Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information for

Exploring the Structure and Hydrogen Storage Capacity of $CeH_n^{0/+}$ Clusters

Correspondence author

Electronic mail: lixusheng@hpu.edu.cn (Xusheng Li)

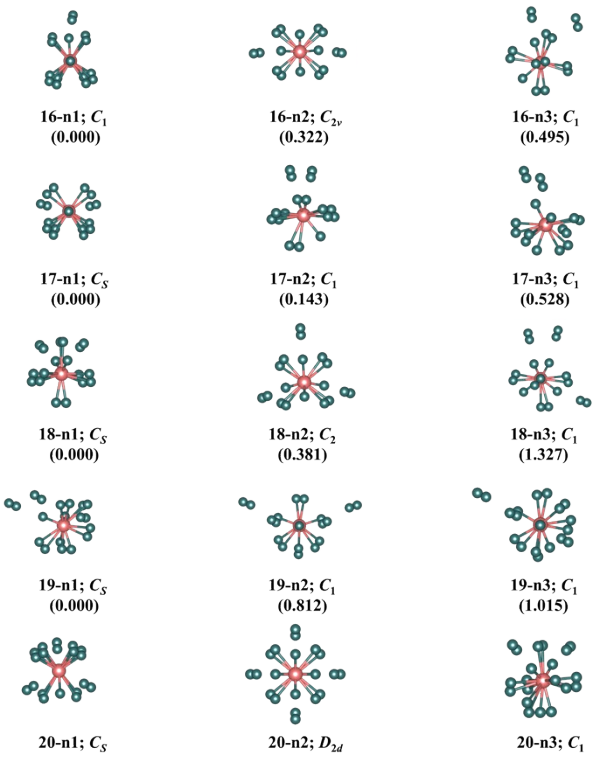

Fig. S1 Geometrical structures of neutral CeH_n (n = 16 − 20) clusters, as well as the reCetive energy (in eV) and point group symmetry.

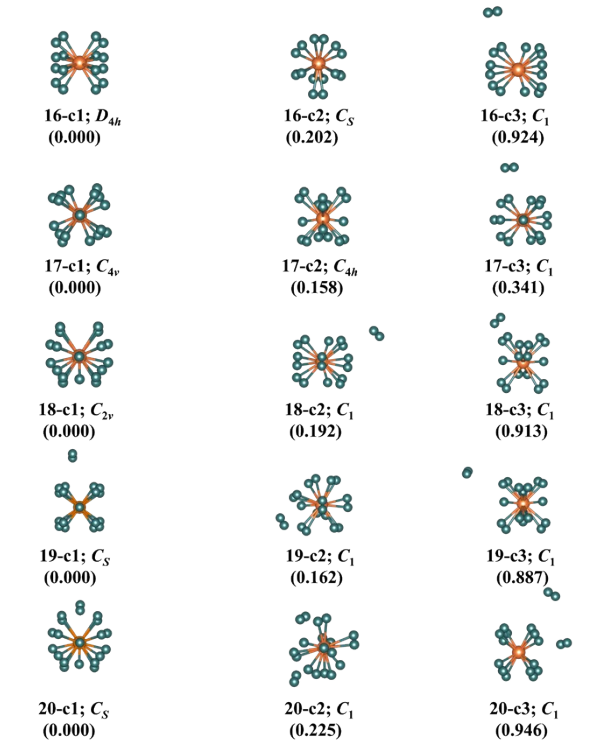

Fig. S2 Geometrical structures of cation CeH_n^+ (n = 16 − 20) clusters, as well as the reCetive energy (in eV) and point group symmetry.

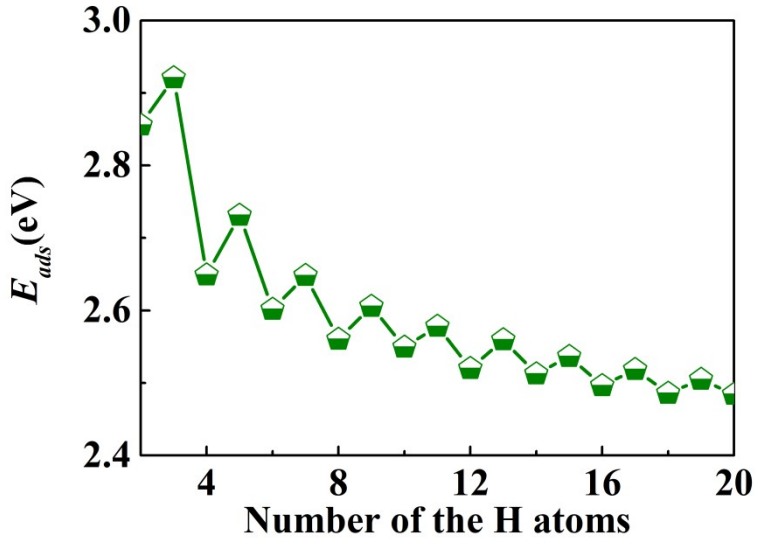

Fig. S3 The adsorption energies of neutral CeH_n (n = 2 − 20) clusters.

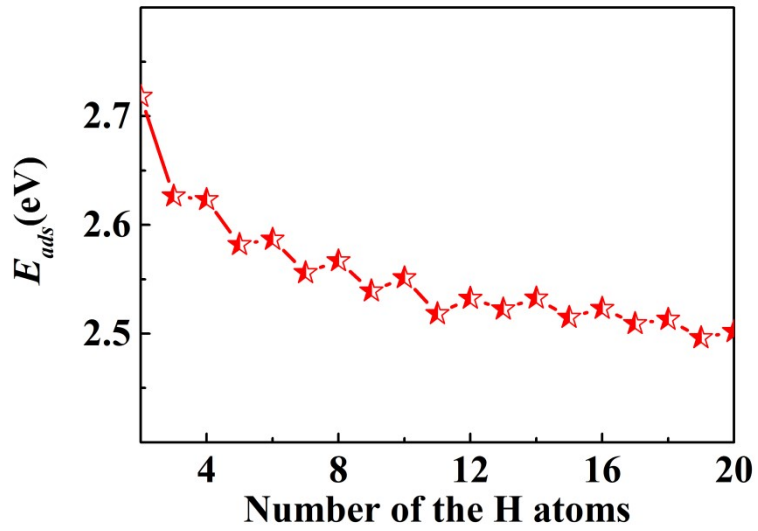

Fig. S4 The adsorption energies of cation CeH_n^+ (n = 2 − 20) clusters.

