

**Quantum chemical study of the activator contribution to stereoinduction
at the step of alkene insertion into the catalytically active centers
Cp₂ZrMe(Cl)–methylalumoxane**

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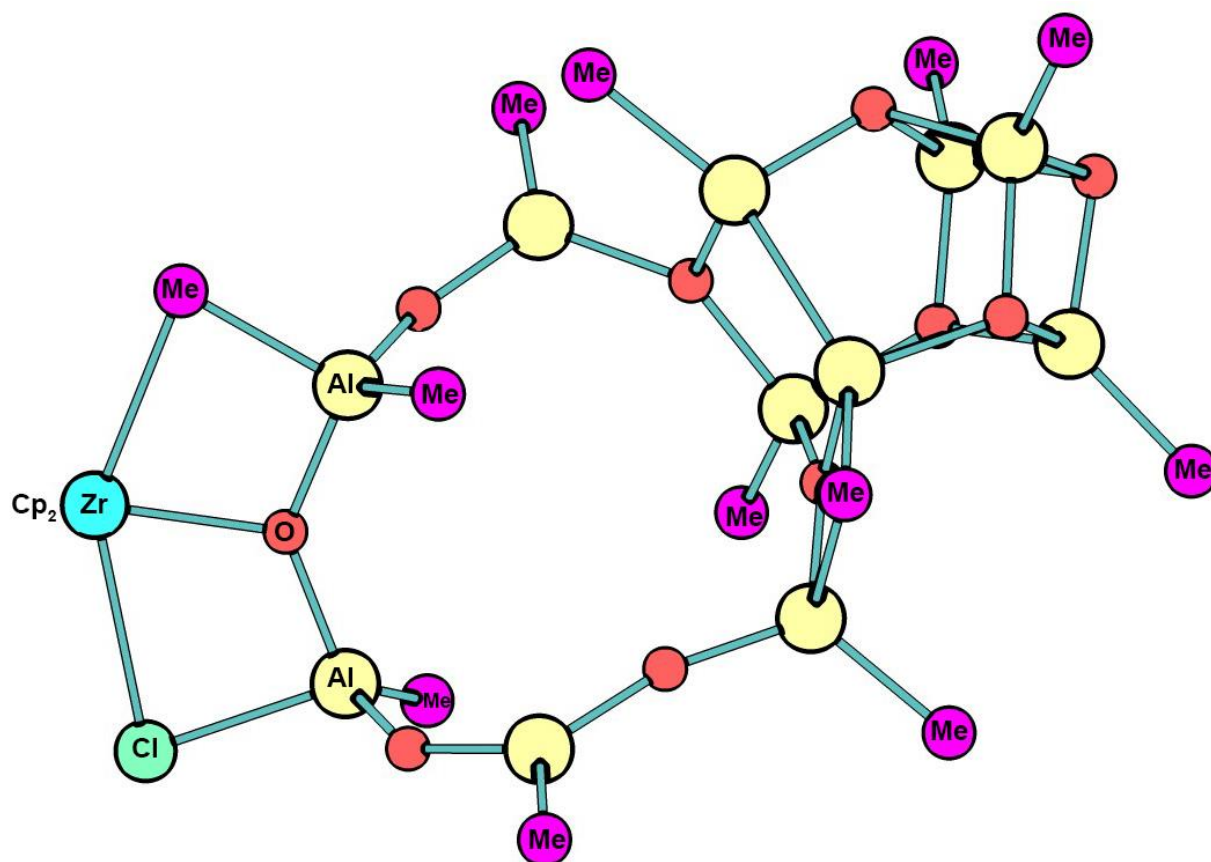
Table S1. Calculated thermodynamic parameters for all optimized compounds and intermediates at $T = 298.15$ K ($[S] = \text{cal mol}^{-1} \text{K}^{-1}$; $[H] = [G] = \text{kcal mol}^{-1}$).

Compound	PBE/3 ζ			M06-2X/cc-pVDZ//cc-pVDZ-PP		
	H	G	S	H	G	S
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1_{SS}	-5198267.2	-5198377.9	371.3	-3007186.2	-3007284.4	329.3
2	-73855.9	-73874.9	63.5	-73894.8	-73913.7	63.2
3A_{RR}	-5272150.3	-5272266.9	390.8	-3081119.4	-3081224.4	352.4
3A_{RS}	-5272140.2	-5272252.7	377.5	-3081115.2	-3081217.8	344.3
3A_{SR}	-5272132.1	-5272249.6	393.8	-3081096.0	-3081199.3	346.5
3A_{SS}	-5272126.4	-5272243.4	392.2	-3081095.6	-3081197.8	342.6
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3B_{SR}	-5272153.9	-5272268.6	384.6	-3081124.8	-3081226.1	340.0
3B_{SS}	-5272150.9	-5272269.3	397.2	-3081119.7	-3081223.4	347.6
4	-147730.0	-147755.8	86.7	-147812.1	-147837.7	85.9
5A_{RR}	-5346019.0	-5346142.2	413.3	-3155034.1	-3155142.7	364.2
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5A_{SR}	-5346005.5	-5346129.1	414.5	-3155013.4	-3155123.3	368.7
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Cartesian coordinates (PBE/3c)

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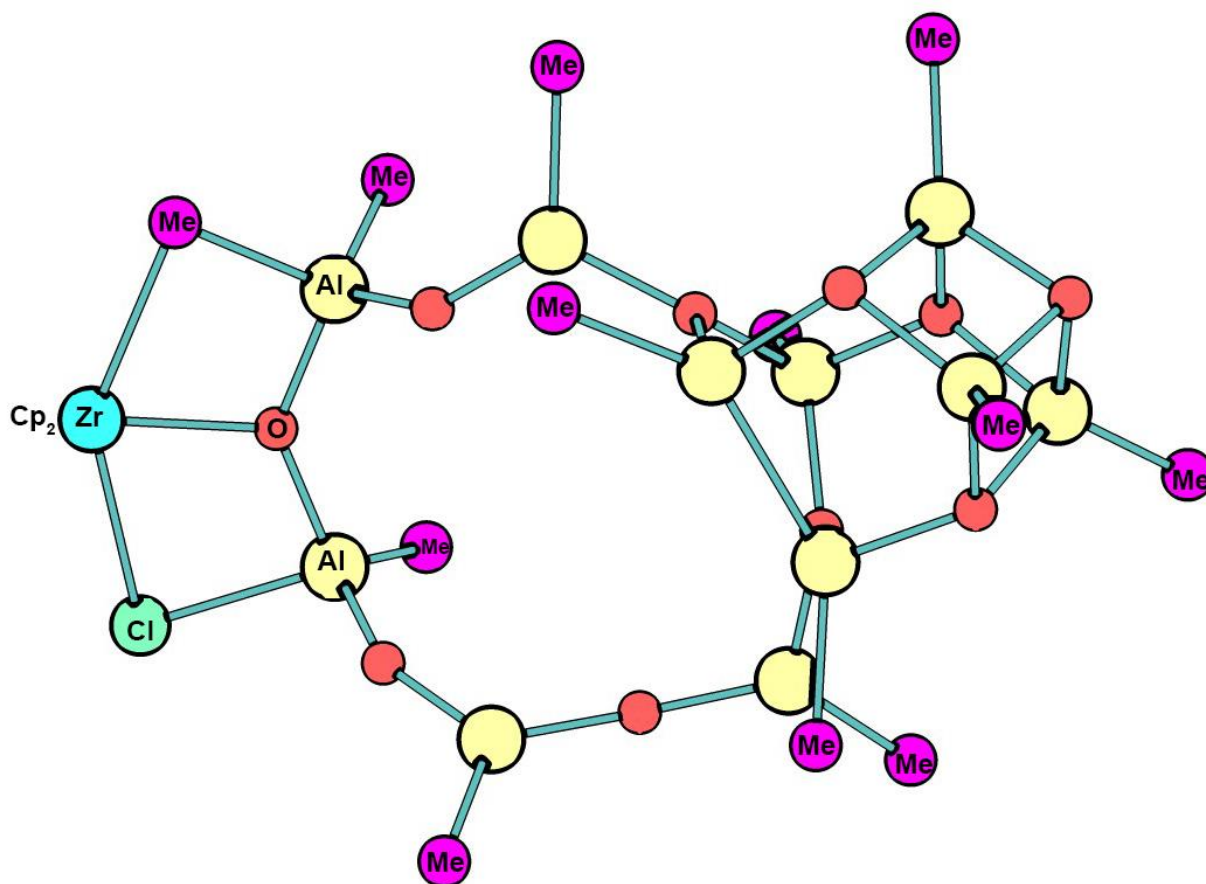


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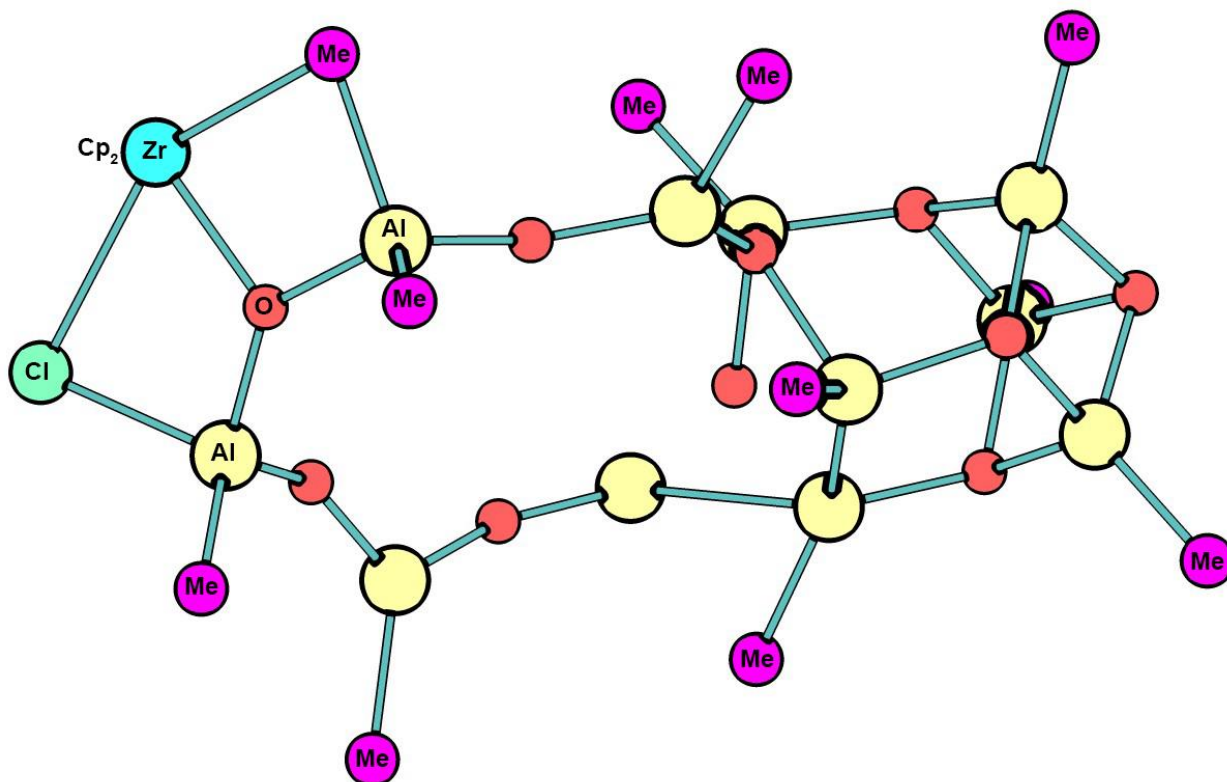


