

## Supplementary Information

### Geometries:

#### Free ligand equilibrium geometry

Si	0.672613	-1.489877	0.466843
C	0.681669	-1.538210	2.349607
C	2.439120	-1.537420	-0.185177
H	-0.070932	-2.674139	-0.050330
C	-0.230425	0.041445	-0.158394
H	2.456680	-1.541345	-1.286527
H	3.013555	-0.659989	0.154792
H	2.966639	-2.439332	0.166301
H	-0.343542	-1.549982	2.752209
H	1.202382	-2.436525	2.719860
H	1.195117	-0.657470	2.769323
C	-1.367603	-0.066526	-0.981652
C	-2.038463	1.068963	-1.448741
C	-1.583197	2.343140	-1.099797
C	-0.455620	2.475956	-0.282742
C	0.209423	1.337453	0.179989
H	-1.737149	-1.056514	-1.263412
H	-2.918778	0.957546	-2.086359
H	-2.105119	3.231552	-1.462853
H	-0.094095	3.469133	-0.005609
H	1.089237	1.466540	0.818236

#### Free ligand with geometry as in complex

Si	-0.604755	-1.588928	0.000000
C	0.042988	-2.446852	1.545128
C	0.042988	-2.446852	-1.545128
H	-2.094214	-1.693599	0.000000
C	-0.127856	0.238094	0.000000
H	-0.370432	-2.005109	-2.465648
H	1.141885	-2.387127	-1.604631
H	-0.238330	-3.512210	-1.535404
H	-0.370432	-2.005109	2.465648
H	-0.238330	-3.512210	1.535404
H	1.141885	-2.387127	1.604631
C	0.042988	0.949923	-1.203957
C	0.368138	2.309797	-1.208171
C	0.531702	2.993814	0.000000
C	0.368138	2.309797	1.208171
C	0.042988	0.949923	1.203957
H	-0.077565	0.436415	-2.161887
H	0.495146	2.836255	-2.157435
H	0.786918	4.056268	0.000000
H	0.495146	2.836255	2.157435
H	-0.077565	0.436415	2.161887

#### Ti complex equilibrium geometry (singlet state)

XX	3.334281	0.972889	-0.464990
H	2.364759	-2.260909	2.263601

H	-4.451426	2.462169	2.186473
H	-2.539376	-0.107487	2.425059
Cl	1.437968	2.520962	2.140372
H	3.806883	0.503208	1.722447
H	4.146315	-2.294121	2.110812
H	3.187880	-3.741823	1.725534
C	3.201728	-2.642006	1.661932
Cl	-0.699534	-3.362658	0.955771
H	-5.479153	2.411743	0.730961
C	-4.517063	2.769962	1.130956
H	-4.526902	3.872030	1.104293
H	-3.252343	-2.664075	2.019907
Cl	0.250437	-0.331363	1.445068
H	4.006602	2.917313	0.559244
C	-2.929986	-0.514838	1.495692
C	3.599722	0.715784	0.676495
C	-3.307890	-1.863379	1.288930
C	3.709567	1.995678	0.066174
H	-1.804991	2.574295	0.754723
C	-3.124238	0.225245	0.282997
Ti	1.416250	1.473356	0.108659
Si	3.063912	-2.111487	-0.129208
Si	-3.063912	2.111487	0.129208
C	3.124238	-0.225245	-0.282997
Ti	-1.416250	-1.473356	-0.108659
H	1.804991	-2.574295	-0.754723
C	-3.709567	-1.995678	-0.066174
C	3.307890	1.863379	-1.288930
H	-4.006602	-2.917313	-0.559244
C	-3.599722	-0.715784	-0.676495
H	5.479153	-2.411743	-0.730961
H	4.526902	-3.872030	-1.104293
C	2.929986	0.514838	-1.495692
H	3.252343	2.664075	-2.019907
C	4.517063	-2.769962	-1.130956
Cl	0.699534	3.362658	-0.955771
H	-3.187880	3.741823	-1.725534
C	-3.201728	2.642006	-1.661932
H	-4.146315	2.294121	-2.110812
Cl	-0.250437	0.331363	-1.445068
H	-3.806883	-0.503208	-1.722447
Cl	-1.437968	-2.520962	-2.140372
H	2.539376	0.107487	-2.425059
H	4.451426	-2.462169	-2.186473
H	-2.364759	2.260909	-2.263601

Zr complex equilibrium geometry (singlet state)

XX	2.939361	1.938019	-0.045426
H	-0.044130	-3.616484	-2.507491
H	-0.074737	3.681386	-2.410358
H	2.238859	2.210275	-2.207357

Cl	-3.172441	1.401057	-1.693193
H	-2.344244	-2.152646	-2.154243
H	-0.744217	-5.043563	-1.692989
H	1.017988	-4.758819	-1.661489
C	0.033722	-4.266670	-1.622808
Cl	3.086064	-1.353824	-1.880854
H	0.664788	5.086932	-1.593270
C	-0.109349	4.307964	-1.506108
H	-1.094020	4.800335	-1.484205
H	4.611762	1.214066	-1.446843
Cl	-0.039480	0.021588	-1.633573
H	-4.677020	-1.178380	-1.253995
C	2.572546	2.093944	-1.178530
C	-2.627788	-2.063736	-1.107791
C	3.828095	1.567744	-0.782328
C	-3.862405	-1.548982	-0.637667
H	-0.950566	2.245923	0.052657
C	1.805971	2.415689	-0.011729
Zr	-2.090362	0.125404	0.052176
Si	-0.132106	-3.281947	-0.040159
Si	0.132106	3.281947	0.040160
C	-1.805971	-2.415689	0.011729
Zr	2.090362	-0.125404	-0.052177
H	0.950566	-2.245923	-0.052658
C	3.862406	1.548982	0.637667
C	-3.828095	-1.567744	0.782327
H	4.677021	1.178380	1.253994
C	2.627788	2.063736	1.107791
H	-0.664788	-5.086930	1.593273
H	1.094020	-4.800333	1.484207
C	-2.572546	-2.093944	1.178529
H	-4.611763	-1.214066	1.446842
C	0.109349	-4.307962	1.506109
Cl	-3.086064	1.353824	1.880854
H	-1.017988	4.758818	1.661491
C	-0.033722	4.266669	1.622810
H	0.744217	5.043561	1.692992
Cl	0.039480	-0.021588	1.633573
H	2.344245	2.152646	2.154243
Cl	3.172441	-1.401057	1.693193
H	-2.238859	-2.210274	2.207357
H	0.074738	-3.681384	2.410359
H	0.044130	3.616482	2.507492

Hf complex equilibrium geometry (singlet state)

XX	3.452642	-0.579839	-0.055472
H	2.399062	2.658185	-2.532305
H	-2.489493	-2.712337	-2.386266
H	-3.183341	-0.063232	-2.124508
Cl	1.305050	-3.137330	-1.760356
H	3.105839	0.016084	-2.237902

H	3.902051	3.223423	-1.750669
H	2.412879	4.204643	-1.662118
C	2.805941	3.176209	-1.650564
Cl	-1.368219	3.099922	-1.778626
H	-3.962477	-3.259677	-1.537671
C	-2.863450	-3.210689	-1.478976
H	-2.470633	-4.239278	-1.482344
H	-4.217409	2.271195	-1.300149
Cl	-0.028881	-0.017119	-1.617635
H	4.169434	-2.300386	-1.400539
C	-3.320829	0.233044	-1.087061
C	3.280205	-0.257757	-1.199833
C	-3.869027	1.467822	-0.657038
C	3.843803	-1.483170	-0.762969
H	-0.809485	-2.280614	0.038447
C	-2.949345	-0.542590	0.058665
Hf	1.441086	-1.500857	-0.009833
Si	2.308409	2.313583	-0.066440
Si	-2.308410	-2.313583	0.066434
C	2.949345	0.542590	-0.058666
Hf	-1.441086	1.500857	0.009835
H	0.809485	2.280614	-0.038443
C	-3.843802	1.483169	0.762975
C	3.869027	-1.467819	0.657044
H	-4.169432	2.300383	1.400546
C	-3.280204	0.257755	1.199835
H	3.962485	3.259685	1.537651
H	2.470640	4.239286	1.482328
C	3.320828	-0.233041	1.087062
H	4.217408	-2.271191	1.300157
C	2.863457	3.210696	1.478963
Cl	1.368219	-3.099922	1.778627
H	-2.412889	-4.204651	1.662103
C	-2.805952	-3.176216	1.650551
H	-3.902062	-3.223430	1.750650
Cl	0.028881	0.017119	1.617637
H	-3.105836	-0.016089	2.237903
Cl	-1.305049	3.137331	1.760357
H	3.183339	0.063238	2.124509
H	2.489505	2.712349	2.386257
H	-2.399077	-2.658197	2.532297

Mo complex equilibrium geometry (singlet state)

C	-2.484646	-3.047637	1.651931
C	2.484652	3.047644	-1.651922
C	2.543721	3.084492	1.487863
C	-2.543729	-3.084499	-1.487854
C	-2.689214	-0.409838	0.053952
C	-3.033057	0.408672	1.204320
C	-3.074861	0.381630	-1.102030
C	-3.645647	1.611791	0.752391

C	-3.671254	1.595155	-0.656680
Cl	0.030126	0.018366	1.645637
Cl	-0.030126	-0.018367	-1.645639
Cl	-1.231101	3.158007	1.670479
Cl	1.231101	-3.158008	-1.670478
Cl	1.292849	-3.121305	1.693503
Cl	-1.292849	3.121305	-1.693504
H	0.533526	2.093003	-0.033120
H	-0.533527	-2.093003	0.033110
H	2.051397	4.059124	-1.655557
H	-2.051404	-4.059122	1.655563
H	-2.082327	-2.513164	2.524734
H	2.082348	2.513168	-2.524730
H	2.113089	4.097085	1.482779
H	-2.113094	-4.097090	-1.482769
H	2.172133	2.572329	2.387273
H	-2.172149	-2.572337	-2.387267
H	2.858207	-0.151409	-2.244327
H	-2.858211	0.151410	2.244325
H	-2.937366	0.100092	-2.141359
H	2.937369	-0.100093	2.141357
H	-3.577997	-3.134139	1.761670
H	3.578002	3.134160	-1.761650
H	3.640511	3.170314	1.555910
H	-3.640519	-3.170326	-1.555893
H	-3.945149	2.445050	1.380149
H	3.945151	-2.445049	-1.380153
H	3.993628	-2.413545	1.292620
H	-3.993629	2.413544	-1.292624
C	2.689214	0.409838	-0.053954
C	3.033055	-0.408671	-1.204322
C	3.074863	-0.381630	1.102028
C	3.645648	-1.611790	-0.752395
C	3.671254	-1.595156	0.656677
Mo	-1.374763	1.389511	0.009715
Mo	1.374764	-1.389512	-0.009716
Si	2.046081	2.176130	-0.062798
Si	-2.046082	-2.176130	0.062801
XX	3.222807	-0.717482	-0.050393

Mo complex equilibrium geometry (triplet state)

H	2.745625	2.901735	-2.546132
H	-2.851954	-2.962313	-2.377640
H	-3.215127	-0.257095	-2.128052
Cl	1.454763	-2.883475	-1.635826
H	3.139968	0.207383	-2.245123
H	4.304556	3.212347	-1.730355
H	3.001430	4.428649	-1.681978
C	3.213884	3.347660	-1.654594
Cl	-1.511957	2.851259	-1.640369
H	-4.373918	-3.252308	-1.487985

C	-3.280903	-3.386118	-1.456023
H	-3.069044	-4.467532	-1.466043
H	-4.276539	2.063903	-1.291507
Cl	-0.026210	-0.014860	-1.498668
H	4.230262	-2.094651	-1.392735
C	-3.352836	0.030406	-1.088728
C	3.313203	-0.056588	-1.204880
C	-3.942438	1.251810	-0.652732
C	3.917998	-1.268096	-0.761509
H	-1.058605	-2.771658	0.043663
C	-2.976761	-0.759625	0.061030
Mo	1.650981	-1.138202	-0.017719
Si	2.522029	2.604766	-0.074282
Si	-2.522036	-2.604768	0.074299
C	2.976757	0.759624	-0.061059
Mo	-1.650977	1.138205	0.017657
H	1.058595	2.771648	-0.043784
C	-3.917988	1.268124	0.761425
C	3.942445	-1.251823	0.652649
H	-4.230248	2.094697	1.392629
C	-3.313197	0.056622	1.204828
H	4.373777	3.252241	1.488185
H	3.068902	4.467463	1.466185
C	3.352837	-0.030434	1.088680
H	4.276549	-2.063933	1.291401
C	3.280765	3.386050	1.456137
Cl	1.511963	-2.851263	1.640301
H	-3.001313	-4.428578	1.682114
C	-3.213763	-3.347589	1.654701
H	-4.304427	-3.212265	1.730547
Cl	0.026200	0.014823	1.498603
H	-3.139962	-0.207320	2.245078
Cl	-1.454738	2.883470	1.635768
H	3.215131	0.257041	2.128012
H	2.851738	2.962205	2.377700
H	-2.745425	-2.901628	2.546179
XX	3.500648	-0.369463	-0.057224

Decontracted basis sets for silicon and hydrogen used in the NMR calculations:

Si 0

S	1	1.00	
		254900.0000000	0.625101D-04
S	1	1.0	
		38190.0000000	0.485553D-03
S	1	1.0	
		8690.0000000	0.254516D-02
S	1	1.0	
		2462.0000000	0.105866D-01
S	1	1.0	
		804.8000000	0.368787D-01