Table. S1 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_2 cluster.

Ce	0.00000000	0.00000000	0.04200500
H	0.00000000	1.65189700	-0.86109800
H	0.00000000	-1.65189700	-0.86109800

Table. S2 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_3 cluster.

Ce	-0.00001500	0.00007600	0.00895100
H	-1.68606000	0.88661500	-0.52107000
H	1.61381100	1.01254600	-0.52107000
H	0.07311500	-1.90347000	-0.52107200

Table. S3 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_4 cluster.

Ce	-1.85743600	0.00000000	-0.92596903
H	1.85743600	0.00000000	-0.92596903
H	0.38315300	-0.00000000	-2.46125504
H	-0.38315300	-0.00000000	-2.46125504
H	0.00000000	0.00000000	0.11884997

Table. S4 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_5 cluster.

Ce	0.08721100	-0.00002200	-0.03582400
H	-0.98482700	1.91585200	0.03026800
H	-2.46267000	-0.38263000	0.40744200
H	-0.98639500	-1.91514400	0.03042200
H	1.92598800	-0.00016700	1.16603500
H	-2.46310500	0.38332400	0.40780800

Table. S5 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_6 cluster.

Ce	0.00031000	-0.08372900	0.00085200
H	0.46163100	2.06096800	0.00645400
H	2.22106300	0.57591900	-0.01290600
H	2.38067500	-0.21341500	-0.01618200
H	-2.40101800	-0.20422100	-0.01032600
H	-0.44817000	2.05997500	0.00148800
H	-2.23218800	0.57705600	-0.01795100

Table. S6 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_7 cluster.

Ce	0.00619400	-0.00352500	-0.02050700
H	2.58456100	0.02991700	0.12424100
H	-2.44418900	-0.32554500	0.22003000
H	-2.42179800	0.44454300	0.23048200
H	-0.96467700	1.83185000	-0.17403800
H	1.26322600	-0.04703600	1.64284700
H	-1.04790200	-1.78822700	-0.22071700
H	2.67154300	0.05896200	-0.63342900

Table. S7 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_8 cluster.

Ce	-0.00473861	0.12026168	0.00000000
H	-0.23074398	-2.10970692	1.48065145
H	-1.64585187	-1.37710404	0.00000000
H	0.37695107	-1.81095118	1.83310657
H	-1.09374128	2.05509386	0.00000000
H	-0.23074398	-2.10970692	-1.48065145
H	1.35912741	0.14643269	1.74627940
H	0.37695107	-1.81095118	-1.83310657
H	1.35912741	0.14643269	-1.74627940

Table. S8 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_9 cluster.

Ce	0.00006300	0.08890000	-0.00002000
H	-1.76828200	1.26067800	0.00025500
H	-0.00024300	-1.99145400	0.00057300
H	1.95299700	-1.60097300	0.00013700
H	-1.95467200	-1.59999200	0.00074200
H	1.76959800	1.25876500	-0.00153300
H	-0.00024200	-0.21427100	2.07984300
H	2.40093400	-1.02645200	0.00057400
H	-2.40205100	-1.02586100	0.00004000
H	-0.00171600	-0.21665700	-2.07948400

Table. S9 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_{10} cluster.

Ce	0.03395800	-0.00015200	0.00252500
H	1.51587800	1.87823100	-0.04965200
H	-1.55439700	-2.01190100	-0.01346300
H	2.06010300	-1.22380200	0.00251900
H	-2.07991100	1.43077100	0.02869000
H	-0.91121000	0.00566600	-2.02005300
H	-0.91344300	-0.00700400	2.02559600
H	2.05233900	1.23995500	-0.04259700
H	-1.56908400	2.00406500	0.00120100
H	-2.06280700	-1.44061600	-0.08889000
H	1.52692200	-1.86672500	0.01274000

Table. S10 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_{11} cluster.

Ce	-0.00921500	-0.07429800	-0.00291400
H	2.32234500	-0.45584500	1.04065800
H	-0.63539800	2.38970600	0.52759100
H	-2.76587000	0.09065700	-0.03359800
H	2.25678000	0.30609300	1.20995700
H	-2.58702500	-0.64759000	-0.02381100
H	2.26055900	-0.21667000	-1.21021800
H	2.20226900	0.56554900	-1.20253300
H	-0.35536100	0.83190700	1.97298000
H	-0.66233300	2.43180400	-0.23710500
H	-0.50502600	1.01169900	-1.85465700
H	-1.00571200	-2.07234400	-0.02316300

Table. S11 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_{12} cluster.

Ce	-0.00100000	0.02689700	0.00000000
H	-2.21205900	1.07558900	0.00000000
H	0.90319600	2.38092100	0.38341900
H	2.49731200	-0.27578100	0.00000000
H	-0.32514600	-2.18910300	-1.10958000
H	-0.32514600	-2.18910300	1.10958000
H	-2.43122500	0.30239600	0.00000000
H	0.90319600	2.38092100	-0.38341900
H	2.29404800	-1.02807600	0.00000000
H	-1.08569100	-1.94229000	-1.08077600
H	-1.08569100	-1.94229000	1.08077600
H	0.51610300	0.91683600	1.99243900
H	0.51610300	0.91683600	-1.99243900

Table. S12 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_{13} cluster.

Ce	-0.01800900	0.00047600	-0.06721200
H	1.32264900	0.87579800	-1.61924000
H	-2.13961586	1.16196123	-0.77208125
H	-0.72443005	-2.28046372	0.71772200
H	-1.74674238	0.83732455	1.56271358
H	2.37044570	-0.61874258	-0.54166087
H	1.80120230	1.35037120	1.01350610
H	0.79955500	-0.38507300	1.95046600
H	-2.41965188	0.46676529	-0.66932984
H	-0.40591058	-2.05550188	1.32969873
H	-1.48377383	1.50930124	1.31498196
H	2.27144079	-1.00073622	0.05088237
H	-0.95045500	-1.62654600	-1.23397000
H	1.85460689	1.59480124	0.39043340

Table. S13 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_{14} cluster.

