

Supporting Information for
Theory and X-ray absorption spectroscopy for aluminum coordination complexes – Al K-edge studies of charge and bonding in (BDI)Al, (BDI)AlR₂, and (BDI)AlX₂ complexes.

Alison B. Altman,^{1,2} C. D. Pemmaraju,² Clément Camp,¹ John Arnold*,^{1,2} Stefan G. Minasian*,² David Prendergast*,³ David K. Shuh*,² Tolek Tyliszczak⁴

¹ Department of Chemistry, University of California, Berkeley, California 94720

² Chemical Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, California 94720

³ Molecular Foundry, Lawrence Berkeley National Laboratory, Berkeley, California 94720

⁴ Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California 94720

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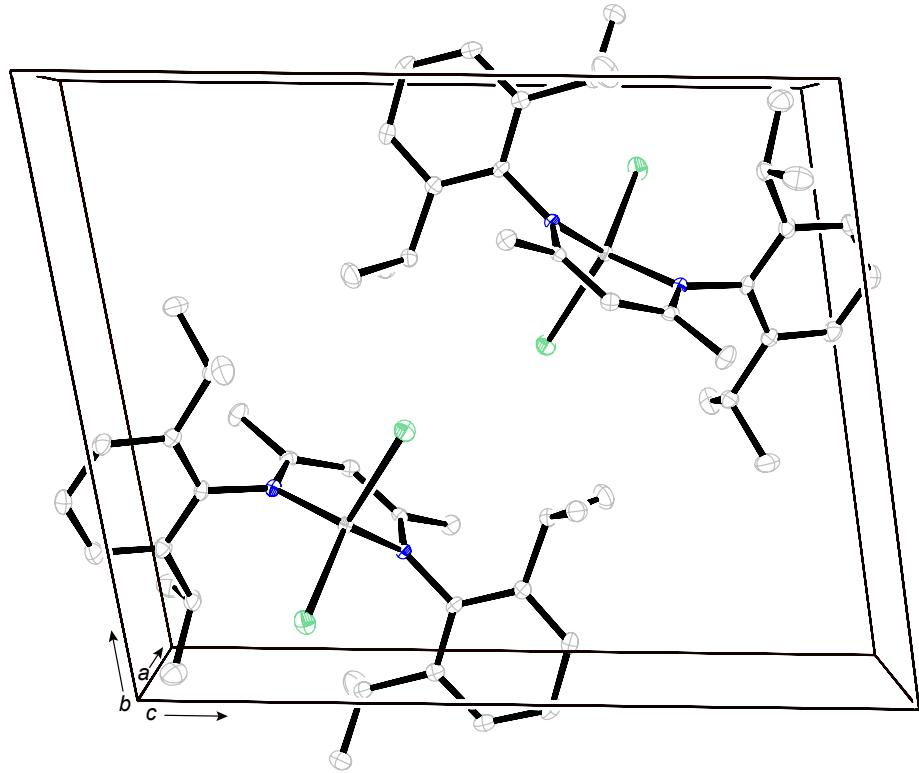


Figure S1. Projection of the crystal structure of $(\text{BDI})\text{AlI}_2$ onto the ac plane. Thermal ellipsoids are shown with 50% probability, with atoms colored as white (carbon), blue (nitrogen), gray (aluminum), and green (iodine). Hydrogen atoms have been omitted for clarity. Block-shaped colorless crystals of $(\text{BDI})\text{AlI}_2$ suitable for X-ray diffraction were grown upon letting stand at -40°C a concentrated toluene solution of the complex over a period of 2 days. The X-ray structural determinations were performed at CHEXRAY, University of California, Berkeley on a Bruker SMART QUAZAR diffractometer which is a 3-circle diffractometer that couples a CCD detector with a sealed-tube source of monochromated Mo K α radiation ($\lambda = 0.71073 \text{ \AA}$). A crystal of appropriate size was coated in Paratone-N oil and mounted on a Kapton[®] loop. The loop was transferred to the diffractometer, centered in the beam, and cooled by a nitrogen flow low-temperature apparatus that had been previously calibrated by a thermocouple placed at the same position as the crystal. Preliminary orientation matrices and cell constants were determined by collection of 36 10 s frames, followed by spot integration and least-squares refinement. The reported cell dimensions were calculated from all reflections with $I > 10 \sigma$. The data were corrected for Lorentz and polarization effects; no correction for crystal decay was applied. An empirical absorption correction based on comparison of redundant and equivalent reflections was applied using SADABS.¹ All software used for diffraction data processing and crystal-structure solution and refinement are contained in the APEX2 program suite (Bruker AXS, Madison, WI).² Thermal parameters for all non-hydrogen atoms were refined anisotropically. $R_1 = \sum(|F_o| - |F_c|)/\sum(|F_o|)$; $wR_2 = [\sum\{w(F_o^2 - F_c^2)^2\}/\sum\{w(F_o^2)^2\}]^{1/2}$. Thermal ellipsoid plot was created using Mercury supplied with Cambridge Structural Database (CCDC: Cambridge, U.K., 2004-2009).

Table S1. Crystallographic parameters for (BDI)AlI₂.

Compound	(BDI)AlI ₂
Formula	C ₂₉ H ₄₁ Al I ₂ N ₂
cryst syst	Triclinic
space group	P-1
volume (Å ³)	1521.41(10)
a (Å)	8.4839(3)
b (Å)	12.6740(5)
c (Å)	15.0089(6)
α (deg)	99.1484(17)
β (deg)	90.5395(17)
γ (deg)	106.9522(18)
Z	2
formula weight (g/mol)	698.42
density (g cm ⁻³)	1.525
absorption coefficient (mm ⁻¹)	2.115
F(000)	696
temp (K)	100(2)
total no. reflections	56457
unique reflections [R(int)]	5594 [0.022]
Final R indices [I > 2σ(I)]	R1 = 0.0144, wR2 = 0.0348
Largest diff. peak and hole (e.Å ⁻³)	0.424 and -0.311
GoF	0.924

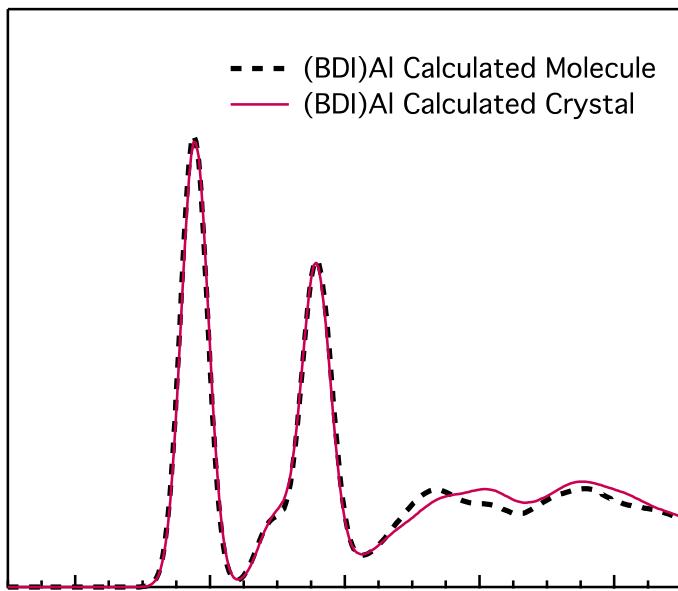


Figure S2. XANES spectra calculated using the XCH approach for an isolated molecular unit (black) and the molecular crystal (red) for the (BDI)Al compound.

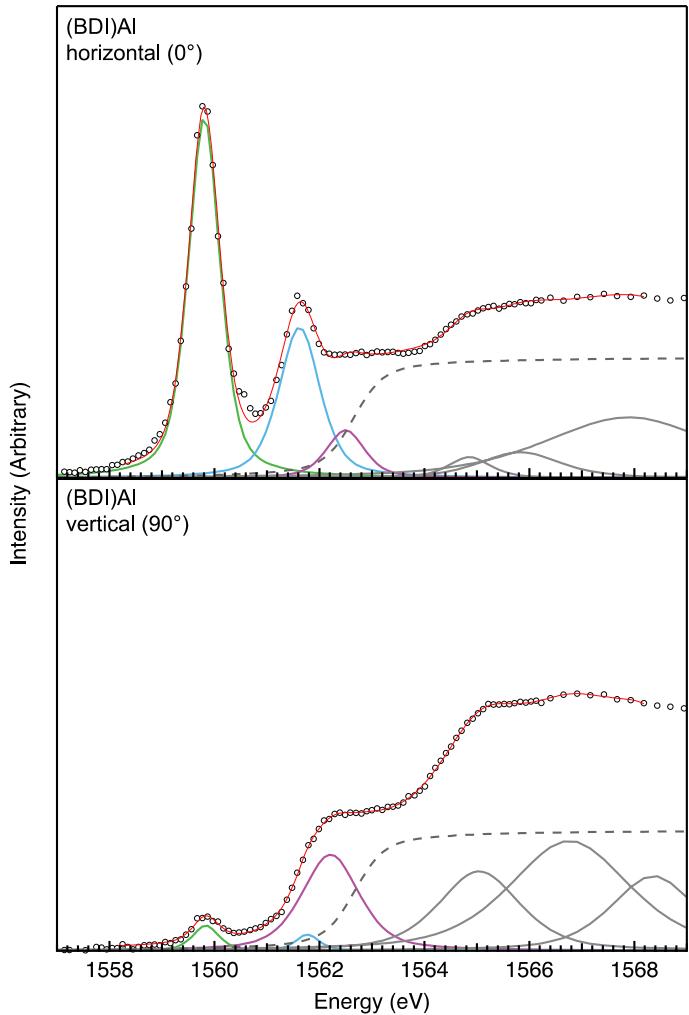


Figure S3. Al K-edge XANES (STXM) experimental data for (BDI)Al at perpendicular light polarization settings (black circles). Pseudo-Voigt functions used to model pre-edge features (green- b_1^* , blue- b_2^* , purple- a_1^* traces), step-function used to model the edge (dashed grey trace), and pseudo-Voigt functions used to model post-edge features (solid grey traces) summed to generate the curve-fits (red traces).