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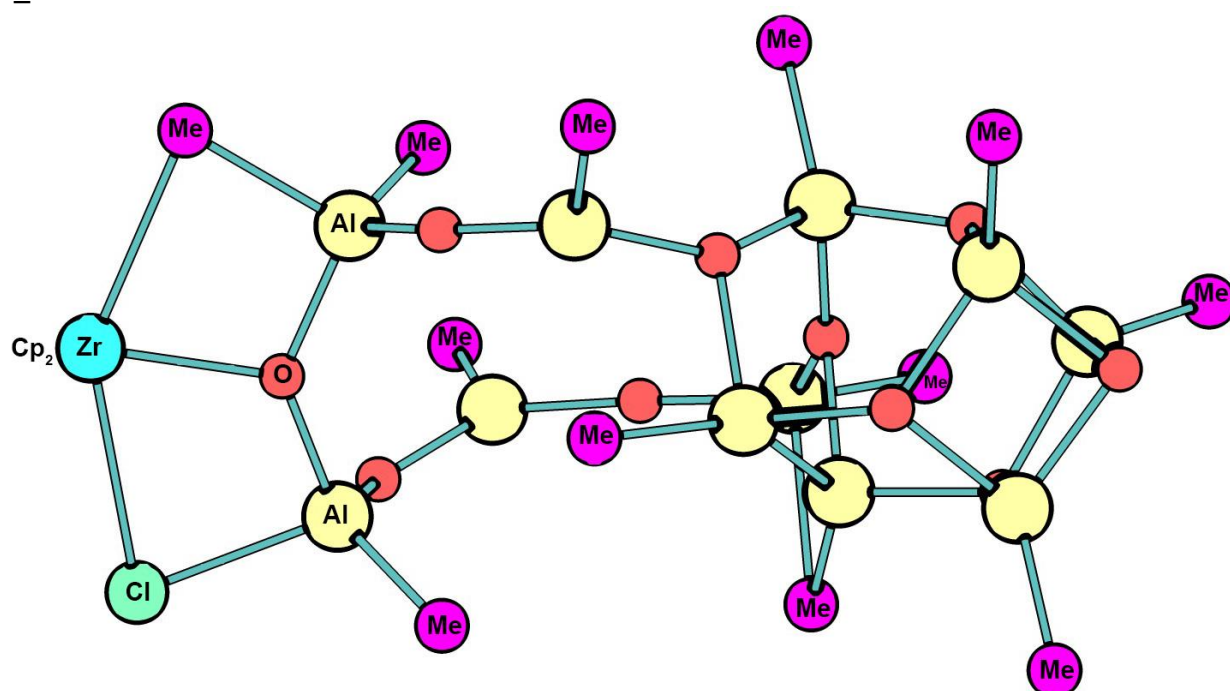


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1 22.85990327 10.54454914 -22.23154610
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6 20.30702552 17.49089231 -24.68295877

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5A_SR

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5A_SS

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5B_RR

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5B_RS

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5B_SR

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5B_SS

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TS(1_{RR}-3A_{RR})

$\nu = 357.75i \text{ cm}^{-1}$

6	32.74407467	9.57996043	-15.16974796
6	32.57071058	8.17208534	-15.26422714
6	31.21620148	7.87550680	-15.00042016
6	30.54476446	9.10117235	-14.70873956
6	31.49075970	10.14754460	-14.80781136
40	31.22790453	9.26102981	-17.17591220
6	30.17071241	11.58163296	-17.37792819
6	31.57726794	11.79363088	-17.49669818
6	32.00197390	11.22026769	-18.71273389
6	30.87431409	10.63926664	-19.35371693
6	29.74091126	10.89944072	-18.54410234
1	33.66703667	10.13602718	-15.31174609
1	33.33632296	7.45885562	-15.55102729
1	30.76513534	6.88807101	-15.01986694
1	29.50721074	9.21238270	-14.41674602
1	31.29888649	11.19878328	-14.62056157
1	29.53443601	11.91984655	-16.56505744
1	32.22289672	12.30311114	-16.78832629
1	33.02556820	11.20208951	-19.06395266
1	30.88052400	10.13003699	-20.31216716
1	28.71873528	10.62219149	-18.78168331
13	37.05879440	9.00641157	-20.19278487
8	35.54517861	8.79199560	-19.33635857
13	34.99155853	9.22980940	-17.61780043
6	38.52488917	9.89069332	-19.25315765
6	35.93938709	8.18805496	-16.23536777
1	38.97162667	9.21744308	-18.50552779
1	38.16792833	10.77974401	-18.71405454
1	39.31955142	10.19211732	-19.94859701
1	35.78827716	7.10457165	-16.36164375
1	35.65848753	8.45118377	-15.20513376
1	37.02219510	8.37520742	-16.31689061
8	33.96380174	6.35778878	-19.77870946
13	33.84612635	8.10052801	-19.76857386
8	33.30243984	8.77914394	-18.12914477
6	33.09708635	8.87313373	-21.42791322
1	32.06655457	8.53990947	-21.62913181

1	33.70243455	8.52720792	-22.28140700
1	33.10220977	9.97298022	-21.45446462
13	33.82496127	4.76417644	-20.32424762
6	32.96865610	3.29954991	-19.35282368
1	33.68351930	2.82808234	-18.66064612
1	32.60326622	2.51438547	-20.02916984
1	32.12396831	3.66475403	-18.75211100
13	33.73200339	4.79369273	-23.29123598
8	34.78163423	4.32477060	-21.77193102
13	36.60105697	4.28578808	-22.05570600
6	31.90574919	5.00072735	-22.49828547
6	37.63902282	4.05059893	-20.40590154
1	31.80903214	5.65886949	-21.61497199
1	31.43264173	4.03575286	-22.25895621
1	31.27466702	5.48452210	-23.26195156
1	37.43445985	4.84199504	-19.66766450
1	38.72172292	4.06760140	-20.60351893
1	37.42053407	3.08821203	-19.91811402
8	33.95112710	3.31404266	-24.37163871
13	35.25253704	2.04895713	-23.98373811
8	36.70173407	3.03031310	-23.36680700
6	34.77708234	0.35864288	-23.13216394
1	35.63770310	-0.32439974	-23.08649388
1	33.97214119	-0.15441050	-23.67815699
1	34.42639875	0.51520012	-22.10090470
13	37.68208461	7.42523272	-23.09365489
6	39.52857927	7.55072669	-23.75031521
1	39.85202648	8.59521817	-23.87591143
1	39.66009229	7.04314361	-24.71797553
1	40.22977501	7.08307483	-23.04157291
8	37.14660578	8.40617354	-21.77667647
13	35.68030836	6.10421288	-24.36561503
8	36.15752914	4.86615784	-25.64066358
13	34.75081061	3.69306877	-26.01634492
6	36.27540220	8.05619036	-24.79680838
6	33.64786395	3.96741347	-27.60393106
1	36.10952968	7.88233974	-25.87718627
1	37.18283081	8.69186153	-24.83832865
1	35.46798456	8.70930426	-24.43758884
1	33.05224977	4.88965122	-27.52810890
1	32.94445347	3.13484336	-27.75112673
1	34.26485720	4.04890440	-28.51077578
8	36.97580362	5.76299216	-23.05065095
13	37.24068459	3.44863314	-25.09999207
8	35.91820944	2.28574182	-25.70446116
6	39.13219617	3.40085637	-25.57526520
1	39.59144330	2.44480409	-25.28464895
1	39.69460380	4.20218561	-25.07331318
1	39.27718188	3.52517679	-26.65824059
6	31.07213260	6.95246136	-18.16298890

1	32.14700533	7.01855738	-17.94110122
1	30.96945245	6.78133834	-19.24016469
1	30.67747751	6.09950302	-17.60687537
17	35.28149249	11.39205025	-17.33568329
6	28.98934953	7.80104122	-18.08808691
6	28.77791442	8.57947574	-16.94315765
1	29.04674200	8.32521710	-19.04571142
1	28.36870657	9.58167422	-17.02393731
1	28.49954177	8.04220025	-16.03609115
6	28.41246517	6.41182209	-18.19929445
1	28.87414528	5.80458533	-18.98652238
1	28.46688333	5.87040900	-17.24565936
1	27.34410654	6.53058957	-18.44832238

TS(1_RS-3A_RS)