Ce	-0.09285000	0.00786000	0.00799900
H	1.07750600	1.35825900	-1.88004000
H	0.47101000	1.88365400	1.66844700
H	2.11780500	-0.40319400	0.11975000
H	0.82401300	2.14530700	1.03287200
H	1.65745300	0.88779800	-1.72225600
H	-0.92283300	1.76560200	-1.04249300
H	5.19509700	-1.05544600	0.42261500
H	-1.15725000	-0.68924800	1.98829100
H	-2.86122700	0.16389600	-0.27936300
H	-0.56761200	-1.71660800	-1.60942400
H	4.46327000	-0.90130400	0.35136000
H	-0.95782300	-2.00597600	-0.94941300
H	-1.33182200	-1.33472200	1.45898400
H	-2.73275100	-0.56806100	-0.08675600

Table. S14 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_{15} cluster.

Ce	-0.06618000	0.01390300	0.01581200
H	2.11913100	-0.07057800	-0.35462100
H	-1.24875300	2.28871800	0.11669700
H	-1.00350800	-0.06361800	-1.97886400
H	1.50521400	-2.00251700	0.57019500
H	1.30021600	2.15026100	0.54206300
H	-0.91034100	-1.23416700	1.63712100
H	-1.06883300	2.31332200	-0.64586800
H	0.78044900	2.19170600	1.12101300
H	-2.98914100	0.09712000	0.20789400
H	-1.28304900	-2.27247200	-0.29430000
H	4.52260100	-0.01552300	-0.59085900
H	-1.24795400	-2.06966800	-1.03044700
H	5.27001600	-0.00885200	-0.65963300
H	-2.87174600	0.09442400	-0.53795400
H	0.89794500	-2.19063700	0.99629200

Table. S15 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_{16} cluster.

Ce	-0.20885400	-0.18684800	-0.01785100
H	-0.91818100	1.04686100	1.99432000
H	-0.86463000	0.34243200	2.30299100
H	-0.40436700	-1.50862600	1.59777700
H	7.93822800	0.56709000	-0.19579200
H	-1.92003300	4.95280000	-0.43040800
H	1.33580100	1.75473300	0.04645700
H	0.92810600	-0.96035400	-2.04847600
H	2.09285800	-0.91813200	0.87246100
H	-2.41164100	-0.56663000	-1.20869500
H	7.67742000	1.26354500	-0.16920800
H	-1.65091000	4.27181800	-0.28801700
H	-2.69397600	-0.26835300	-0.55919000
H	1.59545200	-1.15552700	1.40534200
H	-0.66825300	1.85016500	0.15188900
H	0.18535400	-1.10710200	-2.26410700
H	1.89229500	1.27247900	-0.17201200

Table. S16 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_{17} cluster.

Ce	0.01172100	-0.15591900	-0.00144200
H	-2.71308200	-1.18620600	-0.35986700
H	-2.56796300	4.46392700	-0.13264300
H	-1.62460100	0.57104200	1.89353300
H	1.48294400	-0.08166200	2.16117200
H	-0.42802000	-1.88003600	1.31677000
H	4.83219800	2.20787200	-0.05512900
H	-2.81249700	-0.43779400	-0.36534400
H	-2.28604900	3.76890900	-0.14536400
H	-1.46234600	-0.13557200	2.13721300
H	1.01275900	-0.65841800	2.33978400
H	1.33824000	-1.05123000	-2.03593800
H	4.15740100	1.88278400	-0.00815400
H	-0.88220700	-0.66120700	-2.35203800
H	-0.93857600	0.11911500	-2.39513900
H	1.68725800	-0.35942400	-1.96929800
H	1.98646600	0.83325300	0.17917800
H	-1.45001900	1.49203300	-0.12651600

Table. S17 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_{18} cluster.

Ce	0.01039400	-0.17757400	0.03995800
H	-1.27078600	-1.38980300	-1.81453900
H	0.64837600	0.23887800	2.50638100
H	1.45888900	-0.22171200	-1.96604600
H	0.31574600	-2.56797600	0.34262700
H	-2.82978400	3.28629400	0.08310100
H	3.98106400	0.29585100	0.14018800
H	2.50976400	4.36733700	-0.70567400
H	-5.14730300	-0.13138700	0.16762800
H	-2.99700500	0.12697800	4.01256400
H	4.59362700	-0.11104000	0.30229900
H	2.28352500	3.65123400	-0.63573600
H	-4.44033300	0.09598300	0.09066200
H	-1.66293300	-0.73374200	-1.78224600
H	0.70219600	0.97441400	2.27612600
H	1.21886500	-0.94539000	-2.05647300
H	0.36196500	-2.34508700	1.10055400
H	1.57321700	1.14893000	-0.41152300
H	-1.90193500	0.67393000	-0.08188400

Table. S18 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_{19} cluster.

Ce	0.09172400	-0.18479100	0.00114500
H	-1.04020200	-1.32431100	-2.04024100
H	2.92788500	-0.33082400	-0.18336900
H	1.43773900	1.55747500	-0.12682500
H	-1.44762500	-0.66313000	-2.03841600
H	2.84491000	-1.08060400	-0.14494000
H	0.56289700	-1.79231800	1.44308100
H	1.14757600	-0.78950900	-2.25008000
H	-3.52787100	3.44688000	-0.16175000
H	1.41758200	0.07858400	2.22292000
H	-1.01433300	-0.62822700	2.30841000
H	-5.05052800	-0.35044700	-0.00952100
H	2.52480800	4.55481100	-0.29095300
H	-1.96976900	0.64494400	-0.01565600
H	-3.13344100	2.80960900	-0.14066600
H	2.25387300	3.85591000	-0.26773400
H	-4.33608500	-0.12372800	-0.02267500
H	1.54126500	0.77910100	1.94209200
H	-1.51216600	-0.09860600	2.06986100
H	1.14520400	-0.01250200	-2.35878800

Table. S19 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_{20} cluster.

