunt+BSSE correction.
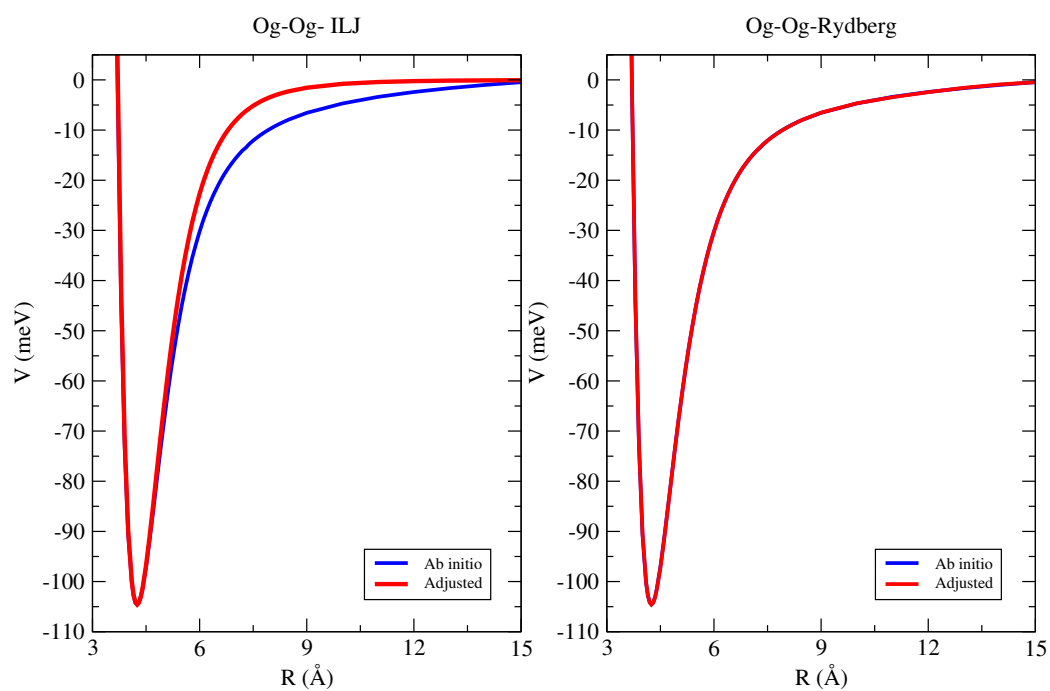
Figure S7: *Ab initio* and adjusted potential energy curves (ILJ and Rydberg) of the Og-Og system with Gaunt+BSSE correction.