S	1	1.0	291.3000000	0.107479D+00
S	1	1.0	113.6000000	0.247936D+00
S	1	1.0	46.7500000	0.390927D+00
S	1	1.0	19.8200000	0.302026D+00
S	1	1.0	7.7080000	0.559236D-01
S	1	1.0	3.3400000	-0.402406D-02
S	1	1.0	1.4020000	0.258030D-02
S	1	1.0	0.4387000	-0.103821D-02
S	1	1.0	0.2070000	0.607930D-03
S	1	1.0	0.0794400	-0.154022D-03
S	1	1.00	254900.0000000	-0.166370D-04
S	1	1.0	38190.0000000	-0.129310D-03
S	1	1.0	8690.0000000	-0.678828D-03
S	1	1.0	2462.0000000	-0.284117D-02
S	1	1.0	804.8000000	-0.100551D-01
S	1	1.0	291.3000000	-0.305774D-01
S	1	1.0	113.6000000	-0.777256D-01
S	1	1.0	46.7500000	-0.154236D+00
S	1	1.0	19.8200000	-0.180368D+00
S	1	1.0	7.7080000	0.798218D-01
S	1	1.0	3.3400000	0.547441D+00
S	1	1.0	1.4020000	0.480119D+00
S	1	1.0	0.4387000	0.474846D-01
S	1	1.0	0.2070000	-0.106996D-01
S	1	1.0	0.0794400	0.219871D-02
S	1	1.00		

		254900.0000000	0.426257D-05
S	1	1.0	
		38190.0000000	0.331062D-04
S	1	1.0	
		8690.0000000	0.174015D-03
S	1	1.0	
		2462.0000000	0.727574D-03
S	1	1.0	
		804.8000000	0.258333D-02
S	1	1.0	
		291.3000000	0.786354D-02
S	1	1.0	
		113.6000000	0.202155D-01
S	1	1.0	
		46.7500000	0.407320D-01
S	1	1.0	
		19.8200000	0.499358D-01
S	1	1.0	
		7.7080000	-0.249396D-01
S	1	1.0	
		3.3400000	-0.190350D+00
S	1	1.0	
		1.4020000	-0.318350D+00
S	1	1.0	
		0.4387000	0.948036D-01
S	1	1.0	
		0.2070000	0.681180D+00
S	1	1.0	
		0.0794400	0.395672D+00
S	1	1.00	
		0.4387000	1.0000000
S	1	1.00	
		0.0794400	1.0000000
P	1	1.00	
		481.5000000	0.192045D-02
P	1	1.0	
		113.9000000	0.153552D-01
P	1	1.0	
		36.2300000	0.713991D-01
P	1	1.0	
		13.3400000	0.213052D+00
P	1	1.0	
		5.2520000	0.390354D+00
P	1	1.0	
		2.1200000	0.393721D+00
P	1	1.0	
		0.8561000	0.132565D+00
P	1	1.0	
		0.2528000	0.395630D-02
P	1	1.0	
		0.0788900	0.331624D-03



P	1	1.00		
		481.5000000		-0.405220D-03
P	1	1.0		
		113.9000000		-0.335896D-02
P	1	1.0		
		36.2300000		-0.152860D-01
P	1	1.0		
		13.3400000		-0.489218D-01
P	1	1.0		
		5.2520000		-0.855008D-01
P	1	1.0		
		2.1200000		-0.112137D+00
P	1	1.0		
		0.8561000		0.618274D-01
P	1	1.0		
		0.2528000		0.551919D+00
P	1	1.0		
		0.0788900		0.523492D+00
P	1	1.00		
		0.8561000		1.0000000
P	1	1.00		
		0.0788900		1.0000000
D	1	1.00		
		0.1590000		1.0000000
D	1	1.00		
		0.4810000		1.0000000
F	1	1.00		
		0.3360000		1.0000000
S	1	1.00		
		0.0330000		1.0000000
P	1	1.00		
		0.0237000		1.0000000
D	1	1.00		
		0.0556000		1.0000000
F	1	1.00		
		0.1250000		1.0000000
****				
H 0				
S	1	1.00		
		33.8700000		0.0060680
S	1	1.0		
		5.0950000		0.0453080
S	1	1.0		
		1.1590000		0.2028220
S	1	1.0		
		0.3258000		0.5039030
S	1	1.0		
		0.1027000		0.3834210
S	1	1.00		
		0.3258000		1.0000000
S	1	1.00		

		0.1027000	1.0000000
P	1	1.00	
		1.4070000	1.0000000
P	1	1.00	
		0.3880000	1.0000000
D	1	1.00	
		1.0570000	1.0000000
S	1	1.00	
		0.0252600	1.0000000
P	1	1.00	
		0.1020000	1.0000000
D	1	1.00	
		0.2470000	1.0000000

\*\*\*\*

Metal basis sets and ECPs:

TI	0		
S	19	1.00	
		3014643.0000000	0.0001120
		451432.9000000	0.0003320
		102733.8000000	0.0009400
		29098.1700000	0.0025320
		9492.3300000	0.0068790
		3426.3460000	0.0187490
		1335.8960000	0.0492940
		553.5026000	0.1166940
		240.6925000	0.2273250
		108.7293000	0.3105540
		50.2645700	0.2205840
		22.5800400	0.0732470
		10.7143200	0.1131540
		5.0935460	0.1136590
		2.2441830	0.0193160
		1.0595700	-0.0004650
		0.4688490	0.0001590
		0.1061430	-0.0000590
		0.0552620	0.0000620
S	19	1.00	
		3014643.0000000	-0.0000630
		451432.9000000	-0.0001890
		102733.8000000	-0.0005350
		29098.1700000	-0.0014430
		9492.3300000	-0.0039330
		3426.3460000	-0.0107960
		1335.8960000	-0.0288290
		553.5026000	-0.0706740
		240.6925000	-0.1487780
		108.7293000	-0.2420600
		50.2645700	-0.2347210
		22.5800400	0.0422060
		10.7143200	0.4983350

		5.0935460	0.4868870
		2.2441830	0.0879040
		1.0595700	-0.0052640
		0.4688490	0.0005520
		0.1061430	-0.0006280
		0.0552620	0.0005530
S	19	1.00	
		3014643.0000000	0.0000130
		451432.9000000	0.0000380
		102733.8000000	0.0001090
		29098.1700000	0.0002940
		9492.3300000	0.0008030
		3426.3460000	0.0022200
		1335.8960000	0.0059990
		553.5026000	0.0151490
		240.6925000	0.0337330
		108.7293000	0.0615630
		50.2645700	0.0694620
		22.5800400	-0.0241550
		10.7143200	-0.2789840
		5.0935460	-0.4386710
		2.2441830	0.0909060
		1.0595700	0.7091310
		0.4688490	0.4311640
		0.1061430	0.0258980
		0.0552620	-0.0110070
S	19	1.00	
		3014643.0000000	-0.0000030
		451432.9000000	-0.0000090
		102733.8000000	-0.0000260
		29098.1700000	-0.0000700
		9492.3300000	-0.0001910
		3426.3460000	-0.0005260
		1335.8960000	-0.0014240
		553.5026000	-0.0035930
		240.6925000	-0.0080220
		108.7293000	-0.0146460
		50.2645700	-0.0166610
		22.5800400	0.0058890
		10.7143200	0.0693470
		5.0935460	0.1159210
		2.2441830	-0.0327170
		1.0595700	-0.2334140
		0.4688490	-0.2869410
		0.1061430	0.2839540
		0.0552620	0.5841130
S	19	1.00	
		3014643.0000000	-0.0000060
		451432.9000000	-0.0000170
		102733.8000000	-0.0000480
		29098.1700000	-0.0001310

		9492.3300000	-0.0003460
		3426.3460000	-0.0010090
		1335.8960000	-0.0025320
		553.5026000	-0.0070420
		240.6925000	-0.0138290
		108.7293000	-0.0302210
		50.2645700	-0.0239810
		22.5800400	-0.0071850
		10.7143200	0.1758840
		5.0935460	0.1462460
		2.2441830	0.0971840
		1.0595700	-1.0017360
		0.4688490	0.1999570
		0.1061430	2.2181040
		0.0552620	-1.3423230
S	19	1.00	
		3014643.0000000	-0.0000090
		451432.9000000	-0.0000270
		102733.8000000	-0.0000750
		29098.1700000	-0.0002080
		9492.3300000	-0.0005370
		3426.3460000	-0.0016170
		1335.8960000	-0.0038870
		553.5026000	-0.0114190
		240.6925000	-0.0208780
		108.7293000	-0.0503970
		50.2645700	-0.0320930
		22.5800400	-0.0269460
		10.7143200	0.3275740
		5.0935460	0.2147230
		2.2441830	0.1170160
		1.0595700	-2.4080240
		0.4688490	2.5936190
		0.1061430	0.1447480
		0.0552620	-2.5253120
S	1	1.00	
		0.0254650	1.0000000
P	15	1.00	
		11912.0300000	0.0001040
		2819.9470000	0.0005330
		915.9479000	0.0025880
		350.3842000	0.0104700
		148.4825000	0.0354710
		67.5394400	0.0981640
		32.3033200	0.2106310
		15.9278600	0.3301970
		8.0380350	0.3305000
		4.0939160	0.1571860
		2.0223900	0.0219670
		0.9761020	-0.0017610
		0.4595950	-0.0014300

		0.1771950	-0.0002900
		0.0734420	0.0000340
P	15	1.00	
		11912.0300000	-0.0000350
		2819.9470000	-0.0001790
		915.9479000	-0.0008700
		350.3842000	-0.0035410
		148.4825000	-0.0121500
		67.5394400	-0.0344710
		32.3033200	-0.0765940
		15.9278600	-0.1256220
		8.0380350	-0.1320480
		4.0939160	0.0193960
		2.0223900	0.3164550
		0.9761020	0.4614890
		0.4595950	0.2980100
		0.1771950	0.0495170
		0.0734420	-0.0041080
P	15	1.00	
		11912.0300000	0.0000080
		2819.9470000	0.0000430
		915.9479000	0.0002090
		350.3842000	0.0008480
		148.4825000	0.0029250
		67.5394400	0.0082760
		32.3033200	0.0185500
		15.9278600	0.0303400
		8.0380350	0.0327150
		4.0939160	-0.0087200
		2.0223900	-0.0886360
		0.9761020	-0.1491650
		0.4595950	-0.0932320
		0.1771950	0.2507080
		0.0734420	0.5861800
P	15	1.00	
		11912.0300000	0.0000100
		2819.9470000	0.0000540
		915.9479000	0.0002610
		350.3842000	0.0010710
		148.4825000	0.0036390
		67.5394400	0.0104610
		32.3033200	0.0229850
		15.9278600	0.0386720
		8.0380350	0.0394990
		4.0939160	-0.0068990
		2.0223900	-0.1146250
		0.9761020	-0.1708870
		0.4595950	-0.1652610
		0.1771950	0.4058580
		0.0734420	0.6742340
P	15	1.00	

		11912.030000	0.0000210
		2819.947000	0.0001010
		915.947900	0.0005360
		350.384200	0.0019840
		148.482500	0.0075290
		67.539440	0.0191510
		32.303320	0.0486770
		15.927860	0.0671790
		8.038035	0.1039430
		4.093916	-0.0555620
		2.022390	-0.1916650
		0.976102	-0.6969070
		0.459595	0.5747490
		0.177195	1.1704990
		0.073442	-1.0063770
P	1	1.00	
		0.029334	1.0000000
D	7	1.00	
		64.340200	0.0038830
		18.841800	0.0262040
		6.719830	0.0968870
		2.656130	0.2316310
		1.073680	0.3519720
		0.420557	0.3725630
		0.154817	0.2505630
D	7	1.00	
		64.340200	-0.0039790
		18.841800	-0.0267640
		6.719830	-0.1018940
		2.656130	-0.2371110
		1.073680	-0.3132860
		0.420557	-0.0465630
		0.154817	0.5840720
D	7	1.00	
		64.340200	0.0063860
		18.841800	0.0433010
		6.719830	0.1702500
		2.656130	0.3719460
		1.073680	0.2303500
		0.420557	-0.7820270
		0.154817	-0.1235850
D	1	1.00	
		0.051490	1.0000000
F	1	1.00	
		1.227400	1.0000000
F	1	1.00	
		0.278800	1.0000000
G	1	1.00	
		0.709200	1.0000000
S	1	1.00	
		0.011730	1.0000000

P	1	1.00	
		0.0117200	1.0000000
D	1	1.00	
		0.0171200	1.0000000
F	1	1.00	
		0.0806900	1.0000000
G	1	1.00	
		0.2041300	1.0000000

\*\*\*\*

-Zr 0

S 11 1.00

0.13682600E+03	0.40900000E-03
0.14512800E+02	-0.38517000E-01
0.90698100E+01	0.21581500E+00
0.56664000E+01	-0.17334000E+00
0.31131900E+01	-0.47006700E+00
0.82348200E+00	0.76346100E+00
0.38119300E+00	0.50374000E+00
0.97792000E-01	0.37859000E-01
0.50839000E-01	-0.15390000E-01
0.23693000E-01	0.48040000E-02
0.11000000E-01	0.00000000E+00