$\nu = 440.19 \text{ i cm}^{-1}$

6	26.85764980	15.16582768	-17.10321062
6	27.30754581	14.83939315	-18.41136401
6	27.96088167	13.58821313	-18.35192996
6	27.95594700	13.15409174	-16.99113701
6	27.28563997	14.12971394	-16.22277846
40	25.48893391	13.16198730	-17.79232871
6	24.36188072	13.11962884	-15.49690760
6	23.83894275	14.22705249	-16.23097062
6	23.04048422	13.71630448	-17.29003638
6	23.09894172	12.30359723	-17.23450524
6	23.90390043	11.93458573	-16.11955831
1	26.31280344	16.06513651	-16.83874286
1	27.11852628	15.42690959	-19.30414001
1	28.39627747	13.05405074	-19.19219307
1	28.40132495	12.24106467	-16.60870396
1	27.13261416	14.10220211	-15.14898749
1	24.97456795	13.17288838	-14.60269731
1	23.98717005	15.27958097	-16.01290961
1	22.52302906	14.29229950	-18.05787702
1	22.56962543	11.63092561	-17.90401603
1	24.10286657	10.92171949	-15.78047923
13	21.62293324	13.50648563	-21.25907215
8	22.38220895	14.75623643	-20.31277881
13	24.01933411	15.29403853	-20.24425554
6	20.63979247	12.10391743	-20.23220666
6	24.97302738	15.94529511	-21.85355840
1	21.26770151	11.24877521	-19.92773866
1	19.79626489	11.68602958	-20.80421733
1	20.21065138	12.52924976	-19.31062988
1	24.60821466	16.96202309	-22.07134605
1	24.79392447	15.34041968	-22.75450055
1	26.06281053	16.01969515	-21.71856202
8	23.13421726	12.58180195	-22.09589310
13	24.74302251	12.50667085	-21.22855511

8 24.87825323 13.59893248 -19.73199791
6 26.36537840 12.69651803 -22.35004824
1 27.15861407 13.18981461 -21.76604017
1 26.20135197 13.31662681 -23.24290962
1 26.75620197 11.72708361 -22.69283538
13 22.92875504 11.64178401 -23.61884563
6 24.43068671 10.50044045 -24.18191370
1 25.24746645 11.09299925 -24.61910539
1 24.08083752 9.80816121 -24.96386638
1 24.87019140 9.89006587 -23.37941982
13 20.54232987 11.38473131 -24.86179028
8 22.09020511 12.46204207 -24.97076101
13 21.74892738 13.98474168 -25.91942348
6 21.29986471 10.14346516 -23.31739988
6 23.08124825 15.41958981 -25.77903089
1 21.86949073 10.16850626 -22.36628531
1 21.55659695 9.18989973 -23.80275194
1 20.27659913 10.05344804 -22.91213108
1 23.17160809 15.83448583 -24.76284118
1 22.84109328 16.25702640 -26.45156592
1 24.08380354 15.06074631 -26.05909403
8 20.61255770 10.57434577 -26.51665323
13 21.60389503 11.41788369 -27.84540508
8 21.40868624 13.24905449 -27.54127089
6 23.32901551 10.70684078 -28.41825478
1 23.69987451 11.23286415 -29.31007159
1 23.25916122 9.63786915 -28.66703566
1 24.09167363 10.81364056 -27.63256123
13 20.04770527 15.23975195 -23.70322999
6 19.40951570 17.06386703 -23.44926755
1 19.54415258 17.38757406 -22.40871574
1 18.34288637 17.14636652 -23.70395090
1 19.95473578 17.76222766 -24.10089200
8 20.69612471 14.11283285 -22.62666313
13 18.73790518 13.15124155 -25.34479879
8 18.56537847 12.70855983 -27.12586935
13 19.01933804 10.91855315 -27.44343314
6 17.17944615 13.96360189 -24.42159899
6 17.62100473 9.55694877 -27.51183111
1 16.36209043 13.22710954 -24.36541951
1 16.78931702 14.84580967 -24.95266948
1 17.37439286 14.26217106 -23.37669032
1 17.15805232 9.40287792 -26.52554862
1 18.02242621 8.58748400 -27.84172535
1 16.81935369 9.84276943 -28.20852592
8 20.07001311 14.52505713 -25.35845836
13 19.76723535 13.28459466 -28.40964548
8 20.05482395 11.50707667 -28.87025215
6 19.33039899 14.75333821 -29.61716428
1 20.10453689 14.88414321 -30.38722225

1	19.24360618	15.70495895	-29.07172248
1	18.37334284	14.58107304	-30.13056654
6	24.72492669	10.63193983	-20.25948730
1	24.35173493	9.79334127	-20.84692983
1	24.06784928	10.96641348	-19.45925025
1	25.80467751	10.67900514	-20.15738454
17	24.30493434	16.75811710	-18.61202406
6	25.52460877	9.73486890	-18.30513517
6	26.28972703	10.79135406	-17.72438058
1	24.53606499	9.54427943	-17.87748467
1	27.34544642	10.76256175	-18.01208560
1	26.15919843	10.85669064	-16.63433676
6	26.18049591	8.52440361	-18.90726845
1	26.51648326	7.88487003	-18.07048994
1	25.49899874	7.93118978	-19.52726332
1	27.07288549	8.78579770	-19.49094560

TS(1_SR-3A_SR)

$\nu = 401.37i \text{ cm}^{-1}$

6	26.54997064	6.53198749	-8.30572781
6	26.86142524	5.15624337	-8.49632965
6	26.54750016	4.82391070	-9.83196114
6	26.00739681	5.98278840	-10.46924424
6	25.99498810	7.02907425	-9.52093196
40	28.46947504	6.53432038	-9.92326540
6	28.15374195	8.84807273	-10.94100689
6	28.40952039	9.01728626	-9.54698641
6	29.76272889	8.66629165	-9.30419735
6	30.34037145	8.26633467	-10.53226467
6	29.34891829	8.38429112	-11.54442370
1	26.71106340	7.08937116	-7.38748349
1	27.33549564	4.51430283	-7.75268734
1	26.68256665	3.84690032	-10.28777326
1	25.65977492	6.04634552	-11.49660330
1	25.62477090	8.03558460	-9.68757246
1	27.21914177	9.05639533	-11.45315075
1	27.71246372	9.37669021	-8.79682910
1	30.23611680	8.65406570	-8.32761509
1	31.36947142	7.94622529	-10.66526732
1	29.48945070	8.18359578	-12.60253493
13	28.52482552	3.10081971	-5.09113343
8	28.78987035	4.27941794	-6.29492571
13	29.86497782	5.57999659	-6.74878134
6	29.04259414	3.36605519	-3.21509331
6	31.69315114	5.48314832	-5.99365664
1	30.10623532	3.11825507	-3.07109736
1	28.46012774	2.73003670	-2.53393291
1	28.91549928	4.41449715	-2.91019045
1	32.30551301	6.37440011	-6.18711300
1	32.26551905	4.59606873	-6.29897146

1	31.55613677	5.42632861	-4.90021038
8	31.81298751	3.39248598	-8.65305603
13	31.59425299	5.02894192	-9.21467561
8	29.89620231	5.66190781	-8.66037326
6	33.06361359	6.35563337	-8.99957618
1	33.55633210	6.57997779	-9.95931101
1	33.83528601	5.94933162	-8.32870490
1	32.73296711	7.30948540	-8.56246815
13	32.37473681	1.83014061	-9.04068150
6	33.67206544	1.52123049	-10.48578066
1	33.18925177	1.63074449	-11.47045489
1	34.12153869	0.51854570	-10.45648277
1	34.48921748	2.25709847	-10.44621486
13	32.18314014	-0.34669487	-7.29413133
8	31.24350483	0.47029148	-8.70580053
13	29.55925011	-0.18134135	-8.97904533
6	33.72202009	0.98967886	-7.14869987
6	28.46620686	0.89866223	-10.20538171
1	33.66190578	2.09474080	-7.24270594
1	34.63278539	0.66147204	-7.66951737
1	33.92189826	0.89444878	-6.06638166
1	28.45891878	1.94929765	-9.87472135
1	27.42136612	0.55751688	-10.25459241
1	28.86556655	0.87043806	-11.23123469
8	32.63076921	-1.95843293	-8.07177237
13	31.75232321	-2.45820934	-9.63786792
8	29.99166182	-1.89346362	-9.43481842
6	32.62416939	-2.33090424	-11.37945064
1	32.07792643	-2.91958062	-12.13130236
1	33.65459659	-2.71316866	-11.34279874
1	32.67020321	-1.29380910	-11.74243400
13	27.61749329	0.02996749	-6.10929907
6	25.89601048	-0.90216290	-6.21515857
1	25.25017349	-0.66293614	-5.35760876
1	26.01611040	-1.99499372	-6.25439424
1	25.34925244	-0.60265662	-7.12296642
8	27.75811644	1.63339007	-5.53972407
13	30.07545637	-1.22666709	-6.09345791
8	30.20305792	-2.96295101	-6.68802604
13	31.94280396	-3.44202774	-7.17148775
6	28.95384689	-1.07243927	-4.38958873
6	33.06132473	-4.44625223	-5.92605589
1	29.31102085	-2.02531823	-3.95521403
1	27.86332645	-1.15739913	-4.21110861
1	29.31381022	-0.26076983	-3.74372083
1	33.32676812	-3.84471933	-5.04363061
1	34.00138012	-4.76584503	-6.39900979
1	32.54453149	-5.34756147	-5.56477797
8	28.85696508	-0.47968987	-7.32063371
13	29.57342321	-3.37168378	-8.39078923

8	31.26364693	-4.04047616	-8.78857294
6	27.87023516	-4.29383947	-8.62833182
1	27.72581251	-4.60163384	-9.67427020
1	27.02140041	-3.64916843	-8.35533577
1	27.81153635	-5.19711678	-8.00392409
6	31.22169113	4.84682454	-11.28861789
1	32.10203793	4.46888911	-11.81096888
1	31.01581855	5.90113656	-11.45207501
1	30.40674053	4.13876306	-11.17445329
17	28.98713445	7.53003122	-6.11092956
6	29.61227099	5.15606370	-12.93966174
6	28.42513193	5.49385242	-12.23358837
1	30.17877617	5.96942054	-13.39965847
1	27.94530667	6.41586923	-12.58581046
1	27.72592790	4.65965250	-12.14313765
6	29.76230779	3.82761574	-13.62354045
1	30.80114457	3.59645448	-13.88382047
1	29.34539139	3.00851705	-13.02270293
1	29.18077840	3.86868405	-14.56294392