Ce	-0.01667600	-0.08919400	-0.01888400
H	0.35699300	2.35316600	0.28426000
H	2.42862700	-1.87673000	0.64588600
H	0.25821600	-0.76060700	2.48555500
H	-1.50560200	0.46239000	-1.91044700
H	1.65695300	0.35382400	-1.75108400
H	-2.32018300	-1.74056300	0.77437000
H	4.92512000	2.63251300	0.35147300
H	-0.05099000	-2.44199600	-0.66750500
H	-1.85908600	0.94426000	-0.05001100
H	4.26794500	2.28218400	0.31854100
H	1.83568400	0.91394300	0.14011300
H	-4.89998300	2.51242900	0.54391300
H	1.34076400	-0.22338900	-2.15453500
H	-2.57440200	-1.06126400	0.55568500
H	-1.09680200	-0.02962900	-2.33624900
H	2.61200000	-1.15473900	0.53776200
H	0.34304000	-0.00732300	2.57454400
H	-0.40875200	2.35426700	0.22523300
H	-0.10043500	-2.52721000	0.11635700
H	-4.24190100	2.18771800	0.41141600

Table. S20 Vibrational frequencies (cm^{-1}) of ground state structures of neutral CeH_n (n=2-20) clusters.

CeH_2	CeH_3	CeH_4	CeH_5	CeH_6
407.7545	319.9185	169.2397	140.7777	152.1273
1147.5837	490.8501	434.8495	329.4417	316.3300
1251.3255	498.4766	448.9397	385.4660	326.3087
	1301.1577	729.7605	466.0694	525.0392
	1317.6393	801.4973	474.6084	663.0862
	1405.0517	1064.3860	700.7447	744.8191
		1294.6905	744.4897	790.2475
		1353.4844	1021.6221	798.9555
		3907.3483	1294.2142	954.9096
			1304.4419	1118.7413
			1385.5545	1203.0056
			3972.3007	1391.6402
				2419.2640
				3269.6316
				3405.5199
CeH_7	CeH_8	CeH_9	CeH_{10}	CeH_{11}
107.8255	89.3883	145.7120	63.4639	126.6044
144.4822	105.8646	173.7845	130.0318	145.4309
247.1720	147.0666	205.4655	173.8170	185.6522
309.7605	213.6255	225.3475	201.6812	207.2609
402.1142	285.2519	256.0466	220.5268	216.9432
457.6902	327.1939	308.1616	229.5253	234.5370
460.1330	362.5447	343.5645	286.6125	323.5426
469.0387	425.6817	447.4496	398.5687	329.2495
619.9802	521.6767	481.4068	426.9522	346.8274
716.1188	557.6736	498.3281	468.8267	442.1204

754.4022	558.1829	521.6885	501.6142	448.7900
859.2180	585.5285	651.4308	558.2788	482.2428
1024.0103	619.2395	661.9675	588.8171	512.5399
1281.0190	821.5896	712.2843	607.4772	611.5093
1297.5087	831.8241	717.8707	655.4327	642.7003
1370.9681	952.9392	933.3895	703.8273	671.3635
3961.3595	1059.1761	939.1635	713.9291	677.6843
4086.5437	1128.5302	975.6725	882.7105	716.1244
	1242.1241	1272.4492	914.2795	728.7441
	4157.1028	1288.0147	965.5618	930.8941
	4158.6410	1360.6251	1045.8549	940.6901
		3994.1523	1267.1413	959.9170
		3997.0596	1301.3938	972.6841
		4033.6487	3591.6584	1256.0128
			3825.6989	1274.2331
			3929.1354	1341.7954
			4029.6118	3989.2279
				4007.4330
				4034.9880
				4043.6580
CeH_{12}	CeH_{13}	CeH_{14}	CeH_{15}	CeH_{16}
109.3030	114.8701	15.1075	30.6440	3.2407
139.1273	144.2109	25.6542	34.6620	6.4115
139.1889	173.6203	57.1457	79.8294	9.8141
187.0619	189.0246	86.5997	127.5349	13.6488
243.6414	219.3657	146.1679	148.2451	26.1158
428.4730	225.5545	161.7933	180.5807	38.2059
429.9016	240.5346	183.9537	200.6736	38.7879
445.6399	268.4226	218.5752	217.6986	56.3618

490.0463	340.4824	223.2721	227.1071	86.2517
490.8464	347.9020	252.0385	243.7549	152.1508
530.4627	374.1993	293.8719	268.5202	160.3134
534.8345	428.7723	304.1138	285.7376	179.2087
567.2199	443.6120	335.2366	294.8251	214.7052
642.1132	481.6083	373.8564	343.2393	220.8938
768.8239	500.2497	401.8726	355.9631	254.9742
795.5119	547.3050	435.6733	377.1011	297.3106
796.8228	619.5880	439.6838	432.8137	301.4687
807.5580	639.2745	460.8364	444.5178	341.8759
811.0045	649.2969	486.3801	484.2001	387.1484
823.1152	684.8857	525.6464	508.2516	412.7020
852.0476	700.4817	572.6423	553.5690	435.8487
1086.1550	732.5589	599.9485	621.5317	445.8062
1092.3773	743.6113	626.3322	640.7094	463.8093
1094.6872	939.0437	658.5187	648.7353	486.8416
1098.1241	943.0975	684.7833	688.9369	525.7551
1324.4546	954.6781	745.1114	700.3906	578.0323
1324.5724	960.5487	852.0855	735.8720	601.4696
1338.4270	982.6880	919.3665	749.3935	628.7321
1387.6620	1248.5279	962.0889	935.6872	658.1656
3823.8767	1250.5624	971.0103	946.6865	687.6100
3833.2542	1316.9333	1038.9238	956.3143	752.0969
3837.5480	3948.2348	1261.6571	961.0481	851.2280
3850.5160	3995.5332	1294.3762	978.8224	932.5662
	3999.0627	3590.2493	1253.0947	951.4066
	4037.8972	3936.4053	1257.1163	969.7182
	4049.8950	3938.1339	1322.9602	1038.6865
		3951.7509	3954.0175	1265.9721