S 11 1.00

0.13682600E+03	-0.14200000E-03
0.14512800E+02	0.13145000E-01
0.90698100E+01	-0.75341000E-01
0.56664000E+01	0.69978000E-01
0.31131900E+01	0.15043600E+00
0.82348200E+00	-0.32538200E+00
0.38119300E+00	-0.35671200E+00
0.97792000E-01	0.30701400E+00
0.50839000E-01	0.62391800E+00
0.23693000E-01	0.26800500E+00
0.11000000E-01	0.00000000E+00

S 11 1.00

0.13682600E+03	-0.31000000E-04
0.14512800E+02	0.19190000E-02
0.90698100E+01	-0.50977000E-01
0.56664000E+01	-0.15384000E-01
0.31131900E+01	0.43516600E+00
0.82348200E+00	-0.11911120E+01
0.38119300E+00	0.12925700E+00
0.97792000E-01	0.26494430E+01
0.50839000E-01	-0.18700320E+01
0.23693000E-01	-0.37790700E+00
0.11000000E-01	0.00000000E+00

S 11 1.00

0.13682600E+03	0.94000000E-04
0.14512800E+02	-0.10988000E-01
0.90698100E+01	-0.30538000E-01

0.56664000E+01 -0.96135000E-01  
0.31131900E+01 0.80230800E+00  
0.82348200E+00 -0.32348630E+01  
0.38119300E+00 0.34978270E+01  
0.97792000E-01 -0.74688400E+00  
0.50839000E-01 -0.17815950E+01  
0.23693000E-01 0.17442010E+01  
0.11000000E-01 0.00000000E+00  
S 1 1.00  
0.23693000E-01 0.10000000E+01  
S 1 1.00  
0.11000000E-01 0.10000000E+01  
P 10 1.00  
0.17411900E+02 -0.11830000E-02  
0.10879900E+02 0.19174000E-01  
0.43280400E+01 -0.16007000E+00  
0.11386400E+01 0.40576200E+00  
0.57585500E+00 0.47362000E+00  
0.28867000E+00 0.23196100E+00  
0.12801400E+00 0.32662000E-01  
0.55290000E-01 0.63400000E-03  
0.23613000E-01 0.39100000E-03  
0.10100000E-01 0.00000000E+00  
P 10 1.00  
0.17411900E+02 -0.13400000E-03  
0.10879900E+02 -0.46090000E-02  
0.43280400E+01 0.48189000E-01  
0.11386400E+01 -0.14548400E+00  
0.57585500E+00 -0.18987400E+00  
0.28867000E+00 -0.77814000E-01  
0.12801400E+00 0.33195100E+00  
0.55290000E-01 0.58379200E+00  
0.23613000E-01 0.24686100E+00  
0.10100000E-01 0.00000000E+00  
P 10 1.00  
0.17411900E+02 -0.10700000E-03  
0.10879900E+02 -0.67180000E-02  
0.43280400E+01 0.68365000E-01  
0.11386400E+01 -0.20455000E+00  
0.57585500E+00 -0.27976500E+00  
0.28867000E+00 -0.98014000E-01  
0.12801400E+00 0.64995900E+00  
0.55290000E-01 0.49861100E+00  
0.23613000E-01 0.23340000E-01  
0.10100000E-01 0.00000000E+00  
P 10 1.00  
0.17411900E+02 0.31900000E-03  
0.10879900E+02 -0.13666000E-01  
0.43280400E+01 0.13165900E+00  
0.11386400E+01 -0.45381600E+00  
0.57585500E+00 -0.80191500E+00



0.28867000E+00 0.12831030E+01  
0.12801400E+00 0.59929200E+00  
0.55290000E-01 -0.10604800E+01  
0.23613000E-01 -0.76248000E-01  
0.10100000E-01 0.00000000E+00  
P 1 1.00  
0.23613000E-01 0.10000000E+01  
P 1 1.00  
0.10100000E-01 0.10000000E+01  
D 8 1.00  
0.18073200E+02 0.11410000E-02  
0.52195900E+01 -0.82810000E-02  
0.16998500E+01 0.93377000E-01  
0.83632300E+00 0.25097300E+00  
0.39335400E+00 0.34390700E+00  
0.17882400E+00 0.32983800E+00  
0.78275000E-01 0.21217700E+00  
0.32248000E-01 0.58590000E-01  
D 8 1.00  
0.18073200E+02 -0.12140000E-02  
0.52195900E+01 0.87890000E-02  
0.16998500E+01 -0.11643700E+00  
0.83632300E+00 -0.31261900E+00  
0.39335400E+00 -0.33881200E+00  
0.17882400E+00 0.10978700E+00  
0.78275000E-01 0.57448300E+00  
0.32248000E-01 0.32282100E+00  
D 8 1.00  
0.18073200E+02 0.16120000E-02  
0.52195900E+01 -0.11812000E-01  
0.16998500E+01 0.19971500E+00  
0.83632300E+00 0.50391400E+00  
0.39335400E+00 0.93700000E-02  
0.17882400E+00 -0.91166100E+00  
0.78275000E-01 0.85915000E-01  
0.32248000E-01 0.72855000E+00  
D 1 1.00  
0.32248000E-01 0.10000000E+01  
D 1 1.00  
0.13300000E-01 0.10000000E+01  
F 1 1.00  
0.73950000E+00 0.10000000E+01  
F 1 1.00  
0.19310000E+00 0.10000000E+01  
F 1 1.00  
0.61800000E-01 0.10000000E+01  
G 1 1.00  
0.41950000E+00 0.10000000E+01  
G 1 1.00  
0.13330000E+00 0.10000000E+01  
\*\*\*\*

```
-Zr 0
ECP28MDF, 4, 28
G-Komponente
1
2 1.000000 0.000000
S-G
2
2 8.636528 150.242994
2 3.717639 18.780036
P-G
4
2 7.626728 33.192791
2 7.453207 66.389039
2 3.358389 4.620726
2 3.229738 9.260270
D-G
4
2 5.938086 13.993383
2 5.825544 20.995882
2 2.205019 2.285166
2 2.206292 3.441260
F-G
2
2 4.800215 -5.239320
2 4.798992 -6.987424

-Hf 0
S 10 1.0
0.26504200E+02 0.32017000E-01
0.16584000E+02 -0.25833800E+00
0.10383100E+02 0.74195800E+00
0.64955000E+01 -0.59724600E+00
0.34643100E+01 -0.46743300E+00
0.98620000E+00 0.78143800E+00
0.45782800E+00 0.53375600E+00
0.13211800E+00 0.36380000E-01
0.66967000E-01 -0.13648000E-01
0.29010000E-01 0.19130000E-02
S 10 1.0
0.26504200E+02 -0.92200000E-02
0.16584000E+02 0.76675000E-01
0.10383100E+02 -0.22564100E+00
0.64955000E+01 0.18556800E+00
0.34643100E+01 0.15654900E+00
0.98620000E+00 -0.31141700E+00
0.45782800E+00 -0.39452300E+00
0.13211800E+00 0.20348300E+00
0.66967000E-01 0.68629600E+00
0.29010000E-01 0.31922600E+00
S 10 1.0
```

0.26504200E+02 -0.51870000E-02  
0.16584000E+02 0.78069000E-01  
0.10383100E+02 -0.26334100E+00  
0.64955000E+01 0.16317300E+00  
0.34643100E+01 0.41214500E+00  
0.98620000E+00 -0.92791900E+00  
0.45782800E+00 -0.35528500E+00  
0.13211800E+00 0.25901110E+01  
0.66967000E-01 -0.12877130E+01  
0.29010000E-01 -0.68288400E+00  
S 10 1.0  
0.26504200E+02 0.26620000E-01  
0.16584000E+02 -0.51092000E-01  
0.10383100E+02 -0.13386000E-01  
0.64955000E+01 -0.24939600E+00  
0.34643100E+01 0.11377230E+01  
0.98620000E+00 -0.32919740E+01  
0.45782800E+00 0.30952960E+01  
0.13211800E+00 0.52338100E+00  
0.66967000E-01 -0.29817690E+01  
0.29010000E-01 0.19815350E+01  
S 1 1.0  
0.29010000E-01 0.10000000E+01  
S 1 1.0  
0.12600000E-01 0.10000000E+01  
P 9 1.0  
0.15272400E+02 -0.24916000E-01  
0.95703500E+01 0.13496700E+00  
0.50361800E+01 -0.31452800E+00  
0.11521500E+01 0.47660400E+00  
0.56240100E+00 0.48419100E+00  
0.27420400E+00 0.18449400E+00  
0.12050500E+00 0.18639000E-01  
0.52812000E-01 0.15040000E-02  
0.22891000E-01 -0.29000000E-04  
P 9 1.0  
0.15272400E+02 0.66140000E-02  
0.95703500E+01 -0.36926000E-01  
0.50361800E+01 0.88777000E-01  
0.11521500E+01 -0.15141700E+00  
0.56240100E+00 -0.20415200E+00  
0.27420400E+00 -0.40135000E-01  
0.12050500E+00 0.36632600E+00  
0.52812000E-01 0.56269600E+00  
0.22891000E-01 0.22037900E+00  
P 9 1.0  
0.15272400E+02 0.94170000E-02  
0.95703500E+01 -0.53087000E-01  
0.50361800E+01 0.12828700E+00  
0.11521500E+01 -0.21700800E+00  
0.56240100E+00 -0.32512200E+00

0.27420400E+00 -0.46510000E-02  
0.12050500E+00 0.73434300E+00  
0.52812000E-01 0.38499800E+00  
0.22891000E-01 0.88690000E-02  
P 9 1.0  
0.15272400E+02 0.19046000E-01  
0.95703500E+01 -0.10395300E+00  
0.50361800E+01 0.25102700E+00  
0.11521500E+01 -0.52896300E+00  
0.56240100E+00 -0.80065700E+00  
0.27420400E+00 0.16510980E+01  
0.12050500E+00 0.11950800E+00  
0.52812000E-01 -0.95902300E+00  
0.22891000E-01 -0.27430000E-02  
P 1 1.0  
0.22891000E-01 0.10000000E+01  
P 1 1.0  
0.99000000E-02 0.10000000E+01  
D 8 1.0  
0.11975600E+02 -0.14780000E-02  
0.74799800E+01 0.18708000E-01  
0.46738300E+01 -0.58087000E-01  
0.11750300E+01 0.18233400E+00  
0.52835000E+00 0.34866400E+00  
0.22775700E+00 0.39335000E+00  
0.94169000E-01 0.27722300E+00  
0.36631000E-01 0.69834000E-01  
D 8 1.0  
0.11975600E+02 0.12390000E-02  
0.74799800E+01 -0.20216000E-01  
0.46738300E+01 0.66945000E-01  
0.11750300E+01 -0.23925600E+00  
0.52835000E+00 -0.47367700E+00  
0.22775700E+00 -0.84303000E-01  
0.94169000E-01 0.63333000E+00  
0.36631000E-01 0.34964300E+00  
D 8 1.0  
0.11975600E+02 -0.31330000E-02  
0.74799800E+01 0.33477000E-01  
0.46738300E+01 -0.10380900E+00  
0.11750300E+01 0.47168200E+00  
0.52835000E+00 0.51918900E+00  
0.22775700E+00 -0.10917460E+01  
0.94169000E-01 0.84120000E-02  
0.36631000E-01 0.72865700E+00  
D 1 1.0  
0.36631000E-01 0.10000000E+01  
D 1 1.0  
0.14200000E-01 0.10000000E+01  
F 1 1.0  
0.55210000E+00 0.10000000E+01

```
F 1 1.0
  0.16050000E+00  0.10000000E+01
F 1 1.0
  0.50500000E-01  0.10000000E+01
G 1 1.0
  0.35790000E+00  0.10000000E+01
G 1 1.0
  0.10740000E+00  0.10000000E+01
****
```

```
Hf 0
ECP60MDF 5 60
H-Komponente
1
2 1.000000 0.000000
S-H-Komponente
3
2 10.248856 478.237404
4 10.729127 0.388024
2 1.964856 -1.071232
P-H-Komponente
6
2 8.683462 101.046818
2 7.916920 212.197761
4 9.379243 0.132646
4 8.244209 0.453108
2 1.596686 -0.407914
2 1.710281 -0.561817
D-H-Komponente
6
2 5.189557 43.115467
2 5.253229 65.934732
4 5.937871 0.025912
4 5.712906 0.033741
2 1.014856 -0.280579
2 0.473712 -0.084849
F-H-Komponente
2
2 1.912608 4.811801
2 1.880740 6.418574;
G-H-Komponente
2
2 2.724180 -4.636585
2 2.708953 -5.767288

Mo 0
S 9 1.00
  170.0690000 0.0004530
  16.7338000 -0.0413800
  10.4587000 0.2326990
  6.5343400 -0.1825190
```