TS(1_SS-3A_SS)

$\nu = 397.35i \text{ cm}^{-1}$

6	24.42961775	7.77993735	-8.08233158
6	25.11204447	6.62008900	-7.62167263
6	25.78477351	6.04908260	-8.72599224
6	25.48022093	6.82622595	-9.88584121
6	24.64157979	7.88806180	-9.48885554
40	26.87228948	8.33850506	-8.31245059
6	26.66382370	10.44834003	-9.72404946
6	25.91992144	10.66388477	-8.52859079
6	26.83782364	10.74455417	-7.44852787
6	28.14561206	10.57456076	-7.96617159
6	28.03910788	10.39943945	-9.37135936
1	23.84038699	8.44187797	-7.45684337
1	25.16561915	6.27095650	-6.58956025
1	26.41234964	5.16207668	-8.69706666
1	25.82752992	6.63556067	-10.89656905
1	24.22796282	8.65238018	-10.13976934
1	26.25631038	10.36413947	-10.72746850
1	24.84299292	10.77126066	-8.44738354
1	26.56401200	10.86027212	-6.40453623
1	29.05753778	10.55922278	-7.37380631
1	28.86624418	10.27470425	-10.06396426
13	26.63977256	5.09793198	-3.42844166
8	26.06298619	6.30211838	-4.50835526
13	26.50697699	7.97169895	-4.76939969
6	26.29316015	3.20397941	-3.81491220
6	27.50097729	8.89918014	-3.33593264
1	25.66638082	3.07506453	-4.70796267
1	25.78915520	2.71431481	-2.96834939

1	27.23638575	2.66078863	-3.97846153
1	28.37920619	8.34962351	-2.97026623
1	26.80380320	9.01421635	-2.49030008
1	27.82552865	9.90490086	-3.63636054
8	30.18761358	8.95201343	-5.16507206
13	29.35165143	7.61075124	-5.88887702
8	27.55732808	7.96853738	-6.38135236
6	29.39184395	5.81494646	-5.03246731
1	28.66348524	5.14725259	-5.52146910
1	29.16624801	5.85694655	-3.95458465
1	30.38358227	5.34656243	-5.12974223
13	31.31914975	9.45588806	-3.97396641
6	33.06487808	10.17679805	-4.51962111
1	33.72218250	9.36651958	-4.87335140
1	33.59105925	10.68662012	-3.69950293
1	32.96333552	10.89256698	-5.34925254
13	30.42860552	9.97613932	-1.42409026
8	31.29676613	8.60082017	-2.37904789
13	31.43713023	7.03591003	-1.43523230
6	30.35035953	11.37279905	-2.93530148
6	32.19425055	5.48054615	-2.36051898
1	30.05888400	11.28790513	-4.00044981
1	31.19034595	12.07938642	-2.87080159
1	29.46287468	11.89170692	-2.52798071
1	31.49029769	5.00020596	-3.05441181
1	32.50685515	4.71772171	-1.63074229
1	33.09068081	5.75485889	-2.93801784
8	31.68180323	10.47397183	-0.16749434
13	33.10397758	9.32650564	0.16858391
8	32.38328587	7.62404262	0.01235682
6	34.89086131	9.70973408	-0.51772184
1	35.64066187	9.04364508	-0.06618102
1	35.19161692	10.74527849	-0.30194267
1	34.94292849	9.57108896	-1.60791001
13	28.29376939	5.81362756	-0.51608770
6	28.26734607	4.52595934	0.96373118
1	27.24652353	4.16899324	1.16558074
1	28.67039331	4.94285239	1.89795885
1	28.87215162	3.64071519	0.71147007
8	27.42505557	5.52030763	-1.96133351
13	29.08630928	8.39778898	0.08779384
8	30.11551836	8.62724478	1.59973046
13	31.04364650	10.25033718	1.57697922
6	27.20857818	7.70876900	0.53462688
6	30.34627119	11.78565762	2.56228686
1	27.12433779	7.37126085	1.57760006
1	26.51513476	7.09853593	-0.07738026
1	26.70793303	8.69302960	0.47796485
1	29.40830436	12.15706119	2.12262011
1	31.06205453	12.62076103	2.56103451

1	30.13620845	11.52594238	3.61022763
8	29.78956985	6.81519067	-0.66237190
13	31.70767959	7.67857744	1.74131240
8	32.59278396	9.30167446	1.95694781
6	31.85447059	6.12131827	2.90838129
1	32.90298548	5.80925217	3.02249262
1	31.29774946	5.26109617	2.50794313
1	31.45817431	6.33214727	3.91228109
6	30.24486089	7.41938440	-7.77960963
1	31.32237669	7.28885125	-7.66765093
1	29.94916449	8.41090069	-8.11672369
1	29.70207645	6.53768243	-8.10410214
17	24.70875902	9.22992961	-5.12305738
6	29.80307440	7.47033787	-10.06363949
6	28.38556244	7.39691592	-10.12686192
1	30.26862674	8.44887147	-10.20603472
1	27.93195107	8.15033106	-10.78513947
1	28.01829785	6.38582431	-10.31916678
6	30.67235313	6.31028387	-10.45444936
1	31.70214749	6.40865780	-10.09380633
1	30.25681352	5.35264639	-10.11471716
1	30.70475946	6.27692692	-11.55916085

TS(1_{RR}-3B_{RR})

$\nu = 487.99 \text{ i cm}^{-1}$

6	32.55342220	6.13086567	-16.20600630
6	31.65094949	6.40676111	-17.26510975
6	30.46070540	6.92347302	-16.69647192
6	30.61255219	6.94287452	-15.27911320
6	31.90173599	6.44186171	-14.97802803
40	32.33077932	8.67471726	-16.20115985
6	32.14598129	10.52475143	-14.38390721
6	32.47609803	9.33394556	-13.69975096
6	33.77626049	8.93224532	-14.12654668
6	34.25970269	9.91289314	-15.03770231
6	33.25030963	10.88427379	-15.21470066
1	33.56130780	5.73938199	-16.31460764
1	31.86516963	6.28486484	-18.32428033
1	29.56926908	7.22158920	-17.24098248
1	29.87034073	7.27772701	-14.55930450
1	32.32205691	6.31498307	-13.98533642
1	31.21563883	11.07739099	-14.28697229
1	31.84356167	8.80659696	-12.99204650
1	34.32628735	8.06242661	-13.77831786
1	35.21756800	9.88668552	-15.54823524
1	33.30388764	11.73322200	-15.89056971
13	34.57893659	9.58638086	-22.16899828
8	34.19747771	9.04383035	-20.47250195
13	34.60188870	9.70502662	-18.80446471
6	34.41349635	11.48199403	-22.63201479

6	36.52420842	9.59416734	-18.38366542
1	35.31312172	12.03154616	-22.31543779
1	33.55624435	11.96132913	-22.13974132
1	34.31457933	11.62120964	-23.71937946
1	36.84069349	8.56216103	-18.16705106
1	36.79243939	10.21318278	-17.51386673
1	37.13802564	9.95379934	-19.22422686
8	32.57414195	6.45085243	-20.66977558
13	32.66387348	8.16207889	-20.87749281
8	33.47244271	8.79788789	-17.75643324
6	32.51328410	8.72894254	-22.86912245
1	31.79858636	7.90908838	-23.06923131
1	33.22292852	8.59508219	-23.70753774
1	31.96863494	9.66810941	-23.04137725
13	32.95755124	4.79441645	-20.90589733
6	32.25144987	3.42051284	-19.69943751
1	32.77050282	3.45285982	-18.72877227
1	32.38250070	2.40626999	-20.10379485
1	31.18073744	3.56566187	-19.49358202
13	33.88363014	4.10677179	-23.42448604
8	34.53573431	4.44801251	-21.69121019
13	36.33929039	4.75779787	-21.60968797
6	31.87427020	4.14588087	-22.99232750
6	37.01196823	5.38531102	-19.88013615
1	31.28403494	4.88670879	-22.41814633
1	31.48928107	3.14744876	-22.73771604
1	31.53342549	4.36131452	-24.02159378
1	36.55828332	6.34442019	-19.58822251
1	38.10252313	5.53180928	-19.89359628
1	36.79635052	4.66310182	-19.07777977
8	34.49214258	2.40097784	-23.74027792
13	35.83025251	1.72219878	-22.63509550
8	36.93817887	3.16566822	-22.26742862
6	35.40142446	0.42531974	-21.24194834
1	36.31343721	0.01543742	-20.78405498
1	34.82117879	-0.41840330	-21.64279204
1	34.80632397	0.88142498	-20.43662208
13	36.99071573	7.55076835	-23.47111680
6	38.84263555	8.08736120	-23.80267492
1	38.89491435	9.00413916	-24.40766776
1	39.41856054	7.30508129	-24.31745254
1	39.35376843	8.30003384	-22.85090958
8	35.77264191	8.61967438	-22.93976260
13	35.80114297	5.32837722	-24.64009155
8	36.70988091	3.81252482	-25.14227765
13	35.61982282	2.29773740	-25.22799657
6	36.26117259	6.95536802	-25.78115079
6	34.91606836	1.69466066	-26.94621369
1	35.51560584	6.79698374	-26.58174314
1	37.24875601	6.87866797	-26.25997685

1	36.08542927	8.01875465	-25.52953641
1	34.19698995	2.41474319	-27.36508447
1	34.39552294	0.73066195	-26.84937256
1	35.72062220	1.56806461	-27.68532425
8	36.69572667	5.82297038	-23.05511064
13	37.81963752	2.99052989	-23.89261498
8	36.85401541	1.42055037	-24.15931888
6	39.75565995	3.20499989	-23.99468336
1	40.27003238	2.55088829	-23.27578567
1	40.05541940	4.23973774	-23.77051366
1	40.13517480	2.96271954	-24.99791778
6	31.08346141	9.07601884	-19.82364405
1	31.06141710	8.23264418	-19.13867340
1	30.29632188	9.15312055	-20.57160448
1	31.71544668	9.94011689	-19.61610720
17	33.83542288	11.78899161	-18.85306605
6	29.90904620	10.07092347	-18.32308370
6	30.51043281	10.09861987	-17.01533527
1	29.09897923	9.35094540	-18.46372020
1	30.90752501	11.08897626	-16.77044532
1	29.82013694	9.72135000	-16.24479971
6	29.71010970	11.37910964	-19.04805685
1	29.36646919	11.25175925	-20.08191166
1	28.94261062	11.95307965	-18.50139146
1	30.63083291	11.97853670	-19.04386744