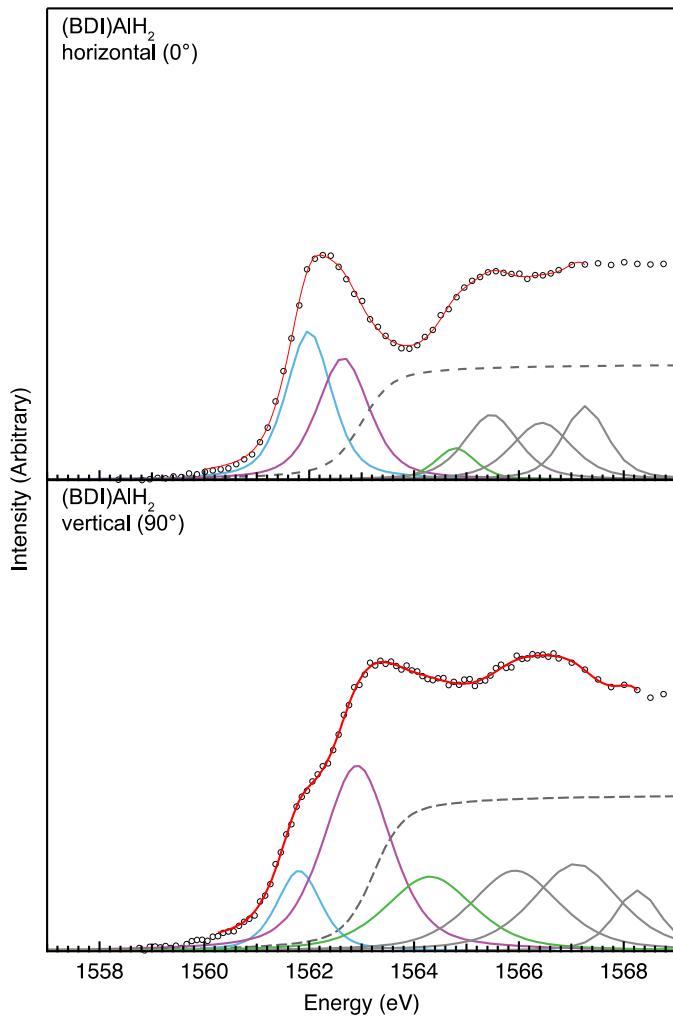


Figure S4. Al K-edge XANES (STXM) experimental data for $(\text{BDI})\text{AlH}_2$ at perpendicular light polarization settings (black circles). Pseudo-Voigt functions used to model pre-edge features (green- b_1^* , blue- b_2^* , purple- a_1^* traces), step-function used to model the edge (dashed grey trace), and pseudo-Voigt functions used to model post-edge features (solid grey traces) summed to generate the curve-fits (red traces).

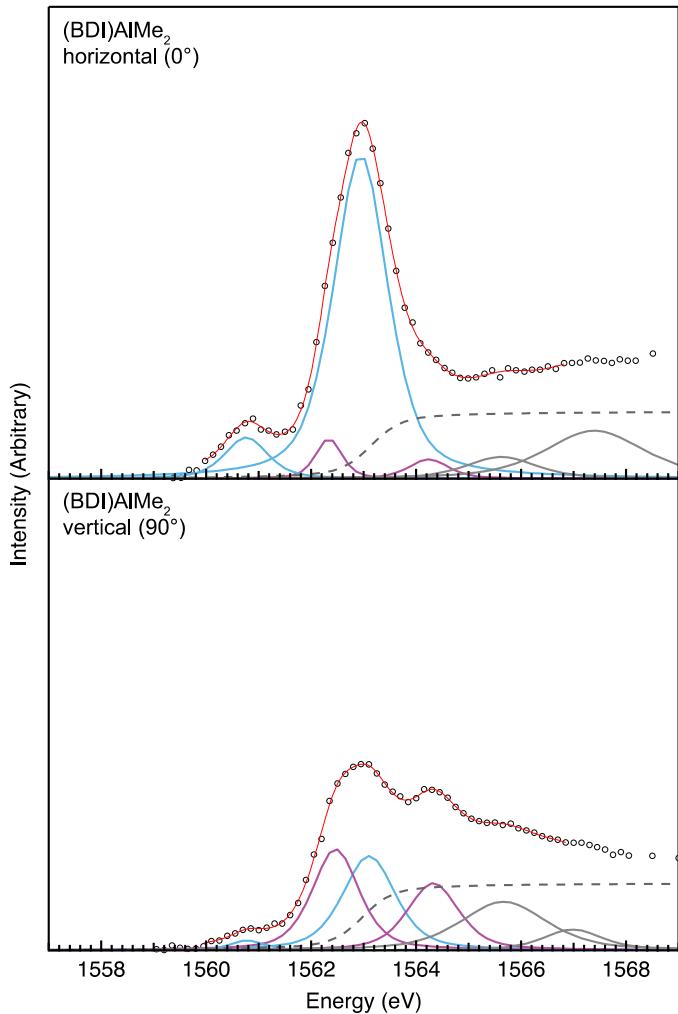


Figure S5. Al K-edge XANES (STXM) experimental data for (BDI)AlMe₂ at perpendicular light polarization settings (black circles). Pseudo-Voigt functions used to model pre-edge features (blue, green, and purple traces), step-function used to model the edge (dashed grey trace), and pseudo-Voigt functions used to model post-edge features (solid grey traces) summed to generate the curve-fits (red traces).

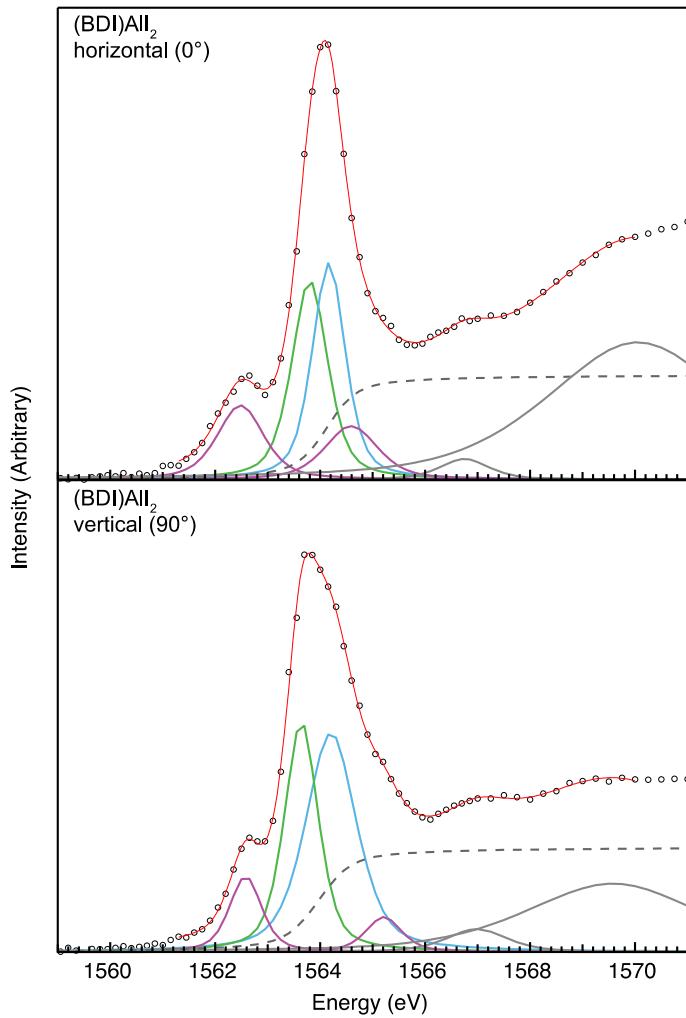


Figure S6. Al K-edge XANES (STXM) experimental data for (BDI)AlI₂ at perpendicular light polarization settings (black circles). Pseudo-Voigt functions used to model pre-edge features (blue, green, and purple traces), step-function used to model the edge (dashed grey trace), and pseudo-Voigt functions used to model post-edge features (solid grey traces) summed to generate the curve-fits (red traces).

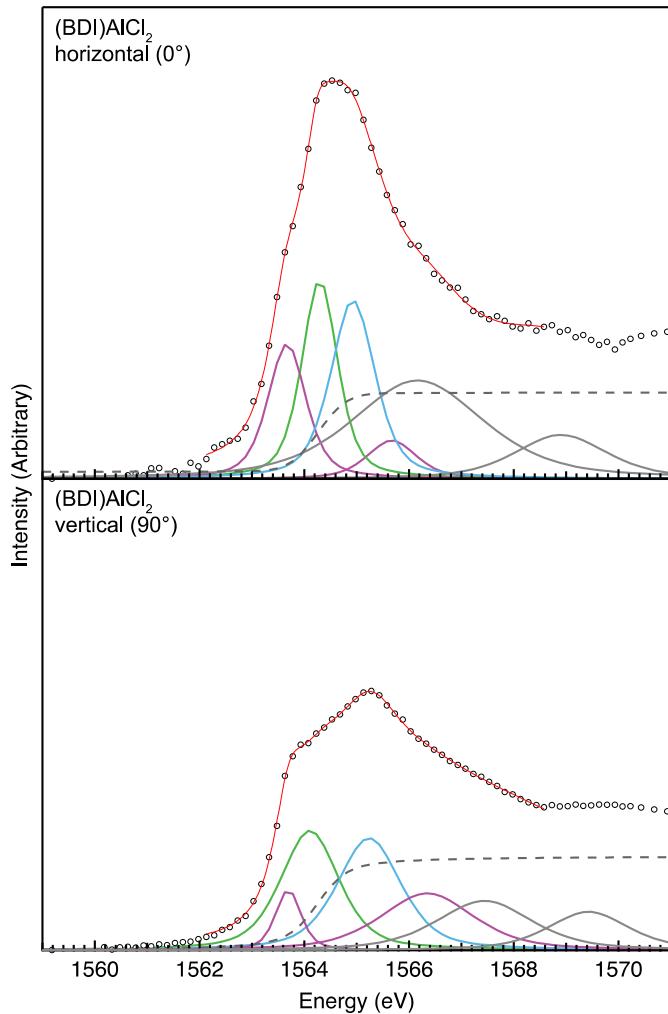


Figure S7. Al K-edge XANES (STXM) experimental data for $(\text{BDI})\text{AlCl}_2$ at perpendicular light polarization settings (black circles). Pseudo-Voigt functions used to model pre-edge features (blue, green, and purple traces), step-function used to model the edge (dashed grey trace), and pseudo-Voigt functions used to model post-edge features (solid grey traces) summed to generate the curve-fits (red traces).