		3.6793500	-0.4983180
		1.0019200	0.7853790
		0.4631400	0.5013700
		0.1187270	0.0358290
		0.0595140	-0.0140370
S	9	1.00	
		170.0690000	-0.0001560
		16.7338000	0.0139920
		10.4587000	-0.0809630
		6.5343400	0.0744540
		3.6793500	0.1588830
		1.0019200	-0.3414150
		0.4631400	-0.3366740
		0.1187270	0.3095560
		0.0595140	0.6149970
S	9	1.00	
		170.0690000	-0.0000750
		16.7338000	0.0015070
		10.4587000	-0.0536740
		6.5343400	-0.0331090
		3.6793500	0.5047010
		1.0019200	-1.3515930
		0.4631400	0.3070100
		0.1187270	2.3973260
		0.0595140	-1.6896850
S	9	1.00	
		170.0690000	-0.0002980
		16.7338000	0.0209690
		10.4587000	-0.1814220
		6.5343400	0.1285330
		3.6793500	0.7288700
		1.0019200	-3.4647110
		0.4631400	3.8855920
		0.1187270	-1.5475660
		0.0595140	-0.7618020
S	1	1.00	
		0.0270390	1.0000000
S	1	1.00	
		0.0123000	1.0000000
P	8	1.00	
		20.3080000	-0.0015140
		12.6907000	0.0221680
		5.1195000	-0.1743690
		1.3778300	0.4279430
		0.6968240	0.4753060
		0.3473670	0.2174030
		0.1528190	0.0285240
		0.0650490	0.0004610
P	8	1.00	
		20.3080000	-0.0000830
		12.6907000	-0.0054470

		5.1195000	0.0532030
		1.3778300	-0.1581500
		0.6968240	-0.1918290
		0.3473670	-0.0524490
		0.1528190	0.3447620
		0.0650490	0.5699340
P	8	1.00	
		20.3080000	-0.0000340
		12.6907000	-0.0086930
		5.1195000	0.0831140
		1.3778300	-0.2494680
		0.6968240	-0.3235300
		0.3473670	0.0156020
		0.1528190	0.6864390
		0.0650490	0.4139530
P	8	1.00	
		20.3080000	0.0001020
		12.6907000	-0.0158590
		5.1195000	0.1536300
		1.3778300	-0.5873860
		0.6968240	-0.6442110
		0.3473670	1.3803170
		0.1528190	0.3384870
		0.0650490	-0.9969510
P	1	1.00	
		0.0273390	1.0000000
P	1	1.00	
		0.0115000	1.0000000
D	7	1.00	
		22.6032000	0.0013060
		6.3391400	-0.0124380
		2.1776300	0.1035120
		1.1070000	0.2776610
		0.5353720	0.3588570
		0.2489800	0.3092260
		0.1104090	0.1740360
D	7	1.00	
		22.6032000	-0.0013410
		6.3391400	0.0130470
		2.1776300	-0.1256280
		1.1070000	-0.3434410
		0.5353720	-0.2978970
		0.2489800	0.2001940
		0.1104090	0.5671490
D	7	1.00	
		22.6032000	0.0020230
		6.3391400	-0.0206910
		2.1776300	0.2714220
		1.1070000	0.5579390
		0.5353720	-0.2102870
		0.2489800	-0.8724070

		0.1104090	0.2634070
D	1	1.00	
		0.0453770	1.0000000
D	1	1.00	
		0.0186000	1.0000000
F	1	1.00	
		1.2203000	1.0000000
F	1	1.00	
		0.3332000	1.0000000
F	1	1.00	
		0.1186000	1.0000000
G	1	1.00	
		0.7324000	1.0000000
G	1	1.00	
		0.2751000	1.0000000

\*\*\*\*

MO	0		
MO-ECP	4	28	
g-ul potential			
	1		
2		1.0000000	0.0000000
s-ul potential			
	2		
2		10.09700000	180.07685300
2		4.37567000	24.71592000
p-ul potential			
	4		
2		9.12656400	41.22767800
2		8.86322300	82.45267000
2		4.04494800	6.34509200
2		3.86665700	12.45842300
d-ul potential			
	4		
2		7.53575400	19.30874400
2		7.27897600	28.97767400
2		2.76320500	3.18951600
2		2.77208500	4.70016900
f-ul potential			
	2		
2		6.30663300	-7.17888800
2		6.35644800	-9.74597800

All-electron basis sets used for the AIM analysis:

TI	0		
S	19	1.00	
		3014643.0000000	0.0001120
		451432.9000000	0.0003320
		102733.8000000	0.0009400
		29098.1700000	0.0025320
		9492.3300000	0.0068790



		3426.3460000	0.0187490
		1335.8960000	0.0492940
		553.5026000	0.1166940
		240.6925000	0.2273250
		108.7293000	0.3105540
		50.2645700	0.2205840
		22.5800400	0.0732470
		10.7143200	0.1131540
		5.0935460	0.1136590
		2.2441830	0.0193160
		1.0595700	-0.0004650
		0.4688490	0.0001590
		0.1061430	-0.0000590
		0.0552620	0.0000620
S	19	1.00	
		3014643.0000000	-0.0000630
		451432.9000000	-0.0001890
		102733.8000000	-0.0005350
		29098.1700000	-0.0014430
		9492.3300000	-0.0039330
		3426.3460000	-0.0107960
		1335.8960000	-0.0288290
		553.5026000	-0.0706740
		240.6925000	-0.1487780
		108.7293000	-0.2420600
		50.2645700	-0.2347210
		22.5800400	0.0422060
		10.7143200	0.4983350
		5.0935460	0.4868870
		2.2441830	0.0879040
		1.0595700	-0.0052640
		0.4688490	0.0005520
		0.1061430	-0.0006280
		0.0552620	0.0005530
S	19	1.00	
		3014643.0000000	0.0000130
		451432.9000000	0.0000380
		102733.8000000	0.0001090
		29098.1700000	0.0002940
		9492.3300000	0.0008030
		3426.3460000	0.0022200
		1335.8960000	0.0059990
		553.5026000	0.0151490
		240.6925000	0.0337330
		108.7293000	0.0615630
		50.2645700	0.0694620
		22.5800400	-0.0241550
		10.7143200	-0.2789840
		5.0935460	-0.4386710
		2.2441830	0.0909060
		1.0595700	0.7091310

		0.4688490	0.4311640
		0.1061430	0.0258980
		0.0552620	-0.0110070
S	19	1.00	
		3014643.0000000	-0.0000030
		451432.9000000	-0.0000090
		102733.8000000	-0.0000260
		29098.1700000	-0.0000700
		9492.3300000	-0.0001910
		3426.3460000	-0.0005260
		1335.8960000	-0.0014240
		553.5026000	-0.0035930
		240.6925000	-0.0080220
		108.7293000	-0.0146460
		50.2645700	-0.0166610
		22.5800400	0.0058890
		10.7143200	0.0693470
		5.0935460	0.1159210
		2.2441830	-0.0327170
		1.0595700	-0.2334140
		0.4688490	-0.2869410
		0.1061430	0.2839540
		0.0552620	0.5841130
S	19	1.00	
		3014643.0000000	-0.0000060
		451432.9000000	-0.0000170
		102733.8000000	-0.0000480
		29098.1700000	-0.0001310
		9492.3300000	-0.0003460
		3426.3460000	-0.0010090
		1335.8960000	-0.0025320
		553.5026000	-0.0070420
		240.6925000	-0.0138290
		108.7293000	-0.0302210
		50.2645700	-0.0239810
		22.5800400	-0.0071850
		10.7143200	0.1758840
		5.0935460	0.1462460
		2.2441830	0.0971840
		1.0595700	-1.0017360
		0.4688490	0.1999570
		0.1061430	2.2181040
		0.0552620	-1.3423230
S	19	1.00	
		3014643.0000000	-0.0000090
		451432.9000000	-0.0000270
		102733.8000000	-0.0000750
		29098.1700000	-0.0002080
		9492.3300000	-0.0005370
		3426.3460000	-0.0016170
		1335.8960000	-0.0038870

		553.5026000	-0.0114190
		240.6925000	-0.0208780
		108.7293000	-0.0503970
		50.2645700	-0.0320930
		22.5800400	-0.0269460
		10.7143200	0.3275740
		5.0935460	0.2147230
		2.2441830	0.1170160
		1.0595700	-2.4080240
		0.4688490	2.5936190
		0.1061430	0.1447480
		0.0552620	-2.5253120
S	1	1.00	
		0.0254650	1.0000000
P	15	1.00	
		11912.0300000	0.0001040
		2819.9470000	0.0005330
		915.9479000	0.0025880
		350.3842000	0.0104700
		148.4825000	0.0354710
		67.5394400	0.0981640
		32.3033200	0.2106310
		15.9278600	0.3301970
		8.0380350	0.3305000
		4.0939160	0.1571860
		2.0223900	0.0219670
		0.9761020	-0.0017610
		0.4595950	-0.0014300
		0.1771950	-0.0002900
		0.0734420	0.0000340
P	15	1.00	
		11912.0300000	-0.0000350
		2819.9470000	-0.0001790
		915.9479000	-0.0008700
		350.3842000	-0.0035410
		148.4825000	-0.0121500
		67.5394400	-0.0344710
		32.3033200	-0.0765940
		15.9278600	-0.1256220
		8.0380350	-0.1320480
		4.0939160	0.0193960
		2.0223900	0.3164550
		0.9761020	0.4614890
		0.4595950	0.2980100
		0.1771950	0.0495170
		0.0734420	-0.0041080
P	15	1.00	
		11912.0300000	0.0000080
		2819.9470000	0.0000430
		915.9479000	0.0002090
		350.3842000	0.0008480

		148.4825000	0.0029250
		67.5394400	0.0082760
		32.3033200	0.0185500
		15.9278600	0.0303400
		8.0380350	0.0327150
		4.0939160	-0.0087200
		2.0223900	-0.0886360
		0.9761020	-0.1491650
		0.4595950	-0.0932320
		0.1771950	0.2507080
		0.0734420	0.5861800
P	15	1.00	
		11912.0300000	0.0000100
		2819.9470000	0.0000540
		915.9479000	0.0002610
		350.3842000	0.0010710
		148.4825000	0.0036390
		67.5394400	0.0104610
		32.3033200	0.0229850
		15.9278600	0.0386720
		8.0380350	0.0394990
		4.0939160	-0.0068990
		2.0223900	-0.1146250
		0.9761020	-0.1708870
		0.4595950	-0.1652610
		0.1771950	0.4058580
		0.0734420	0.6742340
P	15	1.00	
		11912.0300000	0.0000210
		2819.9470000	0.0001010
		915.9479000	0.0005360
		350.3842000	0.0019840
		148.4825000	0.0075290
		67.5394400	0.0191510
		32.3033200	0.0486770
		15.9278600	0.0671790
		8.0380350	0.1039430
		4.0939160	-0.0555620
		2.0223900	-0.1916650
		0.9761020	-0.6969070
		0.4595950	0.5747490
		0.1771950	1.1704990
		0.0734420	-1.0063770
P	1	1.00	
		0.0293340	1.0000000
D	7	1.00	
		64.3402000	0.0038830
		18.8418000	0.0262040
		6.7198300	0.0968870
		2.6561300	0.2316310
		1.0736800	0.3519720

		0.4205570	0.3725630
		0.1548170	0.2505630
D	7	1.00	
		64.3402000	-0.0039790
		18.8418000	-0.0267640
		6.7198300	-0.1018940
		2.6561300	-0.2371110
		1.0736800	-0.3132860
		0.4205570	-0.0465630
		0.1548170	0.5840720
D	7	1.00	
		64.3402000	0.0063860
		18.8418000	0.0433010
		6.7198300	0.1702500
		2.6561300	0.3719460
		1.0736800	0.2303500
		0.4205570	-0.7820270
		0.1548170	-0.1235850
D	1	1.00	
		0.0514900	1.0000000
F	1	1.00	
		1.2274000	1.0000000
F	1	1.00	
		0.2788000	1.0000000
S	1	1.00	
		0.0117300	1.0000000
P	1	1.00	
		0.0117200	1.0000000
D	1	1.00	
		0.0171200	1.0000000
F	1	1.00	
		0.0806900	1.0000000

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Zr	0		
S	26	1.00	
		1.374650E+08	3.900000E-05
		2.198390E+07	1.020000E-04
		4.663660E+06	2.830000E-04
		1.230450E+06	6.530000E-04
		3.829710E+05	1.417000E-03
		1.347840E+05	2.929000E-03
		5.189420E+04	6.014000E-03
		2.131980E+04	1.243500E-02
		9.179920E+03	2.619900E-02
		4.092810E+03	5.546400E-02
		1.875390E+03	1.132890E-01
		8.796740E+02	2.051980E-01
		4.217030E+02	2.861040E-01
		2.065130E+02	2.401140E-01
		1.032640E+02	9.437900E-02

	5.264030E+01	7.068400E-02
	2.724980E+01	9.376700E-02
	1.421930E+01	3.962600E-02
	7.390030E+00	1.037500E-02
	3.757850E+00	8.367000E-03
	1.823910E+00	1.955000E-03
	8.720740E-01	-5.900000E-05
	3.965840E-01	1.300000E-05
	1.045330E-01	-1.100000E-05
	5.568500E-02	8.000000E-06
	2.496200E-02	-2.000000E-06
S 26	1.00	
	1.374650E+08	-2.100000E-05
	2.198390E+07	-5.600000E-05
	4.663660E+06	-1.540000E-04
	1.230450E+06	-3.550000E-04
	3.829710E+05	-7.720000E-04
	1.347840E+05	-1.599000E-03
	5.189420E+04	-3.296000E-03
	2.131980E+04	-6.857000E-03
	9.179920E+03	-1.460800E-02
	4.092810E+03	-3.151900E-02
	1.875390E+03	-6.687900E-02
	8.796740E+02	-1.304680E-01
	4.217030E+02	-2.120310E-01
	2.065130E+02	-2.295690E-01
	1.032640E+02	-4.800500E-02
	5.264030E+01	3.457620E-01
	2.724980E+01	5.209040E-01
	1.421930E+01	2.244900E-01
	7.390030E+00	3.782600E-02
	3.757850E+00	2.020800E-02
	1.823910E+00	4.371000E-03
	8.720740E-01	-1.770000E-04
	3.965840E-01	-1.300000E-05
	1.045330E-01	-2.300000E-05
	5.568500E-02	1.400000E-05
	2.496200E-02	-4.000000E-06
S 26	1.00	
	1.374650E+08	6.000000E-06
	2.198390E+07	1.500000E-05
	4.663660E+06	4.300000E-05
	1.230450E+06	9.900000E-05
	3.829710E+05	2.150000E-04
	1.347840E+05	4.470000E-04
	5.189420E+04	9.250000E-04
	2.131980E+04	1.930000E-03
	9.179920E+03	4.153000E-03
	4.092810E+03	9.071000E-03
	1.875390E+03	1.982800E-02
	8.796740E+02	4.053000E-02