TS(1_RS-3B_RS)

$\nu = 389.23 \text{ i cm}^{-1}$

6	27.07980408	14.45279440	-17.98114340
6	27.59850014	13.22248882	-18.45271706
6	27.60858973	12.30526452	-17.36871239
6	27.09133457	12.96551751	-16.22440039
6	26.76316926	14.29862403	-16.60589532
40	25.09703914	12.84099248	-17.81190139
6	23.50449987	11.98563325	-15.95300093
6	23.99958144	13.23313500	-15.51922311
6	23.53038414	14.23181009	-16.42189231
6	22.70056943	13.59652830	-17.38742767
6	22.70677973	12.21083122	-17.11705784
1	26.89504448	15.34677361	-18.56897261
1	27.93141459	13.03244139	-19.46844725
1	27.97610753	11.28368419	-17.39877554
1	26.99061712	12.53730108	-15.23151160
1	26.36384798	15.07561623	-15.96223951
1	23.69309411	11.02698735	-15.47888219
1	24.62993592	13.40140403	-14.65165935
1	23.73731266	15.29650299	-16.38564525
1	22.21210079	14.08063499	-18.23526167
1	22.18315523	11.45181167	-17.69217775
13	20.51878351	14.86433660	-20.81937871

8 22.08662923 14.75924744 -20.16269005
 13 23.80067498 15.06251431 -20.30538799
 6 19.00609918 14.24823174 -19.72192170
 6 24.47214548 15.73968613 -22.03549946
 1 19.23359006 14.30179253 -18.64778303
 1 18.75997731 13.19896437 -19.95058160
 1 18.09892661 14.84012451 -19.91069061
 1 23.82651677 16.59898897 -22.28357320
 1 24.39911616 15.03051355 -22.87051898
 1 25.50293302 16.11640297 -21.98697245
 8 24.16502196 12.35978392 -22.48649746
 13 25.44685433 12.69650287 -21.34522103
 8 24.70498940 13.45368073 -19.77526259
 6 27.10571484 13.59721432 -21.98551599
 1 27.38414018 14.47959147 -21.39086088
 1 26.95932338 13.94795298 -23.01834299
 1 27.96908969 12.91262918 -21.99762201
 13 23.77081866 11.60840173 -23.96181451
 6 24.98919665 10.38540098 -24.89606441
 1 25.77821628 10.95259378 -25.41469494
 1 24.47755385 9.77125354 -25.65015580
 1 25.49308014 9.70678158 -24.19193947
 13 21.00804149 11.08267646 -24.57724428
 8 22.43283128 12.28480874 -24.93431137
 13 21.94556666 13.79380978 -25.86653506
 6 21.93667540 9.81152293 -23.30084233
 6 23.32347317 15.17258217 -26.05519033
 1 22.57512819 10.19559858 -22.48066778
 1 22.46517766 8.98196111 -23.79371157
 1 21.08906196 9.36154027 -22.75506490
 1 23.58870385 15.64280944 -25.09695852
 1 22.98484972 15.97375753 -26.73002092
 1 24.25091447 14.76557742 -26.48685665
 8 20.70634162 10.36459733 -26.25212422
 13 21.43900909 11.19553504 -27.74576879
 8 21.31752468 13.01250134 -27.39134545
 6 23.01376668 10.46657755 -28.63991322
 1 23.14197870 10.91797715 -29.63480130
 1 22.93231788 9.37843747 -28.77648190
 1 23.93554620 10.66068088 -28.07198328
 13 19.61458920 15.50926078 -23.99699906
 6 18.90924538 17.14189769 -24.81788003
 1 18.27852392 17.71269675 -24.12079456
 1 18.31525037 16.93017296 -25.71917628
 1 19.73545976 17.80404738 -25.12019959
 8 20.20698011 15.45962505 -22.39319397
 13 19.17031321 12.89412933 -24.76086578
 8 18.58410470 12.44131443 -26.44547650
 13 18.97795898 10.67099665 -26.88691312
 6 17.74922521 13.93263660 -23.71567821

6	17.60852794	9.29030592	-26.70512053
1	16.88720512	13.42285081	-24.18583391
1	17.42729341	14.99165253	-23.77843121
1	17.74782984	13.66758731	-22.65045518
1	17.34138562	9.12204181	-25.65087924
1	17.95282677	8.32875853	-27.11328299
1	16.68653981	9.56862641	-27.23634008
8	20.36003972	14.31076830	-25.11844319
13	19.53750038	13.06229444	-27.91624115
8	19.72598904	11.29298657	-28.46585749
6	18.86320967	14.55165050	-28.98135992
1	19.45966659	14.69378392	-29.89426608
1	18.89898214	15.49505463	-28.41602773
1	17.81910021	14.38971090	-29.28604300
6	25.99922034	10.80513732	-20.59954614
1	26.71261709	11.15803417	-19.86016763
1	26.42656001	10.16767635	-21.37547030
1	24.98498760	10.55493288	-20.30325092
17	24.39429615	16.54239731	-18.74312684
6	25.91106098	9.50525472	-18.66246867
6	25.22187428	10.30743119	-17.71334649
1	27.00080550	9.46406844	-18.59909332
1	25.76098822	10.43154974	-16.76479456
1	24.17927875	10.00934040	-17.57694811
6	25.27695719	8.28202200	-19.26001834
1	25.32609357	7.47659761	-18.50431963
1	24.21562524	8.44186163	-19.49182898
1	25.79518954	7.92924360	-20.15844339

TS(1_SR-3B_SR)

$\nu = 351.84i \text{ cm}^{-1}$

6	25.77485823	12.77401259	-17.04336692
6	27.12138863	12.32670633	-17.10398288
6	27.38588123	11.59962318	-15.91731861
6	26.19204922	11.53695572	-15.15540090
6	25.19582818	12.28400258	-15.85424990
40	25.68801013	10.17690035	-17.26294389
6	24.63915179	8.29917567	-15.86164233
6	23.81897935	9.43908786	-15.70019318
6	23.20833654	9.72523956	-16.95310455
6	23.63273937	8.73370032	-17.87987328
6	24.52734163	7.86706824	-17.21796812
1	25.27557061	13.37167433	-17.79539891
1	27.80789175	12.53450494	-17.91765168
1	28.34233821	11.16734518	-15.64130366
1	26.07344721	11.04954333	-14.19186981
1	24.17477669	12.45996615	-15.52934947
1	25.21221369	7.81715803	-15.07840145
1	23.66620713	9.98775605	-14.77700054
1	22.49813039	10.52672738	-17.13667482

1 23.36103645 8.68828758 -18.92907349
1 25.04331374 7.02311126 -17.66543636
13 23.18873018 14.55669388 -20.47386965
8 23.96041356 12.95754131 -20.77864985
13 23.20315172 11.77625623 -19.59781737
6 21.57075883 14.90536540 -21.53256900
6 21.71593945 10.60743201 -20.12634331
1 21.83386921 15.23019577 -22.55177419
1 20.96042275 15.70267485 -21.08323091
1 20.93522433 14.01344499 -21.63166474
1 21.20410170 10.11726579 -19.28600965
1 22.04704104 9.82326906 -20.82409763
1 20.96042747 11.21094868 -20.65206900
8 26.99426678 13.03682799 -20.28234389
13 25.60921948 12.06167376 -20.65878863
8 24.83913955 11.17846601 -19.16842571
6 25.77851715 10.92064233 -22.27012391
1 26.70934328 10.33284308 -22.28288759
1 25.77064446 11.53555280 -23.18531744
1 24.94597760 10.20645821 -22.37107827
13 28.49911027 13.72237457 -20.71780592
6 30.19017112 12.76728591 -20.41673148
1 30.40701993 12.69248431 -19.33898496
1 31.04741540 13.27572784 -20.88144594
1 30.15360034 11.74103995 -20.81205738
13 28.29918756 15.90552257 -22.39223334
8 28.57074439 15.51560350 -20.57232912
13 28.12973739 16.87385535 -19.42993379
6 28.56416049 14.00970895 -23.13198810
6 28.11644839 16.42823702 -17.52056774
1 28.08167341 13.05686597 -22.83727040
1 29.62019663 13.79264005 -23.35064717
1 28.07138610 14.19052753 -24.10478384
1 27.35985607 15.66631675 -17.27920830
1 27.89868983 17.31157210 -16.90107067
1 29.09048407 16.03698635 -17.18895736
8 29.70254691 17.03649256 -22.75135644
13 30.60517335 17.79269158 -21.30786141
8 29.30463057 18.13544531 -20.02759622
6 32.35661641 17.11664944 -20.77495306
1 32.81415322 17.75314081 -20.00366965
1 33.04930917 17.07502313 -21.62798348
1 32.28260248 16.09975167 -20.36100016
13 24.79789804 17.44678224 -19.85785865
6 23.96659380 18.82740246 -18.74251150
1 22.87211021 18.84046558 -18.85114774
1 24.34421057 19.83348057 -18.97696610
1 24.18158899 18.63826535 -17.67916159
8 24.20499454 15.84974182 -19.99229337
13 26.54223077 17.73718197 -21.97504573