		4012.8729	3988.6373	1298.6679
		4383.1896	4009.4718	3591.4014
			4040.7498	3935.2626
			4050.7124	3938.5202
			4389.6211	3969.8995
				3997.4768
				4383.1492
				4417.9611
CeH_{17}	CeH_{18}	CeH_{19}	CeH_{20}	-
12.3711	7.6837	2.3179	9.2187	
16.2810	11.7869	13.7065	17.1885	
27.4063	22.6104	16.0714	26.0169	
37.6678	27.1126	29.5273	40.0305	
78.6447	35.7321	30.6688	78.7097	
79.1440	73.0788	39.2441	85.2149	
129.1683	81.9879	67.8852	122.1946	
142.1757	85.7765	75.3175	148.1131	
173.2402	101.5850	78.6489	151.7350	
199.7920	156.7047	123.9221	166.5373	
216.3596	180.8100	144.3870	185.9131	
230.0492	196.2056	176.1509	187.8096	
241.3182	200.3740	197.5049	207.0918	
262.3789	207.9146	216.1275	210.7037	
277.2530	224.4276	226.7635	228.1340	
279.0760	237.7182	238.5532	251.8168	
281.9287	277.3377	243.6012	259.0912	
291.2276	279.5094	250.1635	262.2587	
336.3781	280.6677	256.4825	265.7278	
350.8078	289.5394	267.3581	273.8476	

370.6071	297.7680	272.4917	291.5990	
435.4501	308.2543	277.5421	294.5138	
445.1863	346.2061	288.5335	311.9165	
479.8707	356.5382	340.8212	372.9910	
503.2744	390.1800	357.0762	404.7902	
555.6192	417.7969	375.3238	410.9388	
608.9138	439.6408	429.5839	419.5313	
638.5912	458.2079	440.5915	436.9825	
647.4775	465.4300	483.6125	447.0954	
693.8941	474.2073	502.9696	462.3936	
700.6059	613.2333	553.2681	467.5452	
735.4243	621.9904	617.9546	527.7760	
752.6339	644.8024	635.8364	556.4293	
923.4979	656.6954	645.3837	595.8858	
941.6194	679.7534	685.3682	597.5957	
960.7954	697.0881	699.0229	629.6144	
968.0875	920.6915	734.2936	663.1863	
986.7175	931.6391	744.2521	668.1405	
1250.8013	947.3330	932.2659	676.6934	
1258.4652	954.2618	935.6453	779.5962	
1325.1658	989.2662	953.3096	914.3633	
3940.1151	1258.4325	956.1366	924.9902	
3999.5111	1300.1525	979.9561	951.1900	
4025.5505	3533.2906	1251.9541	960.1227	
4032.0115	3955.6824	1259.1338	966.7499	
4045.8534	3964.9165	1324.7673	1007.7579	
4389.5173	3979.3453	3951.7943	1237.2952	
4389.7456	3984.5587	4009.0269	1274.1829	
	4376.8114	4015.2563	3628.8832	

	4380.9093	4045.6332	3943.4279	
	4388.5785	4053.0029	3949.5134	
		4390.3549	3978.9236	
		4391.3854	3993.4068	
		4394.7608	3994.9522	
			4309.5572	
			4384.9705	
			4388.4581	

Table. S21 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_2^+ cluster.

Ce^+	0.00000000	0.00000000	0.00000000
H	0.02700000	-0.31500000	2.22146900
H	0.02700000	-0.31500000	-2.22146900

Table. S22 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_3^+ cluster.

Ce^+	-0.06178200	0.03976000	-0.00001800
H	-1.39441000	-1.50489200	0.00074700
H	2.53934100	-0.02368400	0.00188000
H	2.43840700	-0.77748400	-0.00155700

Table. S23 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_4^+ cluster.

Ce^+	0.07026500	-0.01607400	-0.02099100
H	-2.32524000	0.01537200	0.20336300
H	-1.45962000	1.47545700	0.05083800
H	-2.35919800	-0.77018300	0.30716800
H	2.06866600	0.21165500	0.65611900

Table. S24 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_5^+ cluster.

Ce^+	0.09982023	-0.04331860	0.00000000
H	-1.57836615	0.08807870	1.73900408
H	-1.97781368	0.38052665	1.13970161
H	-1.57836615	0.08807870	-1.73900408
H	1.28901896	1.57359422	0.00000000
H	-1.97781368	0.38052665	-1.13970161

Table. S25 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_6^+ cluster.

Ce^+	-0.11243800	-0.08079600	0.01161800
H	0.47430500	2.19701600	-0.12928900
H	1.34995700	0.16391000	1.33660800
H	2.36077800	-0.43758900	-0.28300500
H	-1.03841000	1.42453800	-0.88579900
H	2.25089600	-0.69385200	-0.99232400
H	1.12388100	2.03212200	0.27995300

Table. S26 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_7^+ cluster.

Ce^+	-0.00087800	0.02503300	-0.03629800
H	2.43077800	-0.51027100	0.50025600
H	-2.67027800	- 0.55484700	0.30000200
H	-2.73954000	0.15045300	0.55245200
H	0.22434100	2.16130600	-0.18339100
H	0.83796600	-0.23287200	1.72667200
H	-0.60269400	-1.96028500	-0.54310500
H	2.57035000	-0.50536900	-0.24758500

Table. S27 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_8^+ cluster.

Ce^+	-0.03112900	-0.03691800	-0.08843000
H	-0.56875500	1.63080000	0.81150900
H	1.18550100	1.91770200	0.53538800
H	2.46078100	-0.68936700	0.31667100
H	-2.62394500	0.39762300	0.73204900
H	-2.74547400	-0.30720400	0.50581800
H	2.01786300	-1.09188400	0.80893600
H	0.25672600	-1.38569800	1.29021300
H	1.82277200	1.66929900	0.12834500

Table. S28 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_9^+ cluster.

Ce^+	0.00161200	-0.00989600	0.00368600
H	-2.46900600	-0.75497200	0.29495100
H	2.08498600	1.30323800	0.43565000
H	2.40676700	0.60598600	0.44155000
H	-0.28018800	2.47891600	-0.49036900
H	0.97961500	-2.28294500	-0.79118900
H	-2.56161600	-0.67357200	-0.45311800
H	1.61751800	-1.94169000	-0.55324000
H	-0.92513800	2.25239700	-0.82820000
H	-0.94645400	-0.41336300	1.73015800

Table. S29 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_{10}^{+} cluster.