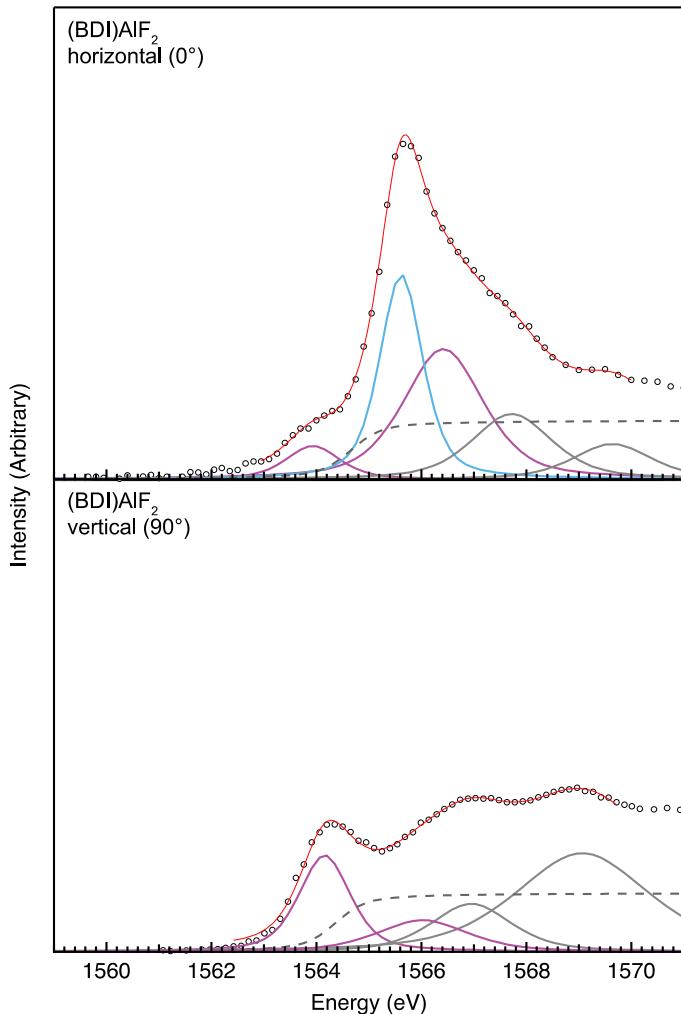


Figure S8. Al K-edge XANES (STXM) experimental data for (BDI)AlF₂ at perpendicular light polarization settings (black circles). Pseudo-Voigt functions used to model pre-edge features (blue, green, and purple traces), step-function used to model the edge (dashed grey trace), and pseudo-Voigt functions used to model post-edge features (solid grey traces) summed to generate the curve-fits (red traces).

Table S2. Background subtracted and calibrated Al K-edge XANES data for (BDI)Al and (BDI)AlR₂ compounds (where R = H, Me). S1 refers to data collected at horizontal polarization while S2 refers to data collected at vertical polarization.

(BDI)Al S1 Energy (eV)	(BDI)Al S1 Intensity	(BDI)Al S2 Energy (eV)	(BDI)Al S2 Intensity	(BDI)AlH ₂ S1 eV	(BDI)AlH ₂ S1 Intensity	(BDI)AlH ₂ S2 Energy (eV)	(BDI)AlH ₂ S2 Intensity	(BDI)AlMe ₂ S1 Energy (eV)	(BDI)AlMe ₂ S 1 Intensity	(BDI)AlMe ₂ S2 Energy (eV)	(BDI)AlMe ₂ S2 Intensity
1519.14	0.008323631	1519.14	0.006349346	1519.76	0.000251741	1519.76	0.034703708	1520	-0.080079977	1520	0.00229141
1521.14	-0.007344867	1521.14	0.022917924	1520.76	0.006272324	1520.76	0.05611684	1521	-0.077435202	1521	-0.009431427
1523.14	0.003280946	1523.14	0.022198749	1521.76	-0.000618132	1521.76	-0.014098046	1522	-0.057307337	1522	-0.010806118
1525.14	-0.000202937	1525.14	0.006313899	1522.76	-0.000477337	1522.76	0.010947458	1523	-0.026262742	1523	-0.046305027
1527.14	-0.002209223	1527.14	-0.008948056	1523.76	0.001099276	1523.76	0.017324184	1524	-0.001715505	1524	-0.003203577
1529.14	-0.018450742	1529.14	-0.024080849	1524.76	0.008201669	1524.76	0.046589511	1525	-0.005501046	1525	-0.0115277
1531.14	-0.014703798	1531.14	0.009035933	1525.76	0.002554083	1525.76	-0.014562516	1526	0.043554904	1526	-0.023078943
1533.14	-0.011442945	1533.14	0.007277811	1526.76	-0.008088773	1526.76	0.033050775	1527	0.030700345	1527	0.006023465
1535.14	5.36E-05	1535.14	-0.007592402	1527.76	0.00407611	1527.76	0.030005777	1528	0.06453574	1528	0.020635416
1537.14	-0.010160824	1537.14	-0.005665202	1528.76	0.008931851	1528.76	-0.010316843	1529	0.078508083	1529	-0.01605058
1539.14	0.000347318	1539.14	0.004230559	1529.76	0.011284421	1529.76	-0.035817048	1530	0.07734487	1530	-0.010252524
1541.14	-0.006845342	1541.14	-0.009156776	1530.76	0.00856411	1530.76	-0.019998402	1531	0.074991124	1531	0.034155071
1543.14	0.007246614	1543.14	-0.008801813	1531.76	0.008333148	1531.76	-0.006810977	1532	0.097144585	1532	-0.014402405
1545.14	0.002824656	1545.14	-0.011580344	1532.76	-0.008839077	1532.76	0.009241322	1533	0.083051559	1533	0.06285195
1547.14	0.002023448	1547.14	-0.001969812	1533.76	0.010811616	1533.76	-0.004295212	1534	0.128973365	1534	0.011417842
1549.14	0.000121121	1549.14	0.003198327	1534.76	0.004216443	1534.76	0.005822015	1535	-0.029895966	1535	-0.022633939
1551.14	0.019765456	1551.14	-0.009748459	1535.76	0.006977547	1535.76	-0.004753657	1536	-0.069029148	1536	-0.001699354
1553.14	0.00678039	1553.14	-0.005148103	1536.76	-0.012330794	1536.76	-0.026305291	1537	-0.052018029	1537	-0.016589087
1555.14	0.022225626	1555.14	0.009844218	1537.76	0.006407312	1537.76	-0.021137533	1538	-0.037688299	1538	0.057923432
1557.14	0.052799985	1557.14	0.007723219	1538.76	0.002047843	1538.76	-0.000377981	1539	-0.071717674	1539	-0.010857913
1557.24	0.048437625	1557.24	0.007076625	1539.76	-0.000139176	1539.76	0.010247509	1540	-0.031959974	1540	0.050535251
1557.34	0.042874525	1557.34	-0.00304769	1540.76	0.004305772	1540.76	-0.045387365	1541	-0.016201096	1541	0.063564783
1557.44	0.063398233	1557.44	-0.008628543	1541.76	-0.002415729	1541.76	-0.017763275	1542	-0.015758526	1542	0.034059341
1557.54	0.049040214	1557.54	0.004488255	1542.76	0.008838965	1542.76	-0.028684516	1543	-0.016161713	1543	0.040828158

1557.65	0.06870681	1557.65	-0.001156264	1543.76	-0.003834262	1543.76	-0.019445953	1544	-0.044200443	1544	0.046809187
1557.75	0.069577993	1557.75	0.030812321	1544.76	0.004544165	1544.76	-0.01690183	1545	-0.043120898	1545	0.023987124
1557.85	0.072450283	1557.85	0.027300278	1545.76	-0.003803185	1545.76	-0.04446929	1546	0.003995202	1546	0.013891051
1557.95	0.072141201	1557.95	0.010397901	1546.76	-0.011051258	1546.76	-0.042007918	1547	0.002675411	1547	-0.006111625
1558.05	0.107134502	1558.05	0.021747536	1547.76	-0.023696276	1547.76	-0.085879508	1548	-0.024521085	1548	-0.03929831
1558.15	0.10915487	1558.15	0.022910096	1548.76	-0.008738374	1548.76	-0.025318308	1549	-0.034035989	1549	0.019262334
1558.25	0.130057888	1558.25	0.05419786	1549.76	-0.023572142	1549.76	0.004453455	1550	-0.025163255	1550	-0.022178435
1558.35	0.135115807	1558.35	0.031561335	1550.76	-0.022940839	1550.76	-0.010387679	1551	-0.001520141	1551	0.014458669
1558.45	0.159200046	1558.45	0.011439935	1551.76	-0.023957667	1551.76	-0.063396634	1552	0.007698476	1552	-0.085381101
1558.55	0.185798508	1558.55	0.030587991	1552.76	-0.022809829	1552.76	-0.061468888	1553	-0.000514916	1553	-0.069482259
1558.66	0.205485078	1558.66	0.044728971	1553.76	-0.008224157	1553.76	-0.01394739	1554	0.000989356	1554	-0.077168657
1558.76	0.23202186	1558.76	0.047847708	1554.76	-0.019741162	1554.76	-0.008751668	1555	-0.006223047	1555	-0.06456815
1558.86	0.308628531	1558.86	0.051951991	1555.76	-0.01567646	1555.76	-0.013932188	1556	-0.003698275	1556	-0.02849497
1558.96	0.360749215	1558.96	0.044860576	1556.76	-0.011957598	1556.76	-0.037099182	1557	-0.019539309	1557	-0.065563826
1559.06	0.455181451	1559.06	0.071130893	1557.76	-0.016689899	1557.76	-0.035184454	1558	-0.020021794	1558	-0.050209763
1559.16	0.62461078	1559.16	0.063051171	1557.91	-0.015462484	1558.76	0.020716289	1558.15	-0.011920352	1558.15	-0.062697381
1559.26	0.780688783	1559.26	0.087235871	1558.06	-0.021750275	1558.86	0.00562037	1558.3	-0.014174804	1558.3	-0.027996329
1559.36	1.133382789	1559.36	0.094749419	1558.21	-0.006620264	1558.96	0.028233453	1558.45	-0.012487837	1558.46	-0.086412495
1559.46	1.581321508	1559.46	0.133973195	1558.36	0.002973208	1559.06	0.029931166	1558.6	-0.028133373	1558.61	-0.062897384
1559.56	2.061124723	1559.56	0.17771831	1558.51	-0.011001011	1559.16	0.02368292	1558.75	-0.045133797	1558.76	-0.048008269
1559.67	2.832496012	1559.67	0.26964726	1558.66	-0.008677273	1559.26	0.033798682	1558.9	-0.005553161	1558.91	-0.001864409
1559.77	3.072560587	1559.77	0.271404502	1558.81	0.000513101	1559.36	0.020052986	1559.05	0.01454312	1559.06	-0.03448363
1559.87	3.027865963	1559.87	0.28147381	1558.96	0.006338089	1559.46	0.034210154	1559.2	0.002027134	1559.22	-0.008346538
1559.97	2.585608438	1559.97	0.245477384	1559.11	0.0192222	1559.56	0.021385089	1559.35	0.074696702	1559.37	0.007388398
1560.07	1.996753332	1560.07	0.24197815	1559.26	0.014490011	1559.66	0.045353093	1559.5	0.035878299	1559.52	0.01214083
1560.17	1.612488089	1560.17	0.185020196	1559.41	0.029951523	1559.76	0.065024707	1559.65	0.020290649	1559.67	0.13102645
1560.27	1.067093877	1560.27	0.163906797	1559.56	0.026264637	1559.86	0.071127295	1559.8	0.024543712	1559.82	0.119515549
1560.37	0.861588166	1560.37	0.145973591	1559.71	0.056113906	1559.96	0.073056245	1559.95	0.061942346	1559.98	0.264294597
1560.47	0.714670054	1560.47	0.151293597	1559.86	0.049014604	1560.06	0.065315968	1560.1	0.136505549	1560.13	0.356633625
1560.57	0.690499717	1560.57	0.157521592	1560.01	0.069346125	1560.16	0.091427393	1560.25	0.145440345	1560.28	0.475712014
1560.68	0.576087188	1560.68	0.171564839	1560.16	0.08115395	1560.26	0.094975723	1560.4	0.21483796	1560.43	0.643956033
1560.78	0.529791124	1560.78	0.185649485	1560.31	0.091205543	1560.36	0.116403605	1560.55	0.251299372	1560.58	0.711345511