8	27.66517419	19.16739972	-22.25690078
13	29.13391442	18.72286953	-23.32568624
6	24.55716941	18.16352281	-22.21599609
6	29.12094458	19.15060365	-25.23075005
1	24.69149650	19.01796936	-22.90531326
1	23.79424074	18.56837142	-21.52082702
1	24.06198964	17.35930512	-22.77630066
1	28.37246812	18.55489654	-25.77472060
1	30.09872921	18.94837844	-25.69201082
1	28.88299330	20.21075273	-25.40147982
8	26.57783494	17.57489310	-20.09903104
13	28.78701346	19.70468470	-20.87236595
8	30.22817495	19.46772553	-22.02734262
6	28.37861114	21.30082232	-19.82691824
1	29.19952916	21.54950113	-19.13872036
1	27.47214026	21.15874720	-19.21953565
1	28.20790051	22.17397233	-20.47320221
6	26.82481185	9.13168061	-19.25629247
1	27.61765969	9.65316634	-19.80315980
1	25.86383067	9.43828376	-19.69222768
1	26.91779161	8.05160559	-19.38665740
17	22.35202763	13.50977581	-18.34185296
6	28.19692139	8.89823414	-17.47322572
6	27.48529133	8.64695677	-16.29394982
1	28.67455477	9.87639782	-17.57334923
1	27.66698984	9.23741466	-15.40121988
1	27.20302844	7.60998511	-16.10861656
6	28.93572885	7.79408668	-18.18596849
1	29.87620302	7.63318957	-17.63161850
1	28.37782510	6.84873860	-18.16381103
1	29.19590549	8.03691617	-19.22250886

TS(1_SS-3B_SS)

$v = 300.94i \text{ cm}^{-1}$

6	26.61864236	5.60084081	-8.33452147
6	27.89189177	5.35373016	-8.90710677
6	27.85451992	5.78958435	-10.25545435
6	26.57000738	6.33388129	-10.51189807
6	25.80134733	6.20788087	-9.31665887
40	27.57748236	7.94649272	-8.83611900
6	26.69715779	9.91303274	-10.26458362
6	25.54479716	9.29864510	-9.73060612
6	25.55842284	9.47590801	-8.32393240
6	26.70881785	10.24815190	-7.99308412
6	27.42033246	10.50590298	-9.18054367
1	26.31755345	5.40342125	-7.31278944
1	28.73865648	4.89741179	-8.40468506
1	28.67036087	5.71040297	-10.96694222
1	26.22695602	6.74494627	-11.45675879
1	24.76819299	6.50455387	-9.16882416

1	26.94803770	9.97259035	-11.31719300
1	24.78000518	8.77970595	-10.29939648
1	24.78931591	9.11965801	-7.64462543
1	27.01053744	10.53716378	-6.99221334
1	28.34789531	11.06597885	-9.25784673
13	26.40270399	6.59990700	-2.52827590
8	26.82821834	7.14355537	-4.13341740
13	25.90240656	8.04819862	-5.45536634
6	24.59703644	6.96652023	-1.87579574
6	25.37746521	9.84962556	-4.83575121
1	23.85534695	6.86222410	-2.68048005
1	24.52175480	7.99730355	-1.49610842
1	24.32224021	6.28916270	-1.05565702
1	26.24995169	10.43834607	-4.51068600
1	24.71585785	9.74523731	-3.96066168
1	24.82407174	10.44906450	-5.57245778
8	29.51903170	8.21803081	-4.49720267
13	28.39683800	7.07387536	-5.18672401
8	27.34210635	7.79034372	-6.54726433
6	28.99425110	5.18736584	-5.31049836
1	28.28165868	4.53695988	-5.84077988
1	29.07868500	4.78353222	-4.28784892
1	29.98002872	5.05565294	-5.78192231
13	30.84287589	8.96091698	-3.75743791
6	32.18424664	10.03375172	-4.69755972
1	32.88142338	9.37716123	-5.24160294
1	32.78148847	10.65458830	-4.01550921
1	31.71448776	10.69479081	-5.44043724
13	30.37012781	9.69086049	-0.94614241
8	31.23631883	8.44351223	-2.09020984
13	31.63812108	6.82076601	-1.32046939
6	29.76509541	11.07674136	-2.26758706
6	32.27795757	5.45466312	-2.57294782
1	29.23520811	10.73914168	-3.18010470
1	30.56145259	11.77162298	-2.57478835
1	29.00402800	11.68116413	-1.74599671
1	31.53553842	5.21084273	-3.34759717
1	32.51971836	4.51699464	-2.04957197
1	33.19619411	5.77662660	-3.08805700
8	31.76916061	10.16955136	0.15859939
13	33.32580792	9.15576687	0.14748375
8	32.76486587	7.39082672	-0.00883463
6	34.90845517	9.76934385	-0.81551723
1	35.77094521	9.11346964	-0.62789733
1	35.19187389	10.78835778	-0.51458732
1	34.73637923	9.78348803	-1.90230149
13	28.63879886	5.45118661	-0.28886100
6	28.73009535	3.64922960	0.47550937
1	27.73161966	3.21301200	0.62756647
1	29.25519331	3.63578404	1.44221962

1	29.27610154	2.97240669	-0.19984398
8	27.59680226	5.80857749	-1.61646575
13	29.48534740	7.85733389	0.64864721
8	30.71566390	8.07223183	1.99599359
13	31.48124086	9.78052205	1.95991754
6	27.75557832	6.93057652	1.31744846
6	30.83205940	11.16242913	3.17657658
1	27.91707587	7.29464817	2.35009008
1	27.41789130	5.89407547	1.52023119
1	26.88168643	7.46007125	0.91465584
1	29.80241691	11.46503369	2.93327544
1	31.45872590	12.06489291	3.12656973
1	30.83334148	10.81108928	4.21880639
8	30.17682641	6.39523049	-0.31374500
13	32.38912910	7.27921360	1.80553096
8	33.14826118	8.96673473	1.99158091
6	32.84537752	5.67169552	2.81270909
1	33.90830262	5.41455941	2.69688000
1	32.25883531	4.80567209	2.47100017
1	32.64792002	5.79951749	3.88689805
6	29.82726094	7.77766290	-7.77990476
1	29.45419023	6.86346817	-7.29805811
1	30.89367763	7.60028025	-7.91956964
1	29.70836267	8.64523190	-7.11772117
17	24.15381142	6.83848866	-6.01946708
6	30.22745324	8.15772027	-10.00177850
6	29.13807483	8.48385186	-10.80857311
1	30.58596569	7.12776315	-10.01829931
1	29.03787520	9.52894877	-11.09076889
1	28.75862722	7.76878980	-11.53322075
6	31.26987227	9.21213216	-9.71807692
1	31.98441772	8.92798531	-8.93771904
1	31.83494713	9.38523389	-10.64861675
1	30.80935571	10.16801615	-9.43515268

TS(1_{RR}-5A_{RR})

$\nu = 280.50i \text{ cm}^{-1}$

6	24.97389988	11.26106143	-15.21849615
6	25.87877686	10.19320630	-14.99761508
6	25.21197077	9.22132741	-14.20489224
6	23.88421276	9.65792626	-13.98610611
6	23.73799706	10.93187944	-14.61567113
40	23.98227055	9.24236048	-16.49726134
6	21.88046846	7.79047883	-16.27598421
6	21.46166284	9.10271771	-15.96106881
6	21.57253889	9.89368842	-17.13213803
6	22.02513168	9.05521440	-18.18875720
6	22.22687890	7.76292346	-17.66430171
1	25.18989040	12.14603141	-15.80318368
1	26.90438420	10.15078313	-15.34960734

1 25.65449130 8.31503855 -13.80931302
1 23.12965705 9.13523543 -13.40640607
1 22.84722916 11.55181970 -14.61839120
1 21.88431474 6.94970892 -15.59165640
1 21.11112823 9.44379620 -14.99226288
1 21.28481479 10.93573980 -17.22717109
1 22.21845979 9.38629898 -19.20412216
1 22.58404267 6.89983244 -18.21905948
13 24.71573115 14.49426805 -20.37754243
8 24.65895947 13.26644363 -19.11990736
13 23.22604386 12.51356548 -18.22581280
6 24.18937583 14.09106879 -22.21256515
6 22.53703645 13.60534288 -16.72955155
1 24.94190301 13.45556339 -22.70300273
1 24.07543759 15.00747092 -22.80677021
1 23.24046254 13.53708217 -22.22305261
1 23.28317112 13.79859096 -15.94436033
1 21.64424537 13.17972443 -16.24650119
1 22.22954535 14.58645595 -17.12587002
8 27.05333465 12.00837624 -17.82879619
13 25.70057194 11.69789774 -18.89032438
8 24.24276941 11.02758755 -17.95404167
6 26.18806316 11.06988402 -20.70600107
1 26.86821108 10.20524909 -20.68070352
1 26.70823182 11.85915542 -21.27652208
1 25.30772668 10.78005699 -21.30032869
13 28.52760803 12.58841976 -17.22008426
6 29.60251793 11.56617559 -15.93497738
1 29.16786551 11.63826588 -14.92519138
1 30.63627926 11.93391087 -15.86704250
1 29.64278534 10.49871037 -16.19848642
13 29.94423549 14.55960961 -18.69759709
8 28.77638977 14.36521628 -17.22560274
13 27.98538892 15.91594627 -16.64528933
6 30.22161670 12.60602934 -19.17027062
6 26.55168052 15.68372500 -15.32904236
1 29.40272711 11.86123964 -19.23325617
1 31.06209121 12.14020411 -18.63511399
1 30.52738810 12.68442444 -20.22856687
1 25.68512373 15.16058272 -15.76123719
1 26.18908015 16.65025847 -14.94764461
1 26.88560979 15.10130712 -14.45663745
8 31.39350099 15.37158421 -17.90144609
13 31.18698756 16.09062761 -16.19576267
8 29.48656276 16.83752980 -16.17332420
6 31.86852621 15.14679437 -14.62971750
1 31.82471900 15.78166615 -13.73275349
1 32.91492879 14.83918841 -14.76989290
1 31.28352059 14.23929556 -14.41819576
13 26.20166882 17.32719667 -19.26085340