4.217030E+02	7.244800E-02
2.065130E+02	8.842200E-02
1.032640E+02	1.506700E-02
5.264030E+01	-2.428610E-01
2.724980E+01	-4.974240E-01
1.421930E+01	-2.335070E-01
7.390030E+00	4.854210E-01
3.757850E+00	7.020170E-01
1.823910E+00	1.631350E-01
8.720740E-01	1.655000E-03
3.965840E-01	3.001000E-03
1.045330E-01	-3.620000E-04
5.568500E-02	2.950000E-04
2.496200E-02	-8.100000E-05
S 26 1.00	
1.374650E+08	-2.000000E-06
2.198390E+07	-6.000000E-06
4.663660E+06	-1.600000E-05
1.230450E+06	-3.700000E-05
3.829710E+05	-8.000000E-05
1.347840E+05	-1.660000E-04
5.189420E+04	-3.430000E-04
2.131980E+04	-7.160000E-04
9.179920E+03	-1.538000E-03
4.092810E+03	-3.362000E-03
1.875390E+03	-7.328000E-03
8.796740E+02	-1.500400E-02
4.217030E+02	-2.671200E-02
2.065130E+02	-3.291500E-02
1.032640E+02	-5.423000E-03
5.264030E+01	9.426200E-02
2.724980E+01	2.112000E-01
1.421930E+01	9.743300E-02
7.390030E+00	-2.577540E-01
3.757850E+00	-6.437290E-01
1.823910E+00	-1.211340E-01
8.720740E-01	7.660700E-01
3.965840E-01	5.479130E-01
1.045330E-01	4.337700E-02
5.568500E-02	-1.667900E-02
2.496200E-02	4.758000E-03
S 26 1.00	
1.374650E+08	1.000000E-06
2.198390E+07	2.000000E-06
4.663660E+06	4.000000E-06
1.230450E+06	1.000000E-05
3.829710E+05	2.200000E-05
1.347840E+05	4.600000E-05
5.189420E+04	9.400000E-05
2.131980E+04	1.970000E-04
9.179920E+03	4.230000E-04

4.092810E+03	9.270000E-04
1.875390E+03	2.018000E-03
8.796740E+02	4.142000E-03
4.217030E+02	7.360000E-03
2.065130E+02	9.119000E-03
1.032640E+02	1.443000E-03
5.264030E+01	-2.614600E-02
2.724980E+01	-5.964900E-02
1.421930E+01	-2.707700E-02
7.390030E+00	7.412400E-02
3.757850E+00	2.051780E-01
1.823910E+00	3.169600E-02
8.720740E-01	-3.079690E-01
3.965840E-01	-3.842290E-01
1.045330E-01	2.243790E-01
5.568500E-02	6.526520E-01
2.496200E-02	3.189420E-01
S 26 1.00	
1.374650E+08	1.000000E-06
2.198390E+07	3.000000E-06
4.663660E+06	8.000000E-06
1.230450E+06	1.800000E-05
3.829710E+05	3.900000E-05
1.347840E+05	8.100000E-05
5.189420E+04	1.710000E-04
2.131980E+04	3.470000E-04
9.179920E+03	7.770000E-04
4.092810E+03	1.605000E-03
1.875390E+03	3.757000E-03
8.796740E+02	7.036000E-03
4.217030E+02	1.413700E-02
2.065130E+02	1.397400E-02
1.032640E+02	8.252000E-03
5.264030E+01	-6.002700E-02
2.724980E+01	-8.058000E-02
1.421930E+01	-1.032140E-01
7.390030E+00	2.392630E-01
3.757850E+00	2.188950E-01
1.823910E+00	3.606080E-01
8.720740E-01	-1.333999E+00
3.965840E-01	5.622500E-02
1.045330E-01	2.598673E+00
5.568500E-02	-1.590164E+00
2.496200E-02	-5.543430E-01
S 26 1.00	
1.374650E+08	2.000000E-06
2.198390E+07	4.000000E-06
4.663660E+06	1.200000E-05
1.230450E+06	2.700000E-05
3.829710E+05	5.800000E-05
1.347840E+05	1.180000E-04



	5.189420E+04	2.540000E-04
	2.131980E+04	5.000000E-04
	9.179920E+03	1.171000E-03
	4.092810E+03	2.282000E-03
	1.875390E+03	5.740000E-03
	8.796740E+02	9.809000E-03
	4.217030E+02	2.221600E-02
	2.065130E+02	1.721700E-02
	1.032640E+02	2.037200E-02
	5.264030E+01	-1.080960E-01
	2.724980E+01	-8.461300E-02
	1.421930E+01	-2.264530E-01
	7.390030E+00	5.213300E-01
	3.757850E+00	1.380690E-01
	1.823910E+00	8.852170E-01
	8.720740E-01	-3.709192E+00
	3.965840E-01	3.475697E+00
	1.045330E-01	-2.666100E-01
	5.568500E-02	-2.271272E+00
	2.496200E-02	1.833948E+00
S 1	1.00	
	2.496200E-02	1.000000E+00
P 21	1.00	
	1.026890E+06	1.400000E-05
	1.663250E+05	5.400000E-05
	3.738190E+04	2.110000E-04
	1.077160E+04	7.820000E-04
	3.733590E+03	2.824000E-03
	1.480440E+03	9.644000E-03
	6.461670E+02	2.992700E-02
	3.016820E+02	8.159300E-02
	1.475910E+02	1.827890E-01
	7.458000E+01	3.108630E-01
	3.853850E+01	3.449150E-01
	2.021330E+01	1.912910E-01
	1.068870E+01	3.583100E-02
	5.653870E+00	-5.564000E-03
	2.959510E+00	-4.994000E-03
	1.509350E+00	-7.890000E-04
	7.426710E-01	3.200000E-05
	3.561060E-01	8.400000E-05
	1.432030E-01	5.000000E-06
	6.136600E-02	3.000000E-06
	2.538000E-02	-1.000000E-06
P 21	1.00	
	1.026890E+06	-6.000000E-06
	1.663250E+05	-2.200000E-05
	3.738190E+04	-8.600000E-05
	1.077160E+04	-3.200000E-04
	3.733590E+03	-1.159000E-03
	1.480440E+03	-3.983000E-03

6.461670E+02	-1.253200E-02
3.016820E+02	-3.505300E-02
1.475910E+02	-8.182300E-02
7.458000E+01	-1.469170E-01
3.853850E+01	-1.665300E-01
2.021330E+01	-1.958000E-03
1.068870E+01	3.022470E-01
5.653870E+00	4.800820E-01
2.959510E+00	2.895230E-01
1.509350E+00	4.606200E-02
7.426710E-01	-1.009000E-03
3.561060E-01	-2.648000E-03
1.432030E-01	-2.700000E-04
6.136600E-02	-5.500000E-05
2.538000E-02	1.200000E-05
P 21 1.00	
1.026890E+06	2.000000E-06
1.663250E+05	8.000000E-06
3.738190E+04	3.000000E-05
1.077160E+04	1.130000E-04
3.733590E+03	4.080000E-04
1.480440E+03	1.403000E-03
6.461670E+02	4.424000E-03
3.016820E+02	1.240700E-02
1.475910E+02	2.911800E-02
7.458000E+01	5.263500E-02
3.853850E+01	5.992900E-02
2.021330E+01	-6.529000E-03
1.068870E+01	-1.338850E-01
5.653870E+00	-2.384410E-01
2.959510E+00	-1.409390E-01
1.509350E+00	2.670430E-01
7.426710E-01	5.264040E-01
3.561060E-01	3.500400E-01
1.432030E-01	6.079500E-02
6.136600E-02	-3.512000E-03
2.538000E-02	1.743000E-03
P 21 1.00	
1.026890E+06	-1.000000E-06
1.663250E+05	-2.000000E-06
3.738190E+04	-8.000000E-06
1.077160E+04	-3.100000E-05
3.733590E+03	-1.120000E-04
1.480440E+03	-3.850000E-04
6.461670E+02	-1.216000E-03
3.016820E+02	-3.403000E-03
1.475910E+02	-8.015000E-03
7.458000E+01	-1.444500E-02
3.853850E+01	-1.657500E-02
2.021330E+01	2.216000E-03
1.068870E+01	3.732300E-02

5.653870E+00	6.903900E-02
2.959510E+00	3.782500E-02
1.509350E+00	-8.772600E-02
7.426710E-01	-2.031560E-01
3.561060E-01	-1.411200E-01
1.432030E-01	2.623720E-01
6.136600E-02	6.031610E-01
2.538000E-02	2.995440E-01
P 21 1.00	
1.026890E+06	-1.000000E-06
1.663250E+05	-3.000000E-06
3.738190E+04	-1.200000E-05
1.077160E+04	-4.400000E-05
3.733590E+03	-1.580000E-04
1.480440E+03	-5.440000E-04
6.461670E+02	-1.717000E-03
3.016820E+02	-4.812000E-03
1.475910E+02	-1.130900E-02
7.458000E+01	-2.043900E-02
3.853850E+01	-2.334200E-02
2.021330E+01	2.934000E-03
1.068870E+01	5.300200E-02
5.653870E+00	9.693500E-02
2.959510E+00	5.530000E-02
1.509350E+00	-1.263110E-01
7.426710E-01	-2.883080E-01
3.561060E-01	-2.127200E-01
1.432030E-01	5.617710E-01
6.136600E-02	5.907190E-01
2.538000E-02	4.064900E-02
P 21 1.00	
1.026890E+06	-1.000000E-06
1.663250E+05	-5.000000E-06
3.738190E+04	-2.000000E-05
1.077160E+04	-7.300000E-05
3.733590E+03	-2.750000E-04
1.480440E+03	-9.030000E-04
6.461670E+02	-3.005000E-03
3.016820E+02	-7.931000E-03
1.475910E+02	-1.998900E-02
7.458000E+01	-3.298400E-02
3.853850E+01	-4.442900E-02
2.021330E+01	1.520600E-02
1.068870E+01	7.215900E-02
5.653870E+00	2.108560E-01
2.959510E+00	2.893500E-02
1.509350E+00	-1.300640E-01
7.426710E-01	-1.052978E+00
3.561060E-01	8.409110E-01
1.432030E-01	1.112199E+00
6.136600E-02	-1.157655E+00

	2.538000E-02	-1.222470E-01
P 1	1.00	
	2.538000E-02	1.000000E+00
D 14	1.00	
	1.873980E+03	1.650000E-04
	5.384570E+02	1.476000E-03
	2.013810E+02	8.701000E-03
	8.772280E+01	3.425200E-02
	4.149510E+01	1.005890E-01
	2.047460E+01	2.180290E-01
	1.031470E+01	3.259560E-01
	5.232370E+00	3.343750E-01
	2.626560E+00	1.951030E-01
	1.252140E+00	4.521400E-02
	5.665690E-01	1.854000E-03
	2.447510E-01	4.680000E-04
	1.007930E-01	-1.050000E-04
	3.872100E-02	5.200000E-05
D 14	1.00	
	1.873980E+03	-3.600000E-05
	5.384570E+02	-3.200000E-04
	2.013810E+02	-1.889000E-03
	8.772280E+01	-7.486000E-03
	4.149510E+01	-2.215500E-02
	2.047460E+01	-4.838300E-02
	1.031470E+01	-6.982500E-02
	5.232370E+00	-6.628400E-02
	2.626560E+00	9.345000E-03
	1.252140E+00	1.800330E-01
	5.665690E-01	3.375510E-01
	2.447510E-01	3.797130E-01
	1.007930E-01	2.816470E-01
	3.872100E-02	9.450100E-02
D 14	1.00	
	1.873980E+03	3.800000E-05
	5.384570E+02	3.410000E-04
	2.013810E+02	2.007000E-03
	8.772280E+01	7.971000E-03
	4.149510E+01	2.359600E-02
	2.047460E+01	5.165200E-02
	1.031470E+01	7.371300E-02
	5.232370E+00	6.816100E-02
	2.626560E+00	-2.217100E-02
	1.252140E+00	-2.243400E-01
	5.665690E-01	-4.064670E-01
	2.447510E-01	-1.230570E-01
	1.007930E-01	5.401810E-01
	3.872100E-02	4.639430E-01
D 14	1.00	
	1.873980E+03	-5.100000E-05
	5.384570E+02	-4.560000E-04