1560.88	0.53575081	1560.88	0.196363733	1560.46	0.101725934	1560.46	0.12413499	1560.7	0.30539079	1560.74	0.822724981
1560.98	0.582308258	1560.98	0.229843504	1560.61	0.137275075	1560.56	0.126776809	1560.85	0.325612606	1560.89	0.891214458
1561.08	0.636100592	1561.08	0.262191845	1560.76	0.1783051	1560.66	0.162226927	1561	0.299249576	1561.04	0.730525753
1561.18	0.8096646	1561.18	0.288409879	1560.91	0.220312077	1560.76	0.186643366	1561.15	0.335825753	1561.19	0.710958065
1561.28	0.931927116	1561.28	0.319382043	1561.06	0.32558896	1560.86	0.207197777	1561.3	0.397745794	1561.34	0.655868588
1561.38	1.188051479	1561.38	0.421778235	1561.21	0.45131369	1560.96	0.228295131	1561.45	0.397634114	1561.5	0.696872575
1561.48	1.38101114	1561.48	0.520549087	1561.36	0.676609315	1561.06	0.316496294	1561.6	0.522898173	1561.65	0.72854407
1561.58	1.505777515	1561.58	0.644812143	1561.51	0.935564359	1561.16	0.355015234	1561.75	0.69963432	1561.8	1.084760638
1561.69	1.443640725	1561.69	0.752039388	1561.66	1.218970767	1561.26	0.427352856	1561.9	1.045797556	1561.95	1.325420453
1561.79	1.388231155	1561.79	0.873252534	1561.81	1.503076994	1561.36	0.554098688	1562.05	1.420321508	1562.1	2.023692822
1561.89	1.236468459	1561.89	0.926176692	1561.96	1.811488317	1561.46	0.627833788	1562.2	1.653466529	1562.26	2.859291227
1561.99	1.108144893	1561.99	1.006776589	1562.11	1.904217885	1561.56	0.743036078	1562.35	2.216020916	1562.41	3.498303319
1562.09	1.037269822	1562.09	1.077111886	1562.26	1.933375682	1561.66	0.807597684	1562.5	2.476772138	1562.56	4.171535889
1562.19	1.025834139	1562.19	1.08921132	1562.41	1.928533762	1561.76	0.920958646	1562.65	2.617241574	1562.71	4.831901209
1562.29	1.018010754	1562.29	1.13177965	1562.56	1.833650772	1561.86	0.982748868	1562.8	2.720569848	1562.86	5.124821456
1562.39	1.020141755	1562.39	1.14279115	1562.71	1.728142357	1561.96	1.020857025	1562.95	2.761100334	1563.02	5.27433522
1562.49	1.020651273	1562.49	1.123731078	1562.86	1.60016737	1562.06	1.07957841	1563.1	2.758888603	1563.17	4.898655261
1562.59	1.018820916	1562.59	1.142987342	1563.01	1.540081806	1562.16	1.124929053	1563.25	2.623768459	1563.32	4.382681502
1562.7	1.031424106	1562.7	1.139011037	1563.16	1.381586336	1562.26	1.177758235	1563.4	2.459918369	1563.47	3.709765629
1562.8	1.043591459	1562.8	1.135166581	1563.31	1.317203242	1562.36	1.194025682	1563.55	2.355254592	1563.62	3.081104708
1562.9	1.016669514	1562.9	1.152968227	1563.46	1.23999282	1562.46	1.279535718	1563.7	2.283973167	1563.78	2.535184229
1563	1.033752405	1563	1.162467173	1563.61	1.17868788	1562.56	1.379025528	1563.85	2.197984152	1563.93	2.319051428
1563.1	1.044472601	1563.1	1.175079856	1563.76	1.133796603	1562.66	1.503623186	1564	2.256572112	1564.08	2.010138256
1563.2	1.039275843	1563.2	1.164215925	1563.91	1.12833142	1562.76	1.566329336	1564.15	2.388073733	1564.23	1.870885053
1563.3	1.041437124	1563.3	1.189628865	1564.06	1.159751621	1562.86	1.678297555	1564.3	2.382451788	1564.38	1.760561461
1563.4	1.04174088	1563.4	1.192518446	1564.21	1.229958929	1562.96	1.694593361	1564.45	2.344356445	1564.54	1.641675354
1563.5	1.034163082	1563.5	1.19987399	1564.36	1.2915965	1563.06	1.76056194	1564.6	2.265032544	1564.69	1.572136455
1563.6	1.026523669	1563.6	1.225528299	1564.51	1.417150849	1563.16	1.834297092	1564.75	2.127598508	1564.84	1.493379779
1563.7	1.033600386	1563.7	1.277151454	1564.66	1.470002445	1563.26	1.818563613	1564.9	2.032449756	1564.99	1.485896656
1563.81	1.042641857	1563.81	1.285257551	1564.81	1.573058852	1563.36	1.847824138	1565.05	1.954136223	1565.14	1.503451016
1563.91	1.048764034	1563.91	1.322126241	1564.96	1.655596629	1563.46	1.828124781	1565.2	1.914501801	1565.3	1.554162104
1564.01	1.090876203	1564.01	1.358462104	1565.11	1.714143515	1563.56	1.841757823	1565.35	1.892645974	1565.45	1.607225572

1564.11	1.106378055	1564.11	1.44369946	1565.26	1.746104992	1563.66	1.813796217	1565.5	1.894503885	1565.6	1.504380988
1564.21	1.142681605	1564.21	1.512653692	1565.41	1.785926505	1563.76	1.792302805	1565.65	1.85946689	1565.75	1.638080165
1564.31	1.185942938	1564.31	1.571831104	1565.56	1.795875116	1563.86	1.817927972	1565.8	1.878939362	1565.9	1.609044636
1564.41	1.228937432	1564.41	1.632991716	1565.71	1.782664385	1563.96	1.786708698	1565.95	1.812012092	1566.06	1.58733275
1564.51	1.265086854	1564.51	1.689318909	1565.86	1.771593335	1564.06	1.779048713	1566.1	1.777229663	1566.21	1.61656743
1564.61	1.29367291	1564.61	1.7602761	1566.01	1.774503139	1564.16	1.749481909	1566.25	1.747756496	1566.36	1.617396939
1564.71	1.333434551	1564.71	1.819472421	1566.16	1.730702213	1564.26	1.73053806	1566.4	1.693995781	1566.51	1.666116182
1564.82	1.35215274	1564.82	1.884618498	1566.31	1.762489887	1564.36	1.723255816	1566.55	1.656245253	1566.66	1.626860123
1564.92	1.359711063	1564.92	1.919195729	1566.46	1.759469583	1564.46	1.736605661	1566.7	1.639909442	1566.82	1.71549627
1565.02	1.384068793	1565.02	1.962517366	1566.61	1.777236104	1564.56	1.737066392	1566.85	1.601084384	1566.97	1.7189416
1565.12	1.401345433	1565.12	1.996826987	1566.76	1.804910705	1564.66	1.692174318	1567	1.595396913	1567.12	1.720969462
1565.22	1.412392771	1565.22	2.039637175	1567.01	1.849103809	1564.76	1.713654297	1567.15	1.594164034	1567.27	1.781560587
1565.32	1.421479933	1565.32	2.036725341	1567.26	1.85516966	1564.86	1.69363878	1567.3	1.565420839	1567.42	1.752048006
1565.42	1.399174582	1565.42	2.035297942	1567.51	1.863689938	1564.96	1.727493309	1567.45	1.530421636	1567.58	1.746353589
1565.52	1.418965243	1565.52	2.040442552	1567.76	1.850782218	1565.06	1.730446938	1567.6	1.496663957	1567.73	1.719251479
1565.62	1.43844798	1565.62	2.038160123	1568.01	1.873866032	1565.16	1.687873109	1567.75	1.417482737	1567.88	1.7719531
1565.72	1.435917957	1565.72	2.046606174	1568.26	1.860000618	1565.26	1.718824086	1567.9	1.45895238	1568.03	1.75100211
1565.83	1.452675354	1565.83	2.057753563	1568.51	1.853871282	1565.36	1.72216019	1568.05	1.404854901	1568.18	1.749843787
1565.93	1.444603525	1565.93	2.051755596	1568.76	1.859704812	1565.46	1.754055481	1568.5	1.399913095	1568.51	1.857064806
1566.03	1.444413121	1566.03	2.06063149	1569.01	1.862033891	1565.56	1.800076891	1569	1.371069154	1569.02	1.883514896
1566.13	1.472064368	1566.13	2.068231953	1569.26	1.847993412	1565.66	1.823058389	1569.5	1.443988629	1569.54	2.054105325
1566.23	1.467112117	1566.23	2.048831181	1569.51	1.839102239	1565.76	1.802651158	1570	1.557474788	1570.05	2.10309434
1566.4	1.490433522	1566.4	2.088798096	1569.76	1.824435435	1565.86	1.805944879	1570.5	1.727831001	1570.56	2.109068305
1566.65	1.465660587	1566.65	2.117599949	1570.01	1.833672877	1565.96	1.879869249	1571	1.801444121	1571.07	2.224542269
1566.91	1.496523874	1566.91	2.125988346	1570.26	1.832076505	1566.06	1.85865947	1571.5	1.923008052	1571.58	2.236384512
1567.16	1.493106046	1567.16	2.112118395	1570.51	1.813533273	1566.16	1.862850283	1572	2.050762542	1572.1	2.135951068
1567.42	1.520930872	1567.42	2.119532441	1570.76	1.81382069	1566.26	1.88965615	1572.5	2.13485045	1572.61	2.082996887
1567.67	1.503812014	1567.67	2.077810085	1571.01	1.774325965	1566.36	1.881713278	1573	2.218204425	1573.12	1.987125392
1567.93	1.496764574	1567.93	2.072922125	1571.26	1.777251827	1566.46	1.887792692	1573.5	2.166981914	1573.63	1.988901081
1568.18	1.507076126	1568.18	2.046131464	1571.51	1.791940659	1566.56	1.873995471	1574	2.120148083	1574.14	1.992188835
1568.44	1.483731232	1568.44	2.027511834	1571.76	1.736798096	1566.66	1.893766701	1574.5	2.079168639	1574.66	1.982063005
1568.69	1.466990455	1568.69	2.016705943	1572.01	1.739435744	1566.76	1.863067267	1575	1.992319424	1575.17	1.93154497