6	25.37826990	19.06507565	-18.88467488
1	24.69834977	19.38072860	-19.68976220
1	26.12877936	19.85765181	-18.74635818
1	24.78164956	19.01802725	-17.96048211
8	25.29138034	16.02614809	-19.91816933
13	28.86478841	16.75850995	-19.50668329
8	30.14748283	17.89888855	-18.84910521
13	31.79629647	17.05402417	-18.60186049
6	27.76681962	17.60005425	-21.03348147
6	33.20531532	17.25106993	-19.93862673
1	28.63215078	18.18008215	-21.40717600
1	26.97129251	18.37031447	-21.08556000
1	27.52130867	16.84786897	-21.79460694
1	32.93288388	16.76948354	-20.88983477
1	34.14580029	16.79395580	-19.59779652
1	33.40714227	18.31069388	-20.15340453
8	27.54716308	16.82634539	-18.16790486
13	30.07430356	18.36650546	-17.04720345
8	31.80735123	17.71164358	-16.86904235
6	29.42715365	20.12565397	-16.50644318
1	29.57393933	20.29202971	-15.42936551
1	28.35220383	20.23831525	-16.71270564
1	29.95114908	20.92995958	-17.04284928
6	25.75895097	8.73713363	-18.18821313
1	26.40118948	9.57351728	-17.87497944
1	25.03050553	9.05154316	-18.94818581
1	26.40486504	7.99761560	-18.66171001
17	21.66944351	12.27484336	-19.76308896
6	25.68978050	6.90709746	-16.81814897
6	24.62423860	6.80536701	-15.91994029
1	25.55166560	6.40624414	-17.77661310
1	24.82360009	6.81032839	-14.85188428
1	23.77971540	6.19545822	-16.22459245
6	27.12454411	6.97788672	-16.35134704
1	27.76258793	7.46632961	-17.10172383
1	27.19846509	7.57415776	-15.43037591
6	27.67356084	5.56211343	-16.07884055
1	27.05725050	5.06928066	-15.30943807
1	27.57721426	4.94959520	-16.99163864
6	29.14014555	5.57619030	-15.63180298
1	29.23727538	6.19731343	-14.72581306
1	29.75126416	6.06683144	-16.40727710
6	29.68964660	4.17414242	-15.35498906
1	29.63525026	3.54237011	-16.25386201
1	29.11681662	3.67304994	-14.56073086
1	30.74052242	4.21226931	-15.03633452

TS(1_RS-5A_RS)

$\nu = 432.24i \text{ cm}^{-1}$

6	26.85177855	15.20031444	-17.10032732
---	-------------	-------------	--------------

6 27.29649990 14.88128461 -18.41207021
6 27.95869954 13.63421803 -18.36042056
6 27.96408251 13.19553367 -17.00149254
6 27.29132953 14.16399981 -16.22587674
40 25.49155477 13.18980384 -17.78804231
6 24.37169572 13.13960413 -15.48967135
6 23.84100108 14.24568388 -16.22009244
6 23.04196001 13.73280037 -17.27754968
6 23.10708652 12.32030058 -17.22452898
6 23.91765093 11.95325765 -16.11298791
1 26.30254123 16.09513306 -16.82977216
1 27.09856743 15.47067466 -19.30167158
1 28.39213918 13.10558061 -19.20516827
1 28.41739787 12.28403272 -16.62482267
1 27.14407159 14.13149369 -15.15140108
1 24.98745984 13.19452085 -14.59764981
1 23.98519001 15.29856639 -16.00101997
1 22.51953622 14.30763334 -18.04272771
1 22.57992900 11.64620162 -17.89427872
1 24.12413045 10.94078481 -15.77744245
13 21.61800173 13.50608349 -21.24902943
8 22.37184834 14.76354306 -20.30924868
13 24.00745657 15.30633374 -20.24219826
6 20.63960261 12.10473785 -20.21602414
6 24.95940145 15.95967696 -21.85170284
1 21.27180595 11.25499649 -19.90545861
1 19.80005002 11.67900472 -20.78812136
1 20.20560798 12.53221013 -19.29778018
1 24.57953475 16.96819480 -22.08160547
1 24.79758468 15.34357511 -22.74832066
1 26.04681210 16.05350293 -21.70949827
8 23.13135009 12.58342106 -22.08215986
13 24.74262298 12.51636271 -21.21743184
8 24.87316950 13.61747474 -19.72740648
6 26.35809502 12.71371834 -22.34855278
1 27.12865853 13.27318615 -21.79505354
1 26.16979157 13.27329902 -23.27594633
1 26.78986766 11.74337539 -22.63605614
13 22.92963985 11.63763065 -23.60143160
6 24.43352877 10.49380052 -24.15484510
1 25.25055287 11.08442818 -24.59413988
1 24.08610317 9.79607029 -24.93302946
1 24.87225433 9.88920708 -23.34756559
13 20.54763631 11.37569092 -24.85250910
8 22.09599086 12.45222770 -24.96003719
13 21.75714699 13.97394732 -25.91118543
6 21.29882154 10.13951087 -23.30166982
6 23.09009703 15.40812585 -25.77160238
1 21.86635381 10.16815858 -22.34935443
1 21.55760435 9.18436686 -23.78284152

1 20.27467649 10.05017191 -22.89856232
1 23.18280057 15.82114569 -24.75491562
1 22.84856318 16.24677322 -26.44216214
1 24.09182059 15.04939568 -26.05475249
8 20.62234507 10.56153909 -26.50557504
13 21.61778439 11.40328579 -27.83224041
8 21.42071404 13.23492111 -27.53260783
6 23.34475358 10.69134308 -28.39857305
1 23.71866072 11.21603569 -29.28988613
1 23.27538109 9.62202646 -28.64603151
1 24.10471545 10.79912418 -27.61040417
13 20.04448406 15.22822871 -23.69984275
6 19.40707061 17.05305913 -23.44858944
1 19.46594415 17.34961549 -22.39305384
1 18.36522789 17.15777985 -23.78403010
1 20.01135842 17.75939501 -24.03674996
8 20.69006104 14.10112981 -22.62141941
13 18.74484471 13.14050278 -25.34520570
8 18.57649023 12.69492370 -27.12596343
13 19.03201554 10.90432081 -27.43773135
6 17.18335159 13.95486489 -24.42817391
6 17.63382042 9.54257220 -27.50807549
1 16.37193859 13.21298523 -24.35846099
1 16.78513996 14.82576671 -24.97180057
1 17.37699646 14.27113123 -23.38815928
1 17.16671281 9.39147519 -26.52329137
1 18.03679486 8.57217476 -27.83332120
1 16.83508027 9.82619850 -28.20899218
8 20.07669022 14.51501226 -25.35564119
13 19.78249445 13.26824173 -28.40685417
8 20.07191466 11.48987166 -28.86260355
6 19.34950174 14.73452017 -29.61884082
1 20.12440791 14.86162003 -30.38873229
1 19.26449068 15.68774607 -29.07591050
1 18.39235153 14.56307309 -30.13232966
6 24.73416992 10.64542385 -20.24375581
1 24.35474166 9.80420100 -20.82359823
1 24.08397698 10.98096438 -19.43815796
1 25.81536285 10.68793104 -20.15075092
17 24.28704436 16.77435795 -18.61166575
6 25.53694457 9.76322166 -18.29101149
6 26.30163483 10.82958102 -17.72273990
1 24.55351201 9.56949935 -17.85025543
1 27.35349267 10.80619068 -18.02721475
1 26.19260571 10.89172815 -16.62997033
6 26.19297420 8.53914933 -18.87659633
1 25.49744571 7.99645932 -19.53170188
1 27.06800268 8.82728554 -19.48004192
6 26.65163643 7.59553695 -17.74103245
1 27.37136816 8.12344842 -17.09528963

1	25.78786214	7.33905105	-17.10429378
6	27.28809929	6.30635147	-18.27610808
1	28.14409739	6.56626554	-18.92024999
1	26.56375891	5.78302199	-18.92132776
6	27.75061947	5.37213230	-17.15481954
1	26.90615725	5.06409414	-16.52092779
1	28.49046949	5.86640934	-16.50800223
1	28.21399030	4.46198808	-17.55951225

TS(1_SR-5A_SR)

$\nu = 387.16 \text{ i cm}^{-1}$

6	26.50232953	6.75211053	-8.34084666
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6	26.52986056	4.91688801	-9.71136123
6	26.00524050	6.01619298	-10.45796625
6	25.97598033	7.14174240	-9.60747589
40	28.46381882	6.60196910	-9.90073138
6	28.23687158	8.90225571	-10.97594786
6	28.43361217	9.09864510	-9.57726634
6	29.76466720	8.71888862	-9.26354658
6	30.38909493	8.28159777	-10.45646894
6	29.44822212	8.39872312	-11.51454858
1	26.63980935	7.38245961	-7.46764719
1	27.26126518	4.77442875	-7.60136052
1	26.67718000	3.90483552	-10.07917396
1	25.67996868	5.99120372	-11.49401188
1	25.61619494	8.13106138	-9.87204332
1	27.33177504	9.12065071	-11.53488674
1	27.71017424	9.49142895	-8.87013954
1	30.19270826	8.71308252	-8.26594331
1	31.41348713	7.93000673	-10.53382910
1	29.63068736	8.16957765	-12.56035081
13	28.52156145	3.06594462	-5.12202294
8	28.76435064	4.26066274	-6.31548220
13	29.84838639	5.55962732	-6.75676013
6	29.06965425	3.31688522	-3.25222335
6	31.67246400	5.44674085	-5.99450756
1	30.13751966	3.07744268	-3.12743737
1	28.50351416	2.67122236	-2.56635416
1	28.93925084	4.36183945	-2.93664306
1	32.29090029	6.33558968	-6.17934845
1	32.24019425	4.55895576	-6.30633239
1	31.53237642	5.38181101	-4.90196130
8	31.75588729	3.37694970	-8.67919301
13	31.56701855	5.02092761	-9.23203770
8	29.87977378	5.67290269	-8.66575671
6	33.06123698	6.31638366	-8.98999628
1	33.54787368	6.56569132	-9.94669650
1	33.83250986	5.87161746	-8.34327171
1	32.75391128	7.25942725	-8.51436425