	2.013810E+02	-2.710000E-03
	8.772280E+01	-1.070100E-02
	4.149510E+01	-3.204500E-02
	2.047460E+01	-6.946400E-02
	1.031470E+01	-9.807300E-02
	5.232370E+00	-8.006300E-02
	2.626560E+00	5.486900E-02
	1.252140E+00	4.033390E-01
	5.665690E-01	4.207990E-01
	2.447510E-01	-7.613030E-01
	1.007930E-01	-3.936520E-01
	3.872100E-02	8.862560E-01
D 1	1.00	
	3.872100E-02	1.000000E+00
F 1	1.00	
	7.043000E-01	1.000000E+00
F 1	1.00	
	1.873000E-01	1.000000E+00
S 1	1.00	
	1.120000E-02	1.000000E+00
P 1	1.00	
	1.050000E-02	1.000000E+00
D 1	1.00	
	1.490000E-02	1.000000E+00
F 1	1.00	
	6.310000E-02	1.000000E+00
	****	
-Hf	0	
S 30	1.00	
	1.209352E+10	4.000000E-06
	1.755709E+09	1.060000E-05
	3.405127E+08	2.850000E-05
	8.319553E+07	6.270000E-05
	2.435708E+07	1.265000E-04
	8.193356E+06	2.352000E-04
	3.058833E+06	4.192000E-04
	1.232418E+06	7.244000E-04
	5.242476E+05	1.238000E-03
	2.315739E+05	2.103600E-03
	1.049682E+05	3.582500E-03
	4.844357E+04	6.099100E-03
	2.266140E+04	1.032270E-02
	1.072633E+04	1.690020E-02
	5.138808E+03	2.521230E-02
	2.496078E+03	2.887580E-02
	1.232232E+03	1.443390E-02
	6.197951E+02	-1.481000E-04
	3.182361E+02	1.093465E-01
	1.669069E+02	3.470565E-01
	8.930310E+01	3.289259E-01

4.855668E+01	1.244939E-01
2.664003E+01	9.489160E-02
1.458614E+01	5.226050E-02
7.846900E+00	1.145840E-02
4.062263E+00	6.834100E-03
1.970383E+00	1.162100E-03
9.749930E-01	-2.420000E-05
4.493950E-01	-9.600000E-06
1.226740E-01	-7.000000E-07
S 32 1.00	
1.209352E+10	2.020000E-05
1.755709E+09	5.330000E-05
3.405127E+08	1.428000E-04
8.319553E+07	3.147000E-04
2.435708E+07	6.354000E-04
8.193356E+06	1.183700E-03
3.058833E+06	2.116000E-03
1.232418E+06	3.674600E-03
5.242476E+05	6.323500E-03
2.315739E+05	1.086350E-02
1.049682E+05	1.880180E-02
4.844357E+04	3.285770E-02
2.266140E+04	5.796340E-02
1.072633E+04	1.021044E-01
5.138808E+03	1.745218E-01
2.496078E+03	2.710215E-01
1.232232E+03	3.349050E-01
6.197951E+02	2.513034E-01
3.182361E+02	8.755700E-03
1.669069E+02	-2.118762E-01
8.930310E+01	-2.094483E-01
4.855668E+01	-7.305620E-02
2.664003E+01	-3.593750E-02
1.458614E+01	-1.881600E-02
7.846900E+00	-3.853100E-03
4.062263E+00	-2.101200E-03
1.970383E+00	-3.737000E-04
9.749930E-01	1.370000E-05
4.493950E-01	1.200000E-06
1.226740E-01	1.200000E-06
6.214100E-02	-7.000000E-07
2.785000E-02	2.000000E-07
S 32 1.00	
1.209352E+10	3.600000E-06
1.755709E+09	9.500000E-06
3.405127E+08	2.550000E-05
8.319553E+07	5.610000E-05
2.435708E+07	1.133000E-04
8.193356E+06	2.114000E-04
3.058833E+06	3.787000E-04
1.232418E+06	6.598000E-04

5.242476E+05	1.140700E-03
2.315739E+05	1.974100E-03
1.049682E+05	3.452000E-03
4.844357E+04	6.134100E-03
2.266140E+04	1.108870E-02
1.072633E+04	2.034370E-02
5.138808E+03	3.708120E-02
2.496078E+03	6.426080E-02
1.232232E+03	9.358410E-02
6.197951E+02	7.855680E-02
3.182361E+02	-8.294720E-02
1.669069E+02	-4.159398E-01
8.930310E+01	-5.334647E-01
4.855668E+01	1.206950E-02
2.664003E+01	6.488933E-01
1.458614E+01	3.805257E-01
7.846900E+00	1.347113E-01
4.062263E+00	1.132714E-01
1.970383E+00	1.959320E-02
9.749930E-01	-3.551000E-04
4.493950E-01	-8.360000E-05
1.226740E-01	-1.530000E-05
6.214100E-02	2.100000E-06
2.785000E-02	-1.900000E-06
S 32 1.00	
1.209352E+10	-2.100000E-06
1.755709E+09	-5.700000E-06
3.405127E+08	-1.520000E-05
8.319553E+07	-3.340000E-05
2.435708E+07	-6.750000E-05
8.193356E+06	-1.259000E-04
3.058833E+06	-2.255000E-04
1.232418E+06	-3.928000E-04
5.242476E+05	-6.788000E-04
2.315739E+05	-1.174300E-03
1.049682E+05	-2.051800E-03
4.844357E+04	-3.643100E-03
2.266140E+04	-6.575000E-03
1.072633E+04	-1.203980E-02
5.138808E+03	-2.187660E-02
2.496078E+03	-3.778160E-02
1.232232E+03	-5.487260E-02
6.197951E+02	-4.622430E-02
3.182361E+02	5.115090E-02
1.669069E+02	2.756854E-01
8.930310E+01	3.901265E-01
4.855668E+01	-4.071420E-02
2.664003E+01	-9.229997E-01
1.458614E+01	-6.832651E-01
7.846900E+00	5.959111E-01
4.062263E+00	8.336312E-01

1.970383E+00	1.541300E-01
9.749930E-01	-2.555000E-03
4.493950E-01	2.130100E-03
1.226740E-01	-4.566000E-04
6.214100E-02	2.920000E-04
2.785000E-02	-9.400000E-05
S 32 1.00	
1.209352E+10	7.000000E-07
1.755709E+09	1.800000E-06
3.405127E+08	4.700000E-06
8.319553E+07	1.030000E-05
2.435708E+07	2.090000E-05
8.193356E+06	3.890000E-05
3.058833E+06	6.970000E-05
1.232418E+06	1.215000E-04
5.242476E+05	2.099000E-04
2.315739E+05	3.631000E-04
1.049682E+05	6.347000E-04
4.844357E+04	1.126600E-03
2.266140E+04	2.035000E-03
1.072633E+04	3.724500E-03
5.138808E+03	6.780000E-03
2.496078E+03	1.170510E-02
1.232232E+03	1.709030E-02
6.197951E+02	1.434770E-02
3.182361E+02	-1.633580E-02
1.669069E+02	-9.138810E-02
8.930310E+01	-1.325812E-01
4.855668E+01	1.478650E-02
2.664003E+01	4.005955E-01
1.458614E+01	2.995483E-01
7.846900E+00	-3.832038E-01
4.062263E+00	-7.994775E-01
1.970383E+00	-8.126500E-02
9.749930E-01	8.274524E-01
4.493950E-01	5.223973E-01
1.226740E-01	3.087970E-02
6.214100E-02	-1.293960E-02
2.785000E-02	1.978900E-03
S 32 1.00	
1.209352E+10	-2.000000E-07
1.755709E+09	-5.000000E-07
3.405127E+08	-1.300000E-06
8.319553E+07	-2.800000E-06
2.435708E+07	-5.600000E-06
8.193356E+06	-1.050000E-05
3.058833E+06	-1.870000E-05
1.232418E+06	-3.260000E-05
5.242476E+05	-5.640000E-05
2.315739E+05	-9.750000E-05
1.049682E+05	-1.705000E-04



4.844357E+04	-3.025000E-04
2.266140E+04	-5.468000E-04
1.072633E+04	-9.998000E-04
5.138808E+03	-1.822400E-03
2.496078E+03	-3.142000E-03
1.232232E+03	-4.598100E-03
6.197951E+02	-3.844100E-03
3.182361E+02	4.375700E-03
1.669069E+02	2.472010E-02
8.930310E+01	3.576180E-02
4.855668E+01	-3.821500E-03
2.664003E+01	-1.109845E-01
1.458614E+01	-8.227100E-02
7.846900E+00	1.087536E-01
4.062263E+00	2.478151E-01
1.970383E+00	2.248250E-02
9.749930E-01	-3.324083E-01
4.493950E-01	-3.848196E-01
1.226740E-01	2.742196E-01
6.214100E-02	6.568257E-01
2.785000E-02	2.799885E-01
S 31 1.00	
1.755709E+09	-1.000000E-06
3.405127E+08	-2.000000E-06
8.319553E+07	-5.000000E-06
2.435708E+07	-9.000000E-06
8.193356E+06	-1.800000E-05
3.058833E+06	-3.100000E-05
1.232418E+06	-5.500000E-05
5.242476E+05	-9.400000E-05
2.315739E+05	-1.640000E-04
1.049682E+05	-2.840000E-04
4.844357E+04	-5.110000E-04
2.266140E+04	-9.040000E-04
1.072633E+04	-1.702000E-03
5.138808E+03	-2.984000E-03
2.496078E+03	-5.424000E-03
1.232232E+03	-7.308000E-03
6.197951E+02	-7.383000E-03
3.182361E+02	9.581000E-03
1.669069E+02	3.630700E-02
8.930310E+01	7.150500E-02
4.855668E+01	-3.010200E-02
2.664003E+01	-1.437050E-01
1.458614E+01	-2.157890E-01
7.846900E+00	3.113400E-01
4.062263E+00	2.494780E-01
1.970383E+00	3.636970E-01
9.749930E-01	-1.288652E+00
4.493950E-01	-5.037200E-02
1.226740E-01	2.562387E+00

	6.214100E-02	-1.513281E+00
	2.785000E-02	-5.518040E-01
S 31	1.00	
	1.755709E+09	-1.000000E-06
	3.405127E+08	-3.000000E-06
	8.319553E+07	-7.000000E-06
	2.435708E+07	-1.400000E-05
	8.193356E+06	-2.700000E-05
	3.058833E+06	-4.800000E-05
	1.232418E+06	-8.400000E-05
	5.242476E+05	-1.440000E-04
	2.315739E+05	-2.540000E-04
	1.049682E+05	-4.300000E-04
	4.844357E+04	-7.970000E-04
	2.266140E+04	-1.359000E-03
	1.072633E+04	-2.682000E-03
	5.138808E+03	-4.420000E-03
	2.496078E+03	-8.715000E-03
	1.232232E+03	-1.030600E-02
	6.197951E+02	-1.354600E-02
	3.182361E+02	1.996000E-02
	1.669069E+02	4.424400E-02
	8.930310E+01	1.367990E-01
	4.855668E+01	-1.013500E-01
	2.664003E+01	-1.291330E-01
	1.458614E+01	-5.067950E-01
	7.846900E+00	7.903790E-01
	4.062263E+00	3.045500E-02
	1.970383E+00	1.220545E+00
	9.749930E-01	-4.234797E+00
	4.493950E-01	3.802694E+00
	1.226740E-01	-4.475330E-01
	6.214100E-02	-2.088291E+00
	2.785000E-02	1.759596E+00
S 1	1.00	
	2.785000E-02	1.000000E+00
P 28	1.00	
	2.756805E+08	2.500000E-06
	4.609476E+07	7.100000E-06
	9.405828E+06	2.140000E-05
	2.278079E+06	5.670000E-05
	6.390263E+05	1.434000E-04
	2.031933E+05	3.510000E-04
	7.187865E+04	8.545000E-04
	2.783122E+04	2.096600E-03
	1.163097E+04	5.210800E-03
	5.183406E+03	1.304140E-02
	2.437996E+03	3.214110E-02
	1.199494E+03	7.506260E-02
	6.125623E+02	1.551916E-01
	3.224974E+02	2.615865E-01

1.739582E+02	3.162618E-01
9.558593E+01	2.279622E-01
5.320039E+01	8.638500E-02
2.981870E+01	2.841650E-02
1.672716E+01	1.366230E-02
9.326823E+00	2.819300E-03
5.129062E+00	5.499000E-04
2.756974E+00	1.161000E-04
1.433454E+00	3.950000E-05
7.197090E-01	-1.190000E-05
3.503200E-01	3.700000E-06
1.415820E-01	-2.100000E-06
6.064300E-02	9.000000E-07
2.519000E-02	-3.000000E-07
P 28 1.00	
2.756805E+08	-1.400000E-06
4.609476E+07	-4.000000E-06
9.405828E+06	-1.190000E-05
2.278079E+06	-3.170000E-05
6.390263E+05	-8.020000E-05
2.031933E+05	-1.967000E-04
7.187865E+04	-4.799000E-04
2.783122E+04	-1.182400E-03
1.163097E+04	-2.952400E-03
5.183406E+03	-7.456000E-03
2.437996E+03	-1.860440E-02
1.199494E+03	-4.448080E-02
6.125623E+02	-9.499680E-02
3.224974E+02	-1.678305E-01
1.739582E+02	-2.055356E-01
9.558593E+01	-7.784810E-02
5.320039E+01	2.505311E-01
2.981870E+01	4.970631E-01
1.672716E+01	3.133613E-01
9.326823E+00	6.791950E-02
5.129062E+00	7.604200E-03
2.756974E+00	1.558400E-03
1.433454E+00	2.678000E-04
7.197090E-01	3.000000E-06
3.503200E-01	4.270000E-05
1.415820E-01	-4.300000E-06
6.064300E-02	3.400000E-06
2.519000E-02	-1.000000E-06
P 28 1.00	
2.756805E+08	6.000000E-07
4.609476E+07	1.800000E-06
9.405828E+06	5.400000E-06
2.278079E+06	1.430000E-05
6.390263E+05	3.620000E-05
2.031933E+05	8.890000E-05
7.187865E+04	2.171000E-04