1568.95	1.486284693	1568.95	2.004017674	1572.26	1.731555455	1567.01	1.835750772	1575.5	1.968035323	1575.68	1.893261976
1569.2	1.445765243	1569.2	1.974914098	1572.51	1.712425836	1567.26	1.792145986	1576	1.935430924	1576.19	1.856830795
1569.45	1.466768073	1569.45	1.965180808	1572.76	1.680976763	1567.51	1.729424833	1576.5	1.912362156	1576.7	1.852539594
1569.71	1.462139491	1569.71	1.948321971	1573.01	1.676011451	1567.76	1.681141559	1577	1.921067559	1577.22	1.875739053
1569.96	1.441425084	1569.96	1.925301106	1573.26	1.674247967	1568.01	1.694339269	1577.5	1.89277435	1577.73	1.824132364
1570.22	1.433326962	1570.22	1.893392076	1573.51	1.669634946	1568.26	1.660602702	1578	1.880349627	1578.24	1.79354016
1570.47	1.402041497	1570.47	1.883330538	1573.76	1.637751004	1568.51	1.611998996	1578.5	1.85661541	1578.75	1.854785027
1570.73	1.382027888	1570.73	1.875996527	1574.01	1.647071513	1568.76	1.635112017	1579	1.852123257	1579.26	1.788395138
1570.98	1.397568588	1570.98	1.854864497	1574.26	1.647645059	1569.01	1.593354606	1579.5	1.789070028	1579.78	1.748026627
1571.24	1.373726216	1571.24	1.836016337	1574.51	1.640988394	1569.26	1.61135965	1580	1.75228778	1580.29	1.686986905
1571.49	1.372805248	1571.49	1.837608876	1574.76	1.623590813	1569.51	1.606546861	1580.5	1.683704657	1580.8	1.613762207
1571.75	1.362487703	1571.75	1.834457757	1575.01	1.605106897	1569.76	1.557094442	1581	1.682823386	1581.31	1.49558868
1572	1.331199588	1572	1.831719089	1575.26	1.59596122	1570.01	1.545658183	1581.5	1.639148675	1581.82	1.383645125
1572.26	1.346731953	1572.26	1.822507409	1575.51	1.58351966	1570.26	1.535874627	1582	1.601715436	1582.34	1.393895884
1572.52	1.336310394	1572.52	1.80052264	1575.76	1.584242795	1570.51	1.486465466	1582.5	1.501397093	1582.85	1.294127348
1572.77	1.306036892	1572.77	1.799733265	1576.01	1.552798688	1570.76	1.448515183	1583	1.453585567	1583.36	1.241583329
1573.03	1.287825289	1573.03	1.784944507	1576.26	1.550279285	1571.01	1.476229002	1583.5	1.379288757	1583.87	1.230137921
1573.28	1.263318292	1573.28	1.759008618	1576.51	1.531837674	1571.26	1.447844647	1584	1.358494314	1584.38	1.196162645
1573.54	1.280777592	1573.54	1.722752946	1576.76	1.525983453	1571.51	1.371364694	1584.5	1.312387008	1584.9	1.173382377
1573.79	1.252698405	1573.79	1.740745768	1578.76	1.487848379	1571.76	1.385113793	1585	1.265455544	1585.41	1.232512349
1574.05	1.264666375	1574.05	1.704104991	1580.76	1.47835736	1572.01	1.403853628	1585.5	1.218084693	1585.92	1.0946478
1574.3	1.258393697	1574.3	1.680813352	1582.76	1.418755687	1572.26	1.356344519	1586	1.151212992	1586.43	1.070792694
1574.56	1.25080072	1574.56	1.652233548	1584.76	1.2342921	1572.51	1.342781884	1586.5	1.132849807	1586.94	1.067335863
1574.81	1.2361111963	1574.81	1.63433203	1586.76	1.089270612	1572.76	1.339880262	1587	1.122757988	1587.46	1.099195369
1575.07	1.258514793	1575.07	1.64223257	1588.76	0.971710319	1573.01	1.336794853	1587.5	1.067424981	1587.97	1.105674608
1575.32	1.248248161	1575.32	1.602077978	1590.76	0.915370226	1573.26	1.308016495	1588	1.101010882	1588.48	1.061385001
1575.58	1.244398945	1575.58	1.580409776	1592.76	0.888136438	1573.51	1.339893026	1588.5	1.056686185	1588.99	1.077333959
1575.83	1.226937458	1575.83	1.564998122	1594.76	0.886104272	1573.76	1.337833248	1589	1.039613532	1589.5	1.066067996
1576.08	1.23922601	1576.08	1.568492025	1596.76	0.879677406	1574.01	1.347926428	1589.5	0.979605145	1590.02	0.968401209
1576.34	1.244108541	1576.34	1.543476126	1598.76	0.906687674	1574.26	1.342973237	1590	0.964568639	1590.53	0.993676563
1576.59	1.255729046	1576.59	1.560285644	1600.76	0.936699511	1574.51	1.323781009	1592	0.944837149	1592.14	0.936732261
1576.85	1.235467816	1576.85	1.523513224	1604.76	0.977313536	1574.76	1.31701562	1594	0.89225665	1594.29	0.913399717

1577.1	1.236352971	1577.1	1.529952097	1609.76	0.975150154	1575.01	1.341075991	1596	0.900270131	1596.43	0.85578531
1577.36	1.2463646	1577.36	1.519374736	1614.76	0.992491354	1575.26	1.334032887	1598	0.87927381	1598.57	0.895622279
1577.61	1.221859712	1577.61	1.509878955	1619.76	0.946732141	1575.51	1.323170664	1600	0.887891304	1600.71	0.896023823
1577.87	1.257649293	1577.87	1.51092143	1624.76	0.956566572	1575.76	1.331014642	1602	0.884220298	1602.86	0.882638642
1578.12	1.24133275	1578.12	1.494879213	1629.76	0.939720741	1576.01	1.297080288	1604	0.930288217	1605	0.918141163
1578.38	1.244794906	1578.38	1.487601595	1634.76	0.921060499	1576.26	1.352761374	1606	0.900849318	1607.14	0.996257165
1578.63	1.226671186	1578.63	1.496037047	1639.76	0.867093001	1576.51	1.308101132	1608	0.966150965	1609.29	0.978525907
1578.89	1.220208618	1578.89	1.478300309	1644.76	0.857994081	1576.76	1.350039424	1610	0.965781219	1611.43	1.006678621
1579.15	1.219061384	1579.15	1.476897787	1649.76	0.840430443	1578.76	1.321154581	1612	1.026271829	1613.57	1.020407667
1579.4	1.215724132	1579.4	1.463532236	1654.76	0.877547633	1580.76	1.281662043	1614	1.01845948	1615.72	1.020437767
1580.19	1.203281014	1580.19	1.467030435	1659.76	0.838459907	1582.76	1.221745522	1616	0.957092282	1617.86	0.903697993
1581.25	1.144653357	1581.25	1.436292462	1664.76	0.854580237	1584.76	1.182692074	1618	0.986050424	1620	0.970422099
1582.3	1.123039413	1582.3	1.391027399	1669.76	0.858609238	1586.76	1.213966058	1620	0.937862207	1622.15	0.987013095
1583.35	1.088218626	1583.35	1.340281683	1674.76	0.861215826	1588.76	1.130151904	1625	0.951576126	1625.33	0.917848829
1584.41	1.058697041	1584.41	1.271729997	1679.76	0.79806472	1590.76	1.046179516	1630	0.907169411	1630.67	0.884219141
1585.46	1.047234345	1585.46	1.193248444	1684.76	0.763798302	1592.76	0.999176505	1635	0.876696064	1636	0.797603139
1586.51	1.035012529	1586.51	1.111310522	1689.76	0.809813356	1594.76	0.978878049	1640	0.827052045	1641.33	0.831954181
1587.56	1.026567353	1587.56	1.060411783	1694.76	0.838784251	1596.76	0.962489038	1645	0.858038359	1646.67	0.868747749
1588.62	1.005276486	1588.62	1.017507229	1699.76	0.895632887	1598.76	0.927785589	1650	0.804219578	1652	0.825274788
1589.67	0.995096604	1589.67	0.975025109			1600.76	0.969811503	1655	0.819128428	1657.33	0.793099794
1590.72	0.961528454	1590.72	0.94489061			1604.76	0.931287313	1660	0.787103267	1662.66	0.765668742
1591.78	0.903014484	1591.78	0.930548392			1609.76	0.91284089	1665	0.846176486	1668	0.896556908
1592.83	0.880948984	1592.83	0.913843453			1614.76	0.885148816	1670	0.87233185	1673.33	0.904463725
1593.88	0.866938487	1593.88	0.907254206			1619.76	0.943370381	1675	0.853082094	1678.66	0.892334834
1594.94	0.863232441	1594.94	0.913681477			1624.76	0.885350515	1680	0.903310033	1684	0.907121045
1595.99	0.860302778	1595.99	0.912998842			1629.76	0.894768116	1685	0.888017829	1689.33	0.839308721
1597.04	0.8516761	1597.04	0.911321713			1634.76	0.904129053	1690	0.87736478	1694.66	0.824093594
1598.09	0.873414047	1598.09	0.918350888			1639.76	0.941606768	1695	0.86346424	1699.99	0.762043864
1599.15	0.851003344	1599.15	0.924417366			1644.76	0.885492383	1700	0.717286493	1705.33	0.647437896
1600.2	0.869001955	1600.2	0.94030921			1649.76	0.878507617				
1604.4	0.887496192	1604.4	0.958457988			1654.76	0.83875826				
1609.67	0.935720967	1609.67	0.997530306			1659.76	0.854652187				