Ce^{+}	-0.09941000	0.03366800	0.12764200
H	-2.15758300	-1.33241400	-0.52021000
H	0.70963600	-1.93229500	-1.14973800
H	0.03589500	1.99260800	-1.33823600
H	0.72389800	1.67968300	-1.46753000
H	4.41554500	-0.23442900	-0.26305700
H	-2.36066100	-0.59891800	-0.59881200
H	0.10503900	-2.30983200	-0.86264700
H	-1.63361200	1.11664900	-0.53604500
H	1.42143600	-0.19297200	-1.13730100
H	4.50617800	-0.14080900	0.47031100

Table. S30 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_{11}^{+} cluster.

Ce^{+}	0.00000000	0.09303200	0.00000000
H	2.19697400	-0.78307300	0.41221600
H	-2.13003000	-0.90329300	0.41368200
H	0.01561000	-2.51501900	0.39312400
H	0.37735400	0.21906100	-2.40417300
H	-0.41232000	0.15719300	-2.39797900
H	0.01561000	-2.51501900	-0.39312400
H	2.19697400	-0.78307300	-0.41221600
H	-2.13003000	-0.90329300	-0.41368200
H	-0.09517900	2.34743300	0.00000000
H	-0.41232000	0.15719300	2.39797900
H	0.37735400	0.21906100	2.40417300

Table. S31 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_{12}^{+} cluster.

Ce^{+}	-0.01396800	0.00664300	0.03632600
H	2.25174200	-1.32628100	0.26446200
H	-2.32202300	-1.32349900	-0.25431600
H	-0.13447300	1.74662600	1.01401500
H	-0.10683600	-1.60010600	1.22137300
H	0.62573300	-0.62801200	-2.65622300
H	0.82297400	0.09628800	-2.68500900
H	1.78643600	1.76076700	0.46365100
H	-1.90851800	1.74042800	-0.02929800
H	1.71135500	-1.69156300	0.66398900
H	-1.91485500	-1.72911500	0.24408300
H	2.29370500	1.29723800	0.13452600
H	-2.29507100	1.27194500	-0.48814500

Table. S32 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_{13}^{+} cluster.

Ce^{+}	0.00203100	-0.00149700	0.00204000
H	-1.82790000	-0.26701000	1.67036800
H	0.28038300	-2.30787800	-1.04287100
H	-2.22856100	0.74607400	-1.15677400
H	1.82426100	-0.40191500	1.64564500
H	-0.28393600	2.59205700	-0.15988600
H	2.12129800	-0.09231200	-1.43228000
H	-2.24722100	0.00818300	-1.33280700
H	-2.21960400	-0.60049600	1.10316800
H	2.25802700	-0.68610000	1.08477600
H	2.19248500	0.63802300	-1.21746700
H	0.47169700	2.56072100	-0.26114500
H	-0.48616000	-2.28305500	-1.02778900
H	0.02743700	0.18052800	2.00876400

Table. S33 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_{14}^{+} cluster.

Ce^{+}	0.00000000	0.00000000	0.04860200
H	0.84123300	1.33722900	1.43439500
H	0.11981200	1.19004000	1.72588000
H	1.30800100	0.26052400	-1.49945100
H	0.00000000	1.95388500	-0.79416400
H	0.37009100	-1.53471100	-1.36767200
H	-0.84123300	-1.33722900	1.43439500
H	1.69072400	0.64069100	-0.87074800
H	-0.37009100	1.53471100	-1.36767200
H	1.55100500	-0.80262300	0.86143900
H	-0.11981200	-1.19004000	1.72588000
H	0.00000000	-1.95388500	-0.79416400
H	-1.30800100	-0.26052400	-1.49945100
H	-1.69072400	-0.64069100	-0.87074800
H	-1.55100500	0.80262300	0.86143900

Table. S34 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_{15}^{+} cluster.

Ce^{+}	-0.11722400	-0.00905200	-0.02093300
H	2.29155100	1.18422300	-0.43082700
H	-1.17202800	2.12334400	-0.76027800
H	1.83069900	1.75048800	-0.62238600
H	1.51465000	-2.00342400	0.56566200
H	0.70898900	1.67665200	1.77409600
H	-0.45254900	-0.70624800	1.84534400
H	-1.61999000	1.62146500	-1.13636800
H	0.56137800	1.04900700	2.18042400
H	-2.27591000	-0.60611600	1.09391100
H	-1.02217300	-1.63134600	-1.80022200
H	4.68990600	-0.35016000	-0.23646100
H	-1.44457900	-1.00731200	-1.93198200
H	4.63646500	-0.34641500	-0.97882700
H	-2.59266500	-0.36703300	0.43801700
H	1.14524300	-1.86213300	1.21401900

Table. S35 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_{16}^{+} cluster.

Ce^{+}	0.00718800	-0.05638800	-0.00248100
H	2.14398200	0.68982300	1.36027300
H	1.96253700	-2.07074400	-0.39297700
H	-2.14460800	1.18195000	-0.33788700
H	0.12506900	2.41753700	-0.33561300
H	-0.50162200	0.85690800	-1.72638300
H	-1.54050000	-0.89986700	1.83973100
H	-1.80094700	-1.43031500	-1.36394300
H	2.04470300	-1.99370300	0.34937900
H	-1.74310200	-1.47808100	1.38944300
H	-0.45281800	0.82981600	1.74864400
H	2.09549100	0.71998300	-1.40822800
H	0.10784900	2.39526000	0.42654900
H	-1.61557500	-0.83783800	-1.80351000
H	1.54671500	0.83481400	1.80925000
H	1.48264200	0.87075400	-1.83502500
H	-2.12674100	1.18417900	0.42420600

Table. S36 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_{17}^{+} cluster.