2.783122E+04	5.356000E-04
1.163097E+04	1.339500E-03
5.183406E+03	3.392100E-03
2.437996E+03	8.500600E-03
1.199494E+03	2.047230E-02
6.125623E+02	4.420830E-02
3.224974E+02	7.932270E-02
1.739582E+02	9.762100E-02
9.558593E+01	2.174690E-02
5.320039E+01	-1.916100E-01
2.981870E+01	-4.074993E-01
1.672716E+01	-1.679732E-01
9.326823E+00	3.824472E-01
5.129062E+00	5.737032E-01
2.756974E+00	2.618374E-01
1.433454E+00	2.529930E-02
7.197090E-01	-5.324300E-03
3.503200E-01	-4.618000E-03
1.415820E-01	-4.554000E-04
6.064300E-02	-6.480000E-05
2.519000E-02	9.800000E-06
P 28 1.00	
2.756805E+08	-2.000000E-07
4.609476E+07	-6.000000E-07
9.405828E+06	-1.800000E-06
2.278079E+06	-4.800000E-06
6.390263E+05	-1.210000E-05
2.031933E+05	-2.970000E-05
7.187865E+04	-7.240000E-05
2.783122E+04	-1.787000E-04
1.163097E+04	-4.471000E-04
5.183406E+03	-1.132400E-03
2.437996E+03	-2.840400E-03
1.199494E+03	-6.846900E-03
6.125623E+02	-1.481760E-02
3.224974E+02	-2.664600E-02
1.739582E+02	-3.284090E-02
9.558593E+01	-6.257400E-03
5.320039E+01	6.973080E-02
2.981870E+01	1.523824E-01
1.672716E+01	4.976060E-02
9.326823E+00	-1.918262E-01
5.129062E+00	-3.179031E-01
2.756974E+00	-1.128710E-01
1.433454E+00	3.380900E-01
7.197090E-01	5.363084E-01
3.503200E-01	3.002415E-01
1.415820E-01	4.290370E-02
6.064300E-02	-1.710300E-03
2.519000E-02	1.064000E-03
P 28 1.00	

2.756805E+08	5.000000E-08
4.609476E+07	1.600000E-07
9.405828E+06	4.700000E-07
2.278079E+06	1.260000E-06
6.390263E+05	3.190000E-06
2.031933E+05	7.840000E-06
7.187865E+04	1.915000E-05
2.783122E+04	4.722000E-05
1.163097E+04	1.182200E-04
5.183406E+03	2.992300E-04
2.437996E+03	7.513600E-04
1.199494E+03	1.809000E-03
6.125623E+02	3.921340E-03
3.224974E+02	7.038070E-03
1.739582E+02	8.705700E-03
9.558593E+01	1.594370E-03
5.320039E+01	-1.842683E-02
2.981870E+01	-4.071822E-02
1.672716E+01	-1.267440E-02
9.326823E+00	5.131997E-02
5.129062E+00	8.822408E-02
2.756974E+00	2.819736E-02
1.433454E+00	-1.015484E-01
7.197090E-01	-2.037969E-01
3.503200E-01	-1.210086E-01
1.415820E-01	2.847885E-01
6.064300E-02	5.961411E-01
2.519000E-02	2.845461E-01

P 26 1.00

9.405828E+06	1.000000E-06
2.278079E+06	2.000000E-06
6.390263E+05	5.000000E-06
2.031933E+05	1.100000E-05
7.187865E+04	2.700000E-05
2.783122E+04	6.800000E-05
1.163097E+04	1.690000E-04
5.183406E+03	4.290000E-04
2.437996E+03	1.076000E-03
1.199494E+03	2.590000E-03
6.125623E+02	5.618000E-03
3.224974E+02	1.007600E-02
1.739582E+02	1.247800E-02
9.558593E+01	2.262000E-03
5.320039E+01	-2.633900E-02
2.981870E+01	-5.844100E-02
1.672716E+01	-1.799600E-02
9.326823E+00	7.316900E-02
5.129062E+00	1.275380E-01
2.756974E+00	3.907100E-02
1.433454E+00	-1.435790E-01
7.197090E-01	-3.050420E-01

	3.503200E-01	-1.787740E-01
	1.415820E-01	6.480570E-01
	6.064300E-02	5.242010E-01
	2.519000E-02	2.004900E-02
P 26	1.00	
	9.405828E+06	1.000000E-06
	2.278079E+06	3.000000E-06
	6.390263E+05	8.000000E-06
	2.031933E+05	1.900000E-05
	7.187865E+04	4.600000E-05
	2.783122E+04	1.130000E-04
	1.163097E+04	2.890000E-04
	5.183406E+03	7.090000E-04
	2.437996E+03	1.849000E-03
	1.199494E+03	4.255000E-03
	6.125623E+02	9.737000E-03
	3.224974E+02	1.626600E-02
	1.739582E+02	2.266200E-02
	9.558593E+01	1.790000E-04
	5.320039E+01	-3.690400E-02
	2.981870E+01	-1.137880E-01
	1.672716E+01	-5.035000E-03
	9.326823E+00	8.338200E-02
	5.129062E+00	2.968810E-01
	2.756974E+00	-4.371200E-02
	1.433454E+00	-1.017150E-01
	7.197090E-01	-1.205985E+00
	3.503200E-01	1.173144E+00
	1.415820E-01	8.868500E-01
	6.064300E-02	-1.199702E+00
	2.519000E-02	-2.668200E-02
P 1	1.00	
	2.519000E-02	1.000000E+00
D 19	1.00	
	3.337742E+04	2.810000E-05
	9.004266E+03	1.805000E-04
	3.049558E+03	1.035100E-03
	1.228148E+03	4.789100E-03
	5.621297E+02	1.789980E-02
	2.817336E+02	5.290040E-02
	1.500302E+02	1.266245E-01
	8.287758E+01	2.344967E-01
	4.660527E+01	3.255258E-01
	2.629149E+01	2.925701E-01
	1.471036E+01	1.356091E-01
	8.088891E+00	2.813650E-02
	4.337181E+00	3.878700E-03
	2.250717E+00	1.371100E-03
	1.090234E+00	1.844000E-04
	4.993750E-01	3.290000E-05
	2.180060E-01	-7.100000E-06

	9.104400E-02	2.800000E-06
	3.572800E-02	-1.100000E-06
D 19	1.00	
	3.337742E+04	-1.400000E-05
	9.004266E+03	-8.970000E-05
	3.049558E+03	-5.168000E-04
	1.228148E+03	-2.395400E-03
	5.621297E+02	-9.040300E-03
	2.817336E+02	-2.693470E-02
	1.500302E+02	-6.581350E-02
	8.287758E+01	-1.214854E-01
	4.660527E+01	-1.629359E-01
	2.629149E+01	-9.309150E-02
	1.471036E+01	1.551805E-01
	8.088891E+00	3.946828E-01
	4.337181E+00	3.967364E-01
	2.250717E+00	1.851120E-01
	1.090234E+00	3.168260E-02
	4.993750E-01	9.961000E-04
	2.180060E-01	3.768000E-04
	9.104400E-02	-9.930000E-05
	3.572800E-02	3.790000E-05
D 19	1.00	
	3.337742E+04	2.800000E-06
	9.004266E+03	1.790000E-05
	3.049558E+03	1.033000E-04
	1.228148E+03	4.791000E-04
	5.621297E+02	1.809600E-03
	2.817336E+02	5.402700E-03
	1.500302E+02	1.323220E-02
	8.287758E+01	2.443540E-02
	4.660527E+01	3.255810E-02
	2.629149E+01	1.630290E-02
	1.471036E+01	-4.083290E-02
	8.088891E+00	-9.443950E-02
	4.337181E+00	-9.211620E-02
	2.250717E+00	1.390530E-02
	1.090234E+00	1.951061E-01
	4.993750E-01	3.477603E-01
	2.180060E-01	3.846470E-01
	9.104400E-02	2.655230E-01
	3.572800E-02	6.451070E-02
D 19	1.00	
	3.337742E+04	-3.000000E-06
	9.004266E+03	-2.000000E-05
	3.049558E+03	-1.130000E-04
	1.228148E+03	-5.260000E-04
	5.621297E+02	-1.984000E-03
	2.817336E+02	-5.932000E-03
	1.500302E+02	-1.451500E-02
	8.287758E+01	-2.684400E-02

	4.660527E+01	-3.563000E-02
	2.629149E+01	-1.757600E-02
	1.471036E+01	4.632900E-02
	8.088891E+00	1.050870E-01
	4.337181E+00	1.010330E-01
	2.250717E+00	-2.680200E-02
	1.090234E+00	-2.588300E-01
	4.993750E-01	-4.612510E-01
	2.180060E-01	-3.332500E-02
	9.104400E-02	6.313280E-01
	3.572800E-02	3.279370E-01
D 19	1.00	
	3.337742E+04	4.000000E-06
	9.004266E+03	2.500000E-05
	3.049558E+03	1.470000E-04
	1.228148E+03	6.620000E-04
	5.621297E+02	2.582000E-03
	2.817336E+02	7.456000E-03
	1.500302E+02	1.899100E-02
	8.287758E+01	3.344100E-02
	4.660527E+01	4.747200E-02
	2.629149E+01	1.761800E-02
	1.471036E+01	-5.598200E-02
	8.088891E+00	-1.491330E-01
	4.337181E+00	-1.084140E-01
	2.250717E+00	3.052500E-02
	1.090234E+00	5.360480E-01
	4.993750E-01	3.680330E-01
	2.180060E-01	-1.074801E+00
	9.104400E-02	7.835400E-02
	3.572800E-02	7.010640E-01
D 1	1.00	
	3.572800E-02	1.000000E+00
F 11	1.00	
	6.712408E+02	3.759000E-04
	2.348865E+02	3.294400E-03
	1.006506E+02	1.740650E-02
	4.839611E+01	5.677050E-02
	2.463601E+01	1.388145E-01
	1.279909E+01	2.433081E-01
	6.633614E+00	3.059279E-01
	3.373708E+00	2.948321E-01
	1.653725E+00	2.145462E-01
	7.604970E-01	1.086476E-01
	3.140770E-01	2.756450E-02
F 1	1.00	
	5.588000E-01	1.000000E+00
F 1	1.00	
	1.597000E-01	1.000000E+00
S 1	1.00	
	1.250000E-02	1.000000E+00



P 1 1.00  
1.050000E-02 1.000000E+00  
D 1 1.00  
1.400000E-02 1.000000E+00  
F 1 1.00  
5.050000E-02 1.000000E+00  
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Mo 0  
S 26 1.00  
1.622270E+08 4.300000E-05  
2.568810E+07 1.130000E-04  
5.428430E+06 3.120000E-04  
1.432080E+06 7.130000E-04  
4.465710E+05 1.532000E-03  
1.575650E+05 3.131000E-03  
6.080040E+04 6.349000E-03  
2.501180E+04 1.295700E-02  
1.077100E+04 2.695900E-02  
4.796840E+03 5.657100E-02  
2.193200E+03 1.154950E-01  
1.025760E+03 2.118170E-01  
4.901640E+02 3.050670E-01  
2.393290E+02 2.726880E-01  
1.194130E+02 1.085990E-01  
6.081930E+01 3.119300E-02  
3.151130E+01 3.375500E-02  
1.649190E+01 1.447600E-02  
8.616140E+00 6.679000E-03  
4.414150E+00 6.892000E-03  
2.162700E+00 1.728000E-03  
1.046100E+00 -5.300000E-05  
4.762780E-01 1.200000E-05  
1.268570E-01 -1.000000E-05  
6.386100E-02 6.000000E-06  
2.810700E-02 -2.000000E-06

S 26 1.00  
1.622270E+08 -1.700000E-05  
2.568810E+07 -4.600000E-05  
5.428430E+06 -1.270000E-04  
1.432080E+06 -2.900000E-04  
4.465710E+05 -6.250000E-04  
1.575650E+05 -1.280000E-03  
6.080040E+04 -2.609000E-03  
2.501180E+04 -5.363000E-03  
1.077100E+04 -1.130700E-02  
4.796840E+03 -2.425500E-02  
2.193200E+03 -5.171200E-02  
1.025760E+03 -1.029860E-01  
4.901640E+02 -1.749000E-01  
2.393290E+02 -2.038080E-01