1614.93	0.934365989	1614.93	1.002022562			1664.76	0.834290787				
1620.19	0.950813661	1620.19	0.999100283			1669.76	0.846139115				
1625.45	0.954686262	1625.45	0.987383252			1674.76	0.850459521				
1630.72	0.945949293	1630.72	0.979313326			1679.76	0.831720407				
1635.98	0.919320659	1635.98	0.917726833			1684.76	0.790126325				
1641.24	0.925483149	1641.24	0.87954955			1689.76	0.83977841				
1646.51	0.888047775	1646.51	0.864931001			1694.76	0.829332192				
1651.77	0.896048572	1651.77	0.852677077			1699.76	0.860679516				
1657.03	0.873148778	1657.03	0.820776409								
1662.3	0.838734808	1662.3	0.794732236								
1667.56	0.820098122	1667.56	0.797523206								
1672.82	0.845143941	1672.82	0.795680165								
1678.08	0.844938925	1678.08	0.8023761								
1683.35	0.823389195	1683.35	0.813438281								
1688.61	0.869892797	1688.61	0.87790337								
1693.87	0.805708001	1693.87	0.856987265								
1699.14	0.806877438	1699.14	0.862604759								
1704.4	0.802745202	1704.4	0.911795112								

Table S3. Background subtracted and calibrated Al K-edge XANES data for (BDI)AlX₂ compounds (where X = I, Cl, F). S1 refers to data collected at horizontal polarization while S2 refers to data collected at vertical polarization.

(BDI)AlI ₂ S1 Energy (eV)	(BDI)AlI ₂ S1 Intensity	(BDI)AlI ₂ S2 Energy (eV)	(BDI)AlI ₂ S2 Intensity	(BDI)AlCl ₂ S1 Energy (eV)	(BDI)AlCl ₂ S1 Intensity	(BDI)AlCl ₂ S2 Energy (eV)	(BDI)AlCl ₂ S2 Intensity	(BDI)AlF ₂ S1 Energy (eV)	(BDI)AlF ₂ S1 Intensity	(BDI)AlF ₂ S2 Energy (eV)	(BDI)AlF ₂ S2 Intensity
1520	0.071546828	1520	-0.004694133	1519.9115	0.097890003	1519.9115	-0.048189444	1519.5	0.117199027	1519.5	-0.044051063
1521	0.019979698	1521	-0.015441167	1520.9115	-0.112491647	1520.9115	0.01507749	1520.5	0.016268894	1520.5	-0.022991962
1522	0.014258672	1522	-0.031402449	1521.9115	-0.027945266	1521.9115	-0.021955597	1521.5	-0.025329118	1521.5	-0.01147514
1523	0.034640563	1523	-0.010582935	1522.9115	-0.03296309	1522.9115	0.009857632	1522.5	0.051416745	1522.5	-0.015303651
1524	-0.011398063	1524	-0.014459288	1523.9115	0.024005431	1523.9115	0.036162452	1523.5	-0.003320791	1523.5	0.002363634
1525	0.01651963	1525	0.003812364	1524.9115	-0.070035603	1524.9115	-0.006901351	1524.5	0.018957141	1524.5	0.030667748
1526	0.018442587	1526	-0.01248603	1525.9115	0.031017998	1525.9115	0.009417145	1525.5	-0.022065078	1525.5	0.012072849
1527	-0.036313769	1527	0.036713738	1526.9115	-0.052572588	1526.9115	0.037498909	1526.5	-0.011508815	1526.5	-0.00132192
1528	0.017658655	1528	0.018352784	1527.9115	-0.004857911	1527.9115	0.033850072	1527.5	0.033457615	1527.5	-0.0015212
1529	0.002166559	1529	0.018629413	1528.9115	0.064452421	1528.9115	-0.023541285	1528.5	-0.002376099	1528.5	-0.021443368
1530	0.024588661	1530	0.033846936	1529.9115	0.1231322	1529.9115	-0.036979673	1529.5	0.023386873	1529.5	0.016365497
1531	-0.023619174	1531	0.017300692	1530.9115	-0.042281412	1530.9115	0.020791384	1530.5	0.002898347	1530.5	-0.029609696
1532	-0.023336672	1532	0.02072849	1531.9115	0.063324461	1531.9115	-0.009900958	1531.5	0.020039703	1531.5	-0.014232054
1533	0.008771877	1533	0.004101263	1532.9115	0.032241523	1532.9115	-0.030972043	1532.5	0.001887974	1532.5	-0.027569784
1534	-0.03816858	1534	-0.005583476	1533.9115	-0.014610701	1533.9115	-0.009068461	1533.5	0.010137153	1533.5	0.00640154
1535	-0.013257289	1535	0.012041296	1534.9115	-0.041687299	1534.9115	-0.007972599	1534.5	-0.002222385	1534.5	-0.00058061
1536	-0.021872516	1536	0.018728177	1535.9115	0.029010486	1535.9115	0.050085745	1535.5	-0.027848453	1535.5	0.032910188
1537	-0.008889813	1537	0.004713803	1536.9115	-0.016269686	1536.9115	0.005926667	1536.5	0.063321966	1536.5	0.030769663
1538	-0.052968881	1538	-0.001854126	1537.9115	0.084042243	1537.9115	0.004451476	1537.5	-0.007616555	1537.5	0.005447197
1539	-0.023734949	1539	-0.001018766	1538.9115	-0.001558033	1538.9115	0.025451387	1538.5	-0.051580522	1538.5	-0.018148633
1540	-0.018355888	1540	-0.032155153	1539.9115	-0.091766797	1539.9115	-0.002314994	1539.5	0.006737258	1539.5	0.001864166
1541	-0.021002322	1541	-0.027670947	1540.9115	0.016647	1540.9115	-0.023765837	1540.5	-0.052110484	1540.5	0.042408178
1542	-0.010730774	1542	0.015683391	1541.9115	0.13225991	1541.9115	0.033952598	1541.5	-0.042923322	1541.5	-0.001887954
1543	-0.012207187	1543	0.025741219	1542.9115	-0.058203182	1542.9115	0.043286622	1542.5	-0.01993834	1542.5	-0.028681997
1544	-0.005114301	1544	-0.010463303	1543.9115	0.014361306	1543.9115	0.002681463	1543.5	-0.062666261	1543.5	0.025064612
1545	-9.78E-05	1545	0.008784376	1544.9115	-0.061854621	1544.9115	0.009702892	1544.5	-0.005176133	1544.5	0.028430116
1546	-0.047428829	1546	0.005183288	1545.9115	0.042135343	1545.9115	0.006963817	1545.5	0.018164486	1545.5	0.029571245