Ce^{+}	-0.03149000	0.04128600	0.00399800
H	1.86696500	-1.87411700	0.31951700
H	-1.57616000	-0.43608600	1.75597700
H	1.95332700	0.77898700	-1.53602000
H	-1.65812400	-0.31914300	-1.74397100
H	0.73378500	2.54091900	-0.00610100
H	2.03250700	0.74271900	1.45122700
H	-1.96251400	0.12843600	1.39014900
H	1.59741000	0.22140600	-1.91361600
H	1.70039700	0.17179000	1.83027200
H	0.21453300	-1.05404500	1.60981000
H	-0.73614700	-2.27560800	0.33805200
H	0.08968300	-0.98150900	-1.66245900
H	-0.02852000	2.55520000	0.01959800
H	-1.49652800	1.34108000	0.08136300
H	-2.06455300	0.17247600	-1.30617000
H	1.89860000	-1.85403300	-0.43290400
H	-0.73826100	-2.25305400	-0.42660800

Table. S37 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_{18}^{+} cluster.

Ce^{+}	0.08320400	0.02656100	0.00057500
H	2.04801800	1.17095400	-1.34744900
H	1.69219100	0.62291400	1.84691800
H	-4.67487800	0.33707300	-0.28752300
H	-1.58416900	-0.69754800	1.79033400
H	0.44817600	-0.89804200	1.75513500
H	-1.50240600	-0.69924500	-1.85648500
H	-2.08745700	-0.47435300	-1.42638500
H	-0.32995300	-2.42061000	0.38411500
H	-0.29142100	-2.42167100	-0.37686800
H	-0.07899700	2.81883700	-0.43634900
H	-2.14553600	-0.45324800	1.33979400
H	2.05769100	-1.43872200	0.41356800
H	1.79331400	0.60512000	-1.78803900
H	1.97064800	1.18544300	1.41388700
H	-4.55694300	0.78328000	0.29718300
H	2.04895800	-1.45696900	-0.34906800
H	0.51683200	-0.93590000	-1.71703200
H	-0.14992200	2.83211900	0.31093900

Table. S38 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_{19}^{+} cluster.

Ce^{+}	-0.12296100	0.00642500	-0.01609200
H	-2.05481000	1.07121200	1.26128800
H	5.13415400	0.25165100	-0.43752200
H	2.25589400	0.95400000	0.26784800
H	-0.91327600	0.03426900	-2.46229200
H	-2.35352300	-1.17903500	-0.76943300
H	0.52956200	-2.42482200	0.77007700
H	-0.58656300	-0.65562600	-2.44844500
H	-2.35121400	-1.22484000	-0.01032100
H	-0.64709900	2.17896500	-1.29018500
H	-0.19762900	2.46385400	-0.74359300
H	1.85310900	1.59487400	0.35877400
H	1.99127300	-1.17257200	-0.89340600
H	5.12836500	-0.10063900	0.21929200
H	0.89809400	0.47455100	2.37370400
H	1.47015200	-1.50531700	-1.34091800
H	-0.04090700	-2.21575200	1.22567900
H	-1.25427200	-0.69955400	1.52945500
H	-1.97945300	1.68442600	0.81794500
H	0.24986000	0.09768300	2.50537600

Table. S39 Cartesian coordinates of the geometrical structure of the lowest total energy state of the CeH_{20}^{+} cluster.

Ce^{+}	-0.10009900	0.00535100	-0.03456600
H	0.26465900	-0.15351500	1.93984300
H	-2.01219600	-0.08612100	-0.66905600
H	0.79892300	1.69343800	1.59880500
H	1.68603000	-1.10635800	-1.99752500
H	2.10142700	-1.21023100	-1.38255900
H	0.76517300	2.22925800	1.05524000
H	1.44129200	1.76126000	-1.76188300
H	1.93429200	1.71563500	-1.19878000
H	1.10187000	-1.80535300	1.26525800
H	-1.53071900	1.75682900	-1.14002700
H	-1.81276700	-1.54368500	0.99308900
H	-1.55202800	0.96331800	1.76242500
H	3.76532200	-0.01084400	1.37071500
H	-1.32374600	-1.73763200	-1.45787100
H	1.13605400	-2.23535000	0.64229900
H	-0.99936300	2.29589600	-1.03981200
H	-1.30785400	-1.54308900	1.56197900
H	-2.05692900	0.97146300	1.19177300
H	-0.71892000	-2.20182300	-1.45011600
H	4.12522900	-0.06346500	0.72105100

Table. S40 Vibrational frequencies (cm^{-1}) of ground state structures of cation CeH_n^+ (n=2-20) clusters.

CeH_2^+	CeH_3^+	CeH_4^+	CeH_5^+	CeH_6^+
493.7392	229.7662	141.2131	198.9796	114.0146
1600.0654	364.8959	308.2876	237.1653	202.3278
1646.4038	411.7832	430.6104	267.6282	324.2203
	770.5201	554.1605	395.2143	482.5131
	1405.1871	562.6526	449.5637	521.5419
	3958.7219	852.4845	470.9164	536.6108
		1535.3265	498.7512	562.7205
		1586.8315	814.7174	819.9364
		4104.5449	821.5402	829.9365
			1441.1045	840.0853
			3947.7068	1121.0484
			3954.9764	1493.7858
				1548.4550
				3809.8028
				4126.6906
CeH_7^+	CeH_8^+	CeH_9^+	CeH_{10}^+	CeH_{11}^+
34.8124	124.9886	64.7688	78.4024	33.0487
62.3141	139.7864	103.5077	103.8520	49.8417
135.7615	260.3104	128.4702	171.8659	69.3361
193.7304	281.6461	164.8988	198.3815	78.6647
235.3465	329.8412	188.3324	245.1313	145.2441
250.4861	409.3192	210.8401	300.1674	174.1229
315.9160	483.6764	300.8810	344.7791	187.6891
330.4408	513.3767	332.5490	417.8878	189.9107
380.2363	578.6601	376.5392	445.5120	194.7873
515.1325	632.1168	395.5902	487.0332	230.1557