1.194130E+02	-5.247400E-02
6.081930E+01	3.315870E-01
3.151130E+01	5.329750E-01
1.649190E+01	2.456630E-01
8.616140E+00	4.181600E-02
4.414150E+00	2.054100E-02
2.162700E+00	4.537000E-03
1.046100E+00	-2.940000E-04
4.762780E-01	-1.050000E-04
1.268570E-01	-2.500000E-05
6.386100E-02	1.200000E-05
2.810700E-02	-4.000000E-06
S 26 1.00	
1.622270E+08	6.000000E-06
2.568810E+07	1.600000E-05
5.428430E+06	4.500000E-05
1.432080E+06	1.040000E-04
4.465710E+05	2.230000E-04
1.575650E+05	4.580000E-04
6.080040E+04	9.350000E-04
2.501180E+04	1.926000E-03
1.077100E+04	4.090000E-03
4.796840E+03	8.838000E-03
2.193200E+03	1.922200E-02
1.025760E+03	3.941100E-02
4.901640E+02	7.130800E-02
2.393290E+02	8.999600E-02
1.194130E+02	2.297700E-02
6.081930E+01	-2.304730E-01
3.151130E+01	-5.003740E-01
1.649190E+01	-2.664810E-01
8.616140E+00	4.671500E-01
4.414150E+00	7.226830E-01
2.162700E+00	1.735690E-01
1.046100E+00	1.823000E-03
4.762780E-01	2.556000E-03
1.268570E-01	-3.390000E-04
6.386100E-02	2.540000E-04
2.810700E-02	-7.400000E-05
S 26 1.00	
1.622270E+08	-2.000000E-06
2.568810E+07	-6.000000E-06
5.428430E+06	-1.800000E-05
1.432080E+06	-4.000000E-05
4.465710E+05	-8.700000E-05
1.575650E+05	-1.780000E-04
6.080040E+04	-3.640000E-04
2.501180E+04	-7.510000E-04
1.077100E+04	-1.592000E-03
4.796840E+03	-3.444000E-03
2.193200E+03	-7.469000E-03

1.025760E+03	-1.532400E-02
4.901640E+02	-2.760100E-02
2.393290E+02	-3.508300E-02
1.194130E+02	-8.845000E-03
6.081930E+01	9.350100E-02
3.151130E+01	2.216680E-01
1.649190E+01	1.190100E-01
8.616140E+00	-2.618900E-01
4.414150E+00	-6.954170E-01
2.162700E+00	-1.131260E-01
1.046100E+00	7.962080E-01
4.762780E-01	5.331810E-01
1.268570E-01	3.875200E-02
6.386100E-02	-1.374600E-02
2.810700E-02	3.949000E-03
S 26 1.00	
1.622270E+08	1.000000E-06
2.568810E+07	2.000000E-06
5.428430E+06	5.000000E-06
1.432080E+06	1.100000E-05
4.465710E+05	2.400000E-05
1.575650E+05	4.900000E-05
6.080040E+04	9.900000E-05
2.501180E+04	2.050000E-04
1.077100E+04	4.350000E-04
4.796840E+03	9.410000E-04
2.193200E+03	2.039000E-03
1.025760E+03	4.189000E-03
4.901640E+02	7.544000E-03
2.393290E+02	9.613000E-03
1.194130E+02	2.413000E-03
6.081930E+01	-2.582500E-02
3.151130E+01	-6.192600E-02
1.649190E+01	-3.345500E-02
8.616140E+00	7.589800E-02
4.414150E+00	2.199000E-01
2.162700E+00	2.977500E-02
1.046100E+00	-3.303870E-01
4.762780E-01	-3.598590E-01
1.268570E-01	2.478020E-01
6.386100E-02	6.410330E-01
2.810700E-02	3.071470E-01
S 26 1.00	
1.622270E+08	1.000000E-06
2.568810E+07	3.000000E-06
5.428430E+06	9.000000E-06
1.432080E+06	2.100000E-05
4.465710E+05	4.500000E-05
1.575650E+05	9.100000E-05
6.080040E+04	1.890000E-04
2.501180E+04	3.780000E-04

	1.077100E+04	8.380000E-04
	4.796840E+03	1.709000E-03
	2.193200E+03	3.990000E-03
	1.025760E+03	7.466000E-03
	4.901640E+02	1.522600E-02
	2.393290E+02	1.551200E-02
	1.194130E+02	1.078600E-02
	6.081930E+01	-6.327300E-02
	3.151130E+01	-8.715200E-02
	1.649190E+01	-1.252170E-01
	8.616140E+00	2.657180E-01
	4.414150E+00	2.413300E-01
	2.162700E+00	4.142440E-01
	1.046100E+00	-1.549714E+00
	4.762780E-01	2.795180E-01
	1.268570E-01	2.319320E+00
	6.386100E-02	-1.439215E+00
	2.810700E-02	-5.052960E-01
S 26	1.00	
	1.622270E+08	2.000000E-06
	2.568810E+07	5.000000E-06
	5.428430E+06	1.400000E-05
	1.432080E+06	3.200000E-05
	4.465710E+05	6.900000E-05
	1.575650E+05	1.400000E-04
	6.080040E+04	2.920000E-04
	2.501180E+04	5.780000E-04
	1.077100E+04	1.301000E-03
	4.796840E+03	2.600000E-03
	2.193200E+03	6.227000E-03
	1.025760E+03	1.129000E-02
	4.901640E+02	2.402200E-02
	2.393290E+02	2.266500E-02
	1.194130E+02	1.987900E-02
	6.081930E+01	-1.063440E-01
	3.151130E+01	-1.260250E-01
	1.649190E+01	-2.195240E-01
	8.616140E+00	4.965450E-01
	4.414150E+00	3.930060E-01
	2.162700E+00	5.776010E-01
	1.046100E+00	-3.754026E+00
	4.762780E-01	3.863439E+00
	1.268570E-01	-1.220996E+00
	6.386100E-02	-1.145399E+00
	2.810700E-02	1.400924E+00
S 1	1.00	
	2.810700E-02	1.000000E+00
P 21	1.00	
	1.206380E+06	1.500000E-05
	2.000840E+05	5.500000E-05
	4.528180E+04	2.070000E-04

1.301010E+04	7.480000E-04
4.474990E+03	2.655000E-03
1.758500E+03	9.006000E-03
7.612450E+02	2.803200E-02
3.531500E+02	7.710400E-02
1.720400E+02	1.752570E-01
8.673700E+01	3.039310E-01
4.478870E+01	3.475700E-01
2.350440E+01	2.025980E-01
1.245200E+01	4.259100E-02
6.612050E+00	-2.898000E-03
3.487030E+00	-3.677000E-03
1.803300E+00	-5.880000E-04
8.939430E-01	1.800000E-05
4.285930E-01	7.000000E-05
1.701960E-01	2.000000E-06
7.166500E-02	2.000000E-06
2.923900E-02	-1.000000E-06
P 21 1.00	
1.206380E+06	-6.000000E-06
2.000840E+05	-2.300000E-05
4.528180E+04	-8.700000E-05
1.301010E+04	-3.160000E-04
4.474990E+03	-1.126000E-03
1.758500E+03	-3.844000E-03
7.612450E+02	-1.212500E-02
3.531500E+02	-3.418300E-02
1.720400E+02	-8.089600E-02
8.673700E+01	-1.480080E-01
4.478870E+01	-1.740180E-01
2.350440E+01	-1.699700E-02
1.245200E+01	2.938150E-01
6.612050E+00	4.869490E-01
3.487030E+00	2.947520E-01
1.803300E+00	4.736300E-02
8.939430E-01	-3.780000E-04
4.285930E-01	-2.364000E-03
1.701960E-01	-1.630000E-04
7.166500E-02	-6.300000E-05
2.923900E-02	1.500000E-05
P 21 1.00	
1.206380E+06	2.000000E-06
2.000840E+05	8.000000E-06
4.528180E+04	3.200000E-05
1.301010E+04	1.160000E-04
4.474990E+03	4.140000E-04
1.758500E+03	1.413000E-03
7.612450E+02	4.467000E-03
3.531500E+02	1.262800E-02
1.720400E+02	3.007200E-02
8.673700E+01	5.543900E-02

4.478870E+01	6.560200E-02
2.350440E+01	-1.462000E-03
1.245200E+01	-1.396540E-01
6.612050E+00	-2.601410E-01
3.487030E+00	-1.484840E-01
1.803300E+00	2.907740E-01
8.939430E-01	5.350980E-01
4.285930E-01	3.336620E-01
1.701960E-01	5.381200E-02
7.166500E-02	-3.376000E-03
2.923900E-02	1.522000E-03
P 21 1.00	
1.206380E+06	1.000000E-06
2.000840E+05	2.000000E-06
4.528180E+04	9.000000E-06
1.301010E+04	3.200000E-05
4.474990E+03	1.130000E-04
1.758500E+03	3.870000E-04
7.612450E+02	1.226000E-03
3.531500E+02	3.459000E-03
1.720400E+02	8.270000E-03
8.673700E+01	1.519500E-02
4.478870E+01	1.814100E-02
2.350440E+01	-8.960000E-04
1.245200E+01	-3.903700E-02
6.612050E+00	-7.572100E-02
3.487030E+00	-3.972000E-02
1.803300E+00	9.760100E-02
8.939430E-01	2.133040E-01
4.285930E-01	1.173450E-01
1.701960E-01	-2.870540E-01
7.166500E-02	-5.891390E-01
2.923900E-02	-2.888420E-01
P 21 1.00	
1.206380E+06	-1.000000E-06
2.000840E+05	-4.000000E-06
4.528180E+04	-1.400000E-05
1.301010E+04	-4.900000E-05
4.474990E+03	-1.750000E-04
1.758500E+03	-5.950000E-04
7.612450E+02	-1.895000E-03
3.531500E+02	-5.319000E-03
1.720400E+02	-1.278500E-02
8.673700E+01	-2.333600E-02
4.478870E+01	-2.820800E-02
2.350440E+01	1.882000E-03
1.245200E+01	5.916500E-02
6.612050E+00	1.192730E-01
3.487030E+00	5.892000E-02
1.803300E+00	-1.483110E-01
8.939430E-01	-3.626210E-01

	4.285930E-01	-1.214220E-01
	1.701960E-01	6.465160E-01
	7.166500E-02	4.914620E-01
	2.923900E-02	2.922700E-02
P 21	1.00	
	1.206380E+06	-2.000000E-06
	2.000840E+05	-6.000000E-06
	4.528180E+04	-2.200000E-05
	1.301010E+04	-7.800000E-05
	4.474990E+03	-2.890000E-04
	1.758500E+03	-9.480000E-04
	7.612450E+02	-3.137000E-03
	3.531500E+02	-8.432000E-03
	1.720400E+02	-2.132800E-02
	8.673700E+01	-3.646100E-02
	4.478870E+01	-4.958900E-02
	2.350440E+01	1.156700E-02
	1.245200E+01	8.328400E-02
	6.612050E+00	2.325200E-01
	3.487030E+00	5.001700E-02
	1.803300E+00	-2.401780E-01
	8.939430E-01	-1.032742E+00
	4.285930E-01	1.066644E+00
	1.701960E-01	8.318460E-01
	7.166500E-02	-1.122290E+00
	2.923900E-02	-8.228100E-02
P 1	1.00	
	2.923900E-02	1.000000E+00
D 14	1.00	
	2.176180E+03	1.630000E-04
	6.237920E+02	1.445000E-03
	2.317980E+02	8.628000E-03
	1.005040E+02	3.440300E-02
	4.750650E+01	1.016110E-01
	2.351030E+01	2.202730E-01
	1.190780E+01	3.299860E-01
	6.082020E+00	3.348450E-01
	3.080710E+00	1.856540E-01
	1.485250E+00	3.933800E-02
	6.892400E-01	1.410000E-03
	3.073880E-01	4.510000E-04
	1.305320E-01	-9.900000E-05
	5.124600E-02	4.500000E-05
D 14	1.00	
	2.176180E+03	-4.200000E-05
	6.237920E+02	-3.760000E-04
	2.317980E+02	-2.246000E-03
	1.005040E+02	-9.032000E-03
	4.750650E+01	-2.688000E-02
	2.351030E+01	-5.884600E-02
	1.190780E+01	-8.479100E-02

	6.082020E+00	-7.842000E-02
	3.080710E+00	2.572800E-02
	1.485250E+00	2.293670E-01
	6.892400E-01	3.725650E-01
	3.073880E-01	3.577360E-01
	1.305320E-01	2.187660E-01
	5.124600E-02	5.978700E-02
D 14	1.00	
	2.176180E+03	4.300000E-05
	6.237920E+02	3.800000E-04
	2.317980E+02	2.285000E-03
	1.005040E+02	9.154000E-03
	4.750650E+01	2.745300E-02
	2.351030E+01	5.986300E-02
	1.190780E+01	8.570700E-02
	6.082020E+00	7.306700E-02
	3.080710E+00	-4.214800E-02
	1.485250E+00	-2.892500E-01
	6.892400E-01	-3.951860E-01
	3.073880E-01	5.206100E-02
	1.305320E-01	5.781250E-01
	5.124600E-02	3.712160E-01
D 14	1.00	
	2.176180E+03	-6.400000E-05
	6.237920E+02	-5.580000E-04
	2.317980E+02	-3.385000E-03
	1.005040E+02	-1.348500E-02
	4.750650E+01	-4.102600E-02
	2.351030E+01	-8.856200E-02
	1.190780E+01	-1.236640E-01
	6.082020E+00	-8.781100E-02
	3.080710E+00	1.169900E-01
	1.485250E+00	5.726770E-01
	6.892400E-01	1.386100E-01
	3.073880E-01	-9.149480E-01
	1.305320E-01	6.012000E-03
	5.124600E-02	7.291860E-01
D 1	1.00	
	5.124600E-02	1.000000E+00
F 1	1.00	
	1.115600E+00	1.000000E+00
F 1	1.00	
	3.136000E-01	1.000000E+00
S 1	1.00	
	1.240000E-02	1.000000E+00
P 1	1.00	
	1.190000E-02	1.000000E+00
D 1	1.00	
	2.010000E-02	1.000000E+00
F 1	1.00	
	1.190000E-01	1.000000E+00



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