1547	0.007515784	1547	0.012812488	1546.9115	0.012346334	1546.9115	-0.049691217	1546.5	0.022497596	1546.5	0.012573128
1548	-0.011039343	1548	0.015435991	1547.9115	-0.106758253	1547.9115	0.012516342	1547.5	-0.038647735	1547.5	0.003352518
1549	-0.019094234	1549	-0.025171051	1548.9115	0.015955796	1548.9115	0.003428994	1548.5	0.00398138	1548.5	0.024937077
1550	-0.012352326	1550	0.016296023	1549.9115	-0.053611055	1549.9115	0.000648298	1549.5	-0.017740666	1549.5	-0.001034566
1551	-0.009826223	1551	-0.019856393	1550.9115	-0.083361762	1550.9115	-0.011909369	1550.5	0.038818636	1550.5	-0.026556148
1552	-0.021204859	1552	-0.02489986	1551.9115	0.028693609	1551.9115	-0.007013476	1551.5	-0.042971076	1551.5	-0.016095663
1553	-0.008236837	1553	-0.010424508	1552.9115	0.004076029	1552.9115	-0.005547361	1552.5	0.025059413	1552.5	0.010173617
1554	-0.0064947	1554	-0.011678233	1553.9115	0.001097275	1553.9115	0.022028557	1553.5	0.052024743	1553.5	-0.014914453
1555	0.011244587	1555	0.0216334	1554.9115	0.080535495	1554.9115	-0.029125099	1554.5	-0.037702735	1554.5	0.013570508
1556	0.027464384	1556	-0.027220352	1555.9115	0.048725948	1555.9115	-0.019036459	1555.5	-0.065992939	1555.5	-0.031636752
1557	-0.003844791	1557	-0.001158096	1556.9115	0.021096995	1556.9115	-0.038963013	1556.5	0.047612576	1556.5	-0.013329295
1558	0.009370877	1558	-0.002228778	1557.9115	-0.053899395	1557.9115	-0.017957936	1557.5	-0.057179053	1557.5	-0.020130778
1558.15	0.011298779	1558.15	-0.00760576	1558.9115	-0.072153396	1558.9115	-0.004379672	1558.5	0.040016673	1558.5	-0.025477415
1558.3	-0.00963035	1558.3	0.008801125	1559.9115	0.026683555	1559.9115	0.014110231	1559.5	-0.00732278	1559.5	-0.044336096
1558.45	-0.004641219	1558.45	-0.013494415	1560.0615	-0.029875223	1560.0615	0.010075739	1559.65	0.042668798	1559.65	0.028805445
1558.6	-0.000678524	1558.6	-0.014524787	1560.2115	0.029541186	1560.2115	-0.020346589	1559.8	0.040831544	1559.8	0.013539559
1558.75	0.017669615	1558.75	0.003071353	1560.3615	-0.009801841	1560.3615	0.066821636	1559.95	0.023785314	1559.95	0.016642248
1558.9	0.030503435	1558.9	0.001631028	1560.5115	0.069585253	1560.5115	0.029000386	1560.1	-0.014563836	1560.1	-0.006005297
1559.05	0.002841799	1559.05	0.012570134	1560.6615	0.011970849	1560.6615	0.011374467	1560.25	0.007115414	1560.25	0.00071538
1559.2	0.039819465	1559.2	0.003570681	1560.8115	0.182863283	1560.8115	-0.003399937	1560.4	0.066792802	1560.4	0.048571323
1559.35	0.013079485	1559.35	0.01549814	1560.9515	0.016066936	1560.9515	0.025251777	1560.55	-0.016543495	1560.55	0.02007285
1559.5	-0.002110418	1559.5	0.00083401	1561.1015	0.039029336	1561.1015	0.04522532	1560.7	0.048460502	1560.7	0.015661033
1559.65	0.02811762	1559.65	0.02015481	1561.2515	-0.008032407	1561.2515	-0.02425974	1560.85	0.075147921	1560.85	0.019656552
1559.8	0.025138662	1559.8	0.032031263	1561.4015	-0.041088451	1561.4015	0.071596447	1561	0.018706304	1561	0.032164756
1559.95	0.025986447	1559.95	0.041492627	1561.5515	0.051916568	1561.5515	0.083273725	1561.15	0.040866801	1561.15	0.04042551
1560.1	0.038192964	1560.1	0.030361443	1561.7015	0.118584008	1561.7015	0.076009269	1561.3	-0.010596045	1561.3	0.079619532
1560.25	0.053391266	1560.25	0.062461814	1561.8515	0.113490324	1561.8515	0.120722074	1561.45	0.041491426	1561.45	0.055505299
1560.4	0.035782658	1560.4	0.024195878	1562.0015	-0.009348356	1562.0015	0.123973424	1561.6	0.119299406	1561.6	0.084007599
1560.55	0.049154224	1560.55	0.057848523	1562.1515	0.175409509	1562.1515	0.109022475	1561.75	0.116918757	1561.75	0.11619247
1560.7	0.05890752	1560.7	0.040462526	1562.3015	0.272950682	1562.3015	0.135113244	1561.9	0.084099967	1561.9	0.142715533
1560.85	0.081480718	1560.85	0.06143673	1562.4415	0.175136187	1562.4415	0.179530538	1562.05	0.162294658	1562.05	0.182777216
1561	0.065071814	1561	0.128980319	1562.5915	0.275297016	1562.5915	0.222947721	1562.2	0.187886276	1562.2	0.203002519

1561.15	0.114119776	1561.15	0.13831353	1562.7415	0.242845616	1562.7415	0.246865408	1562.35	0.139450594	1562.35	0.232282373
1561.3	0.146329339	1561.3	0.132173705	1562.8915	0.259961847	1562.8915	0.399854155	1562.5	0.15756386	1562.5	0.326833685
1561.45	0.137625971	1561.45	0.19783974	1563.0415	0.35551168	1563.0415	0.563036764	1562.65	0.268128204	1562.65	0.450106459
1561.6	0.184620929	1561.6	0.260414175	1563.1915	0.470362362	1563.1915	0.792128814	1562.8	0.299962944	1562.8	0.613070252
1561.75	0.21580379	1561.75	0.34795256	1563.3415	0.540506277	1563.3415	1.154352251	1562.95	0.300607669	1562.95	0.944078924
1561.9	0.300510625	1561.9	0.510318883	1563.4915	0.659517391	1563.4915	1.307734088	1563.1	0.343515311	1563.1	1.176719223
1562.05	0.424790687	1562.05	0.630870671	1563.6415	0.771307409	1563.6415	1.541774762	1563.25	0.437001981	1563.25	1.551297298
1562.2	0.555854644	1562.2	0.734754155	1563.7915	1.091806277	1563.7915	1.651370929	1563.4	0.616688703	1563.4	1.752345522
1562.35	0.786869539	1562.35	0.839177077	1563.9315	1.342267404	1563.9315	1.685895395	1563.55	0.746623006	1563.55	1.952878332
1562.5	0.985199305	1562.5	0.961369642	1564.0815	1.534120916	1564.0815	1.758996475	1563.7	0.862358595	1563.7	2.034172156
1562.65	1.087352534	1562.65	0.991297376	1564.2315	1.930807744	1564.2315	1.902456496	1563.85	0.859793181	1563.85	2.093387725
1562.8	1.054086365	1562.8	0.894838024	1564.3815	2.144640082	1564.3815	1.976993054	1564	1.002167756	1564	2.077723932
1562.95	1.054896656	1562.95	0.80850301	1564.5315	2.723903782	1564.5315	1.997277669	1564.15	1.078213948	1564.15	2.12015422
1563.1	1.250216542	1563.1	0.930056805	1564.6815	2.92990584	1564.6815	2.097948778	1564.3	1.155907977	1564.3	2.160729954
1563.25	1.717801235	1563.25	1.155960098	1564.8315	3.14811114	1564.8315	2.180404734	1564.45	1.183636438	1564.45	2.140646089
1563.4	2.670251093	1563.4	1.664311371	1564.9815	3.216679959	1564.9815	2.276998199	1564.6	1.40960175	1564.6	2.155558698
1563.55	3.18801981	1563.55	2.177667559	1565.1315	3.252486236	1565.1315	2.333855621	1564.75	1.694619352	1564.75	2.274866109
1563.7	3.788535889	1563.7	3.102946746	1565.2715	3.212559557	1565.2715	2.313696887	1564.9	2.249048585	1564.9	2.421014359
1563.85	3.785848984	1563.85	3.70044353	1565.4215	2.872319269	1565.4215	2.176058014	1565.05	2.817077972	1565.05	2.694354092
1564	3.646403396	1564	4.125478004	1565.5715	2.637090558	1565.5715	2.181980242	1565.2	3.519441843	1565.2	2.753702007
1564.15	3.484657319	1564.15	4.149118086	1565.7215	2.453894983	1565.7215	2.133546797	1565.35	4.653576943	1565.35	2.955830674
1564.3	3.292522254	1564.3	3.706908155	1565.8715	2.133530075	1565.8715	1.97777929	1565.5	5.474169068	1565.5	2.903595214
1564.45	2.917218678	1564.45	3.107301261	1566.0215	1.996902341	1566.0215	1.921947414	1565.65	5.685790015	1565.65	2.884370046
1564.6	2.589385644	1564.6	2.495333779	1566.1715	1.760983098	1566.1715	1.85310229	1565.8	5.646468348	1565.8	2.821805198
1564.75	2.350127399	1564.75	2.123031927	1566.3215	1.582223977	1566.3215	1.909281039	1565.95	5.450822954	1565.95	2.804333505
1564.9	2.073922202	1564.9	1.779325161	1566.4715	1.408505608	1566.4715	1.892112889	1566.1	4.881110396	1566.1	2.775693258
1565.05	1.889040108	1565.05	1.607017031	1566.6215	1.444411397	1566.6215	1.817800077	1566.25	4.508119403	1566.25	2.742971693
1565.2	1.811414793	1565.2	1.542576692	1566.7615	1.428091304	1566.7615	1.854945588	1566.4	4.257645651	1566.4	2.66650386
1565.35	1.648554361	1565.35	1.464896218	1566.9115	1.279123489	1566.9115	1.78628459	1566.55	4.041590324	1566.55	2.666036799
1565.5	1.511212117	1565.5	1.333200334	1567.0615	1.228527631	1567.0615	1.801421842	1566.7	3.853107566	1566.7	2.677423572
1565.65	1.41921824	1565.65	1.285285979	1567.2115	1.303386056	1567.2115	1.696486391	1566.85	3.706416624	1566.85	2.664701235
1565.8	1.33905274	1565.8	1.281505531	1567.3615	1.216532956	1567.3615	1.770785644	1567	3.54264282	1567	2.622873649