535.9240	645.1609	422.5278	510.6597	238.5883
606.6240	725.1466	438.7025	524.7449	327.2068
800.4929	787.8045	459.3583	570.4535	333.5312
825.8670	921.2220	484.0172	612.4839	353.6089
1141.4660	935.0497	489.5301	664.0835	411.1049
1573.8699	1009.9097	721.6020	762.0214	420.8877
4138.5847	1452.8669	763.2984	800.1515	429.7955
4296.8291	1496.7249	772.1980	835.6308	448.6114
	3965.4284	825.0313	862.0637	469.5084
	4010.5713	1435.1179	929.6185	473.3686
	4027.5742	3955.4006	1047.7564	741.1711
		4061.3988	1423.3715	758.7542
		4099.7454	1473.5100	769.9616
		4186.5704	3910.6965	785.0907
			4022.5668	1468.9285
			4098.1138	4045.0763
			4127.1822	4067.2212
				4077.2426
				4092.5784
				4378.4767
CeH_{12}^+	CeH_{13}^+	CeH_{14}^+	CeH_{15}^+	CeH_{16}^+
70.4573	65.4044	150.6088	27.3315	78.4620
96.0069	89.6693	165.6372	86.8294	129.6898
108.5492	144.9214	174.0282	115.7334	150.2880
150.5764	172.1254	189.5195	145.6249	169.8788
164.6018	200.5764	197.5155	194.2079	178.5555
187.8767	211.6368	201.5156	206.2970	179.3568
224.8727	217.5071	215.5937	224.3190	198.0373
248.0488	237.0029	225.8027	238.1095	207.0802

265.0319	286.0788	306.8100	289.2087	219.6232
318.7811	294.2397	319.6619	296.5618	227.3485
349.5088	323.9318	337.4440	299.4582	235.3407
376.6041	367.9608	388.9901	346.8056	305.0384
416.2077	375.2250	420.4928	349.1960	311.4379
445.3292	390.5574	445.5962	367.0737	333.4225
483.0183	410.6746	453.9924	388.0559	340.7034
508.2082	438.4953	462.3438	413.0913	387.7895
525.9703	439.4070	469.7937	414.2758	423.9323
562.6764	456.8648	474.8025	429.7600	446.4119
597.2672	466.3611	485.1587	436.9863	453.0313
647.7125	476.9189	495.8643	440.5743	469.1427
657.7040	537.8103	571.0391	462.7665	477.8668
685.8093	614.3700	615.5066	463.0637	487.9931
836.5714	695.8669	627.5630	465.5686	513.3522
844.5093	734.8836	678.1301	477.0302	516.9462
892.1925	750.5478	746.2430	509.6732	545.2558
899.7772	757.3207	795.5243	633.1110	555.6031
1427.2265	787.6615	810.9112	692.1731	621.6270
1471.4450	881.0620	818.9000	741.4122	628.1995
4063.4356	925.7751	838.2019	755.2431	683.8456
4071.6975	1403.0889	916.1158	763.4286	762.1667
4113.3146	4025.4802	933.9339	774.8965	804.7135
4119.5138	4063.8798	1407.4005	823.1139	827.6503
4310.0835	4068.0328	1448.1952	862.7770	843.9152
	4069.1288	4075.8971	907.8027	855.7586
	4079.7877	4094.0403	1377.2315	891.7815
	4101.7361	4127.2685	4032.6161	915.4222
		4143.1771	4050.4938	1395.0781

		4153.6143	4064.8645	1432.7319
		4159.7872	4089.4646	4091.6296
			4093.8368	4112.0759
			4101.9001	4116.0855
			4155.5846	4117.2984
				4131.4779
				4151.7519
				4323.4105
CeH_{17}^{+}	CeH_{18}^{+}	CeH_{19}^{+}	CeH_{20}^{+}	-
67.6036	117.4141	19.0698	112.7222	
110.5215	131.6508	35.5452	130.0184	
134.3922	158.7353	60.1556	141.4046	
148.6453	171.4362	63.3340	149.8216	
209.5942	187.5414	67.0893	155.3001	
213.8019	190.6470	109.7713	175.2986	
222.3165	191.6334	130.0449	187.3457	
227.4826	200.7400	149.5015	189.2670	
254.2744	214.8671	177.5745	194.3055	
281.4424	220.4845	204.5422	201.2422	
301.6185	263.1443	207.5027	217.5193	
302.5492	269.5525	221.2597	220.1625	
304.7941	282.0966	229.5116	239.6117	
354.5157	286.5061	247.5172	241.1374	
355.6905	290.0521	270.1825	263.6551	
392.2626	305.5522	289.5039	281.0091	
405.8032	318.8235	297.5261	287.3265	
411.2174	341.9187	304.8020	289.2648	
422.3813	355.8629	350.8329	301.3820	
422.5755	403.4964	356.6453	301.8857	

430.6456	425.0714	393.9793	326.3957	
432.6569	442.1303	408.9345	327.6860	
435.6885	447.3410	411.6534	379.9887	
451.4048	459.8285	419.6454	391.7861	
456.1419	515.9764	425.3265	396.5927	
459.6872	527.5024	430.2741	422.5520	
466.3398	528.1154	435.5718	439.3307	
471.4899	530.4288	437.8894	440.3560	
472.3848	533.5080	452.2068	456.5080	
683.3605	545.1681	457.9717	507.4628	
690.8403	562.2618	461.3734	519.6865	
753.0604	638.7331	468.0800	522.3185	
763.9808	678.1204	470.7447	536.9790	
765.0224	725.0576	477.5232	541.2141	
766.1726	765.3497	678.7286	544.0795	
816.8089	850.9005	694.5411	565.5106	
829.2386	859.3236	748.6229	637.7203	
869.2161	864.9014	763.3341	658.6466	
878.7897	889.2305	765.7221	721.5004	
1349.5261	899.6871	771.1507	767.9973	
4034.4143	908.5684	814.9590	843.8377	
4041.1211	1383.9480	826.3768	854.6808	
4062.5615	1420.8057	866.7745	856.7872	
4075.5432	4085.5055	878.7720	881.8651	
4131.5777	4091.9585	1349.8788	888.3938	
4135.8736	4098.7490	4032.1973	901.1859	
4136.7300	4101.7858	4038.9877	1377.9903	
4154.6260	4117.6133	4062.8482	1415.9569	
	4127.2547	4075.5546	4090.1233	

	4331.3261	4132.1587	4101.4099	
	4335.1200	4136.1363	4113.1882	
		4137.6074	4121.5131	
		4155.1704	4124.0005	
		4409.6006	4134.0094	
			4332.6049	
			4335.8093	
			4366.0596	