1565.95	1.282665938	1565.95	1.297975714	1567.5115	1.353685696	1567.5115	1.712130795	1567.15	3.405218477	1567.15	2.578590067
1566.1	1.26232125	1566.1	1.362368639	1567.6615	1.225308361	1567.6615	1.643653923	1567.3	3.155688111	1567.3	2.579716161
1566.25	1.317574633	1566.25	1.402966838	1567.8115	1.326129174	1567.8115	1.632810445	1567.45	3.106269171	1567.45	2.581846886
1566.4	1.356302727	1566.4	1.41886815	1567.9615	1.260391716	1567.9615	1.614791253	1567.6	2.984854349	1567.6	2.59336387
1566.55	1.397118086	1566.55	1.457162619	1568.1115	1.369837278	1568.1115	1.619211937	1567.75	2.798233659	1567.75	2.617246526
1566.7	1.416746308	1566.7	1.536907281	1568.2515	1.405420607	1568.2515	1.539938667	1567.9	2.599154143	1567.9	2.640599074
1566.85	1.441036249	1566.85	1.511847955	1568.4015	1.348091124	1568.4015	1.615741343	1568.05	2.59406948	1568.05	2.637766083
1567	1.464491099	1567	1.533922099	1568.5515	1.468288706	1568.5515	1.485971649	1568.2	2.383393309	1568.2	2.666047607
1567.25	1.46323185	1567.25	1.56403311	1568.7015	1.397871469	1568.7015	1.517599949	1568.35	2.232611426	1568.35	2.67732244
1567.5	1.49394407	1567.5	1.562250116	1568.8515	1.314415256	1568.8515	1.571369745	1568.5	2.068416701	1568.5	2.643467061
1567.75	1.475497916	1567.75	1.598960046	1569.0015	1.505029869	1569.0015	1.572185053	1568.75	1.938765543	1568.75	2.580022388
1568	1.452476563	1568	1.687153306	1569.1515	1.34054672	1569.1515	1.5897584	1569	1.854068219	1569	2.546031318
1568.25	1.509627914	1568.25	1.788287394	1569.3015	1.40665328	1569.3015	1.548033856	1569.25	1.854693026	1569.25	2.441670175
1568.5	1.535015822	1568.5	1.890792771	1569.4515	1.359282943	1569.4515	1.573866478	1569.5	1.865054683	1569.5	2.414101981
1568.75	1.612448907	1568.75	1.969365397	1569.6015	1.258847903	1569.6015	1.634553409	1569.75	1.766674653	1569.75	2.328999202
1569	1.631260792	1569	2.069832364	1569.7415	1.172859043	1569.7415	1.551253023	1570	1.68435	1570	2.342703809
1569.25	1.653012092	1569.25	2.144133882	1569.8915	1.07950813	1569.8915	1.511531335	1570.25	1.669941122	1570.25	2.326982398
1569.5	1.625291896	1569.5	2.240825958	1570.1615	1.043681477	1570.1615	1.523451505	1570.5	1.652161117	1570.5	2.302314514
1569.75	1.660714844	1569.75	2.290897376	1570.4115	1.12517435	1570.4115	1.529995112	1570.75	1.572707771	1570.75	2.301699048
1570	1.646631541	1570	2.315480062	1570.6615	1.142392462	1570.6615	1.472813867	1571	1.549970021	1571	2.33551876
1570.25	1.642080268	1570.25	2.346869488	1570.9115	1.088583998	1570.9115	1.445022254	1571.25	1.586394467	1571.25	2.315430777
1570.5	1.64601734	1570.5	2.388290687	1571.1615	1.103820453	1571.1615	1.469568047	1571.5	1.538442048	1571.5	2.362280391
1570.75	1.651728351	1570.75	2.409478004	1571.4115	1.083106612	1571.4115	1.47426105	1571.75	1.538855636	1571.75	2.333479027
1571	1.649680859	1571	2.460498431	1571.6615	1.16201276	1571.6615	1.518669617	1572	1.578948791	1572	2.303074781
1571.25	1.628707358	1571.25	2.434226756	1571.9115	1.118996373	1571.9115	1.523857962	1572.25	1.521916186	1572.25	2.322138394
1571.5	1.613021533	1571.5	2.395456882	1572.1615	1.314672267	1572.1615	1.535812529	1572.5	1.490905147	1572.5	2.305592306
1571.75	1.583332467	1571.75	2.398901595	1572.4115	1.207179727	1572.4115	1.562459403	1572.75	1.479081086	1572.75	2.268980468
1572	1.604470929	1572	2.332023103	1572.6615	1.341181194	1572.6615	1.525978364	1573	1.444358672	1573	2.207472748
1572.25	1.562274222	1572.25	2.268027399	1572.9115	1.329558528	1572.9115	1.506252251	1573.25	1.521287597	1573.25	2.233111812
1572.5	1.546656547	1572.5	2.218822331	1573.1615	1.328978184	1573.1615	1.431518909	1573.5	1.482663176	1573.5	2.149334225
1572.75	1.542936609	1572.75	2.141354901	1573.4115	1.198724338	1573.4115	1.491756136	1573.75	1.571817267	1573.75	2.087593721
1573	1.517698817	1573	2.111108927	1573.6615	1.29790831	1573.6615	1.383103319	1574	1.427534251	1574	2.063614797

1573.25	1.423594289	1573.25	2.024387214	1573.9115	1.273647697	1573.9115	1.378871598	1574.25	1.486693644	1574.25	2.032601647
1573.5	1.470805531	1573.5	1.964882815	1574.1615	1.241621379	1574.1615	1.363167456	1574.5	1.55416544	1574.5	2.05384089
1573.75	1.450645999	1573.75	1.952216568	1574.4115	1.268283715	1574.4115	1.375724749	1574.75	1.651833994	1574.75	1.985014771
1574	1.424710985	1574	1.855740828	1574.6615	1.209239362	1574.6615	1.40025045	1575	1.591134663	1575	1.998310165
1574.25	1.397001338	1574.25	1.813297633	1574.9115	1.184154747	1574.9115	1.347482866	1575.25	1.629842923	1575.25	1.944517679
1574.5	1.220860664	1574.5	1.76029609	1575.1615	1.143964291	1575.1615	1.333224826	1575.5	1.621052959	1575.5	1.958687339
1574.75	1.350121842	1574.75	1.752982686	1575.4115	1.182036558	1575.4115	1.313332004	1577.5	2.038082656	1577.5	2.098791894
1575	1.312252508	1575	1.665964471	1575.6615	1.194870491	1575.6615	1.378389272	1579.5	2.053516161	1579.5	2.262678641
1575.25	1.249229792	1575.25	1.679279573	1575.9115	1.195026704	1575.9115	1.41892426	1581.5	1.699290993	1581.5	2.248920355
1575.5	1.287566761	1575.5	1.632059738	1577.9115	1.237243607	1577.9115	1.308440417	1583.5	1.267925862	1583.5	2.187778564
1575.75	1.221133934	1575.75	1.594714458	1579.9115	1.285333831	1579.9115	1.233780808	1585.5	1.174738857	1585.5	2.142614256
1576	1.211564651	1576	1.621708516	1581.9115	1.079489195	1581.9115	1.183947234	1587.5	1.153972697	1587.5	1.824815903
1576.25	1.212118858	1576.25	1.604473296	1583.9115	0.973922665	1583.9115	1.166595421	1589.5	1.162293901	1589.5	1.463927432
1576.5	1.190494211	1576.5	1.557961255	1585.9115	0.912671726	1585.9115	1.097304579	1591.5	1.042850772	1591.5	1.17085947
1576.75	1.191378209	1576.75	1.56149025	1587.9115	0.858684821	1587.9115	0.961275585	1593.5	0.954858132	1593.5	1.052700592
1577	1.192870671	1577	1.55531824	1589.9115	0.887451351	1589.9115	0.886572164	1595.5	0.905181884	1595.5	0.927509933
1579	1.124624518	1579	1.525129817	1591.9115	0.750154747	1591.9115	0.756628325	1597.5	0.843945677	1597.5	0.877758621
1581	1.07853432	1581	1.432769102	1593.9115	0.760468639	1593.9115	0.70477453	1599.5	0.86825754	1599.5	0.905835795
1583	1.067246334	1583	1.280191201	1595.9115	0.680586854	1595.9115	0.672625084	1604.5	0.92505929	1604.5	0.973335435
1585	1.1018239	1585	1.227738745	1597.9115	0.706440288	1597.9115	0.660441626	1609.5	0.922788446	1609.5	0.878785718
1587	1.159845151	1587	1.189118215	1599.9115	0.659542398	1599.9115	0.653139671	1614.5	1.046641457	1614.5	0.956860113
1589	1.124607872	1589	1.173388835	1604.9115	0.592033033	1604.9115	0.65405629	1619.5	1.08755929	1619.5	0.866922182
1591	1.104482454	1591	1.085010445	1609.9115	0.612868716	1609.9115	0.702058528	1624.5	1.068872517	1624.5	0.901242023
1593	1.044431618	1593	0.969081502	1614.9115	0.66494425	1614.9115	0.684356625	1629.5	0.993205764	1629.5	0.91652913
1595	0.974270388	1595	0.928457808	1619.9115	0.681339362	1619.9115	0.64160885	1634.5	0.859637236	1634.5	0.918100618
1597	0.89394672	1597	0.864081014	1624.9115	0.681367661	1624.9115	0.661316079	1639.5	0.844811606	1639.5	0.895624447
1599	0.873753563	1599	0.898247389	1629.9115	0.712779058	1629.9115	0.643907178	1644.5	0.807601209	1644.5	0.935056433
1601	0.874848315	1601	0.848250682	1634.9115	0.641526627	1634.9115	0.706887703	1649.5	0.907547195	1649.5	0.921395162
1605	0.928325598	1605	0.88660072	1639.9115	0.470226216	1639.9115	0.565132287	1654.5	0.66640157	1654.5	0.874117267
1610	1.055305068	1610	0.911595343	1644.9115	0.591040005	1644.9115	0.526137201	1659.5	0.758605507	1659.5	0.809915749
1615	0.972568742	1615	1.014988706	1649.9115	0.445606715	1649.9115	0.420099871	1664.5	0.880638111	1664.5	0.804469094
1620	1.009352457	1620	1.019850553	1654.9115	0.328069205	1654.9115	0.398837304	1669.5	0.764004606	1669.5	0.827462326

1625	0.947718163	1625	1.058042038	1659.9115	0.322729226	1659.9115	0.356383098	1674.5	0.812531909	1674.5	0.872310139
1630	0.914146771	1630	1.000489735	1664.9115	0.280355004	1664.9115	0.314209648	1679.5	1.040022517	1679.5	0.852420484
1635	0.908466915	1635	0.945158117	1669.9115	0.437488191	1669.9115	0.318047363	1684.5	0.85212895	1684.5	0.842704426
1640	0.866615822	1640	0.965812606	1674.9115	0.323738307	1674.9115	0.294515976	1689.5	0.942124241	1689.5	0.867739784
1645	0.833457551	1645	0.912022382	1679.9115	0.292950682	1679.9115	0.298218883	1694.5	0.727332604	1694.5	0.830672131
1650	0.802819501	1650	0.83574443	1684.9115	0.34422053	1684.9115	0.295237201	1699.5	0.814600592	1699.5	0.784970149
1655	0.823096861	1655	0.834108747	1689.9115	0.322124518	1689.9115	0.272109236				
1660	0.844786416	1660	0.738394314	1694.9115	0.207864873	1694.9115	0.316504502				
1665	0.856566658	1665	0.769477721	1699.9115	0.300057705	1699.9115	0.301908644				
1670	0.801332776	1670	0.778845099								
1675	0.888713249	1675	0.834217803								
1680	0.86236213	1680	0.808168716								
1685	0.841402238	1685	0.837543144								
1690	0.834237947	1690	0.848611963								
1695	0.82107646	1695	0.849827991								
1700	0.836727579	1700	0.881578724								

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