13	32.33085488	1.82064834	-9.07043180
6	33.62110749	1.52179681	-10.52408892
1	33.12584593	1.60950047	-11.50476823
1	34.09110401	0.52879367	-10.48767500
1	34.42334434	2.27454312	-10.50132444
13	32.17639981	-0.35103269	-7.31024380
8	31.22072152	0.44730223	-8.72225316
13	29.54434347	-0.22782707	-8.98750527
6	33.70279669	0.99970183	-7.18017678
6	28.42830854	0.83030406	-10.21166284
1	33.62724965	2.10344311	-7.27726144
1	34.61194085	0.68075395	-7.70952789
1	33.91533725	0.90991425	-6.09982018
1	28.38365578	1.87632648	-9.86925089
1	27.39550008	0.45589623	-10.27279059
1	28.83517281	0.82913514	-11.23490051
8	32.63916537	-1.96261778	-8.07972398
13	31.76197475	-2.48462513	-9.63873993
8	29.99625933	-1.93781140	-9.43385946
6	32.62753729	-2.35938220	-11.38376717
1	32.08176937	-2.95299259	-12.13204903
1	33.65990565	-2.73654547	-11.34905180
1	32.66739601	-1.32310693	-11.74985968
13	27.61385606	-0.01074331	-6.11545350
6	25.89705635	-0.95362237	-6.19935119
1	25.25581760	-0.70850187	-5.34002770
1	26.02309999	-2.04612285	-6.22733989
1	25.34259733	-0.66706418	-7.10664217
8	27.74966017	1.60116421	-5.56951535
13	30.08285188	-1.24755779	-6.09597330
8	30.22854191	-2.98649568	-6.67906389
13	31.97206425	-3.44687294	-7.16545680
6	28.96584830	-1.08999121	-4.38948440
6	33.11062598	-4.42619296	-5.91822943
1	29.33176834	-2.03619926	-3.94786441
1	27.87634494	-1.18264044	-4.20863648
1	29.32042780	-0.27023630	-3.75087457
1	33.36334490	-3.81777294	-5.03677745
1	34.05732086	-4.72494264	-6.39170211
1	32.61524473	-5.33868186	-5.55544170
8	28.85112389	-0.52673371	-7.32538193
13	29.59810169	-3.41297866	-8.37724541
8	31.29433542	-4.06596118	-8.77588289
6	27.90424102	-4.35540760	-8.60236420
1	27.75451067	-4.66338672	-9.64748614
1	27.05020647	-3.72119940	-8.32117602
1	27.86159763	-5.26013775	-7.97875211
6	31.20181852	4.86425368	-11.30465464
1	32.07120305	4.47246135	-11.83544666
1	31.00995745	5.92077499	-11.47166567

1	30.37617512	4.16802163	-11.18996691
17	28.96976534	7.50378677	-6.10187128
6	29.56700955	5.18175043	-12.92439573
6	28.39958069	5.54185484	-12.19365244
1	30.13073977	5.98478537	-13.40777416
1	27.91619303	6.45968015	-12.55405407
1	27.69775761	4.71176213	-12.07762481
6	29.68104165	3.84912559	-13.61649836
1	30.73225279	3.60378302	-13.82111502
1	29.26951804	3.05379135	-12.97531860
6	28.90289852	3.87321475	-14.95234313
1	27.84051574	4.08683532	-14.75348150
1	29.27632641	4.69982360	-15.58071383
6	29.02882312	2.55297163	-15.72289599
1	28.66432199	1.72815413	-15.08894679
1	30.09402614	2.34565778	-15.91648465
6	28.25740010	2.56717761	-17.04521385
1	28.62382446	3.36303130	-17.71033538
1	27.18429291	2.74025930	-16.87694910
1	28.36181317	1.61216698	-17.57831440

TS(1_SS-5A_SS)

$\nu = 388.21 \text{ i cm}^{-1}$

6	24.39671191	7.76296929	-8.06231107
6	25.08935022	6.61072487	-7.59771427
6	25.76011357	6.03724754	-8.70192973
6	25.44447394	6.80470437	-9.86520821
6	24.60063829	7.86341232	-9.47051675
40	26.83532866	8.33607405	-8.30989189
6	26.59632158	10.43363870	-9.73462698
6	25.86997667	10.65489509	-8.52914329
6	26.80438009	10.74974634	-7.46463523
6	28.10446568	10.58127319	-8.00140550
6	27.97686504	10.39447564	-9.40348573
1	23.80604693	8.42517364	-7.43840718
1	25.15123664	6.26983612	-6.56319414
1	26.39401983	5.15483833	-8.67057060
1	25.78837532	6.60996364	-10.87632721
1	24.17829408	8.62071538	-10.12401543
1	26.17382801	10.33898031	-10.73083962
1	24.79387097	10.75668941	-8.43146274
1	26.54618537	10.87287959	-6.41759055
1	29.02589526	10.57682102	-7.42401282
1	28.79349813	10.26733982	-10.10789667
13	26.61805324	5.12287426	-3.42026871
8	26.03613747	6.33188034	-4.49168299
13	26.48275495	7.99974482	-4.76145627
6	26.26558500	3.23060340	-3.81062474
6	27.48049850	8.92899652	-3.33140302
1	25.65126436	3.10395317	-4.71260599

1	25.74526646	2.74588414	-2.97100697
1	27.20762630	2.68096883	-3.95840725
1	28.35899593	8.37888374	-2.96707227
1	26.78547551	9.04624130	-2.48425321
1	27.80609860	9.93380500	-3.63393284
8	30.16694177	8.95157712	-5.16473193
13	29.32122525	7.61846155	-5.89246708
8	27.52766343	7.98657341	-6.37628537
6	29.34951532	5.82025343	-5.03939528
1	28.60443964	5.16562854	-5.52124064
1	29.13839932	5.86408842	-3.95849987
1	30.33233778	5.33625902	-5.14991577
13	31.31129203	9.45182871	-3.98564380
6	33.05511221	10.16685105	-4.54507700
1	33.70796288	9.35314676	-4.89922859
1	33.58766394	10.67846512	-3.73020350
1	32.95034590	10.87940666	-5.37702516
13	30.44748531	9.97690600	-1.42596184
8	31.29905413	8.59779110	-2.39044927
13	31.43219488	7.02727371	-1.45499666
6	30.36008912	11.37530123	-2.93363361
6	32.17122831	5.47014457	-2.39173163
1	30.06154639	11.28909491	-3.99688391
1	31.20269171	12.07939595	-2.87663473
1	29.47647634	11.89742496	-2.52217755
1	31.46163192	5.00246823	-3.08843438
1	32.47559522	4.69900307	-1.66722192
1	33.07041353	5.73858398	-2.96768476
8	31.71504653	10.46145128	-0.17615107
13	33.12820221	9.29750414	0.14530592
8	32.39286535	7.60170371	-0.01167556
6	34.91327309	9.66788898	-0.55290890
1	35.65911764	8.98639673	-0.11815875
1	35.22884735	10.69659697	-0.32585970
1	34.95277977	9.54398102	-1.64540533
13	28.28679466	5.82583152	-0.51363183
6	28.26082228	4.53955386	0.96755352
1	27.23845693	4.19189793	1.17776897
1	28.67478341	4.95369318	1.89823247
1	28.85568987	3.64870518	0.71142151
8	27.40789039	5.53692757	-1.95318769
13	29.10346201	8.40195151	0.08836094
8	30.14368525	8.61664501	1.59499249
13	31.08447139	10.23224149	1.57041044
6	27.22227619	7.72773359	0.54340137
6	30.40453081	11.76863655	2.56654878
1	27.13968824	7.39084829	1.58668999
1	26.52083596	7.12367193	-0.06565430
1	26.72998458	8.71630732	0.48872627
1	29.46723037	12.14925786	2.13337008

1	31.12676586	12.59818621	2.56485434
1	30.19785384	11.50628908	3.61449176
8	29.78906266	6.81621706	-0.67067671
13	31.72930081	7.65515527	1.72197107
8	32.62875081	9.27023987	1.93702258
6	31.87354652	6.09263856	2.88237746
1	32.92084005	5.77356385	2.98816315
1	31.30864133	5.23747207	2.48261603
1	31.48548317	6.30229346	3.88973319
6	30.20941404	7.42970566	-7.78449050
1	31.28858899	7.30944130	-7.67634920
1	29.90605602	8.41815252	-8.12463051
1	29.67576502	6.54170295	-8.10813905
17	24.68567925	9.25837900	-5.12010894
6	29.76311596	7.48099572	-10.06157310
6	28.34444713	7.39104554	-10.11765664
1	30.21523661	8.46548901	-10.21495693
1	27.87813219	8.12500739	-10.78912409
1	27.99007768	6.37175088	-10.29380372
6	30.64915444	6.33359369	-10.46844384
1	31.65463351	6.44586100	-10.04035230
1	30.23217555	5.38343415	-10.09965646
6	30.76484518	6.27081182	-12.00910581
1	29.76369754	6.12845537	-12.44659264
1	31.13856842	7.23675255	-12.38940327
6	31.69805345	5.14656253	-12.47612499
1	31.32739974	4.18393122	-12.08721709
1	32.69571178	5.29499594	-12.03158096
6	31.81811160	5.07488279	-14.00067537
1	32.21787508	6.01332611	-14.41221034
1	30.83900030	4.89512330	-14.46848193
1	32.48993551	4.26209116	-14.30904833

TS(1_{RR}-5B_{RR})

$\nu = 484.20\text{i cm}^{-1}$

6	27.87965551	7.27044577	-23.93122112
6	28.57107429	8.49824726	-23.76648343
6	27.64300821	9.45780016	-23.29247766
6	26.36549678	8.83324115	-23.18967140
6	26.51167635	7.48566133	-23.59629635
40	27.87516416	7.66675212	-21.40911978
6	26.16910089	7.33766452	-19.47452227
6	25.60227866	6.71423227	-20.60848389
6	26.43914011	5.61618304	-20.96564938
6	27.49403089	5.54229513	-20.01311481
6	27.34233683	6.61300587	-19.10486027
1	28.31671274	6.33416663	-24.26776280
1	29.63530293	8.65027081	-23.93071723
1	27.85593098	10.50094284	-23.07701970
1	25.44438619	9.30803109	-22.86215292

1	25.72087551	6.74372827	-23.64492241
1	25.77433111	8.21257597	-18.96559597
1	24.70214771	7.02843251	-21.12821309
1	26.27424568	4.92331202	-21.78606967
1	28.30404298	4.81924508	-20.01852354
1	28.02348318	6.85241903	-18.29297054
13	34.26762100	7.74138043	-20.64258874
8	32.53663038	7.44989612	-21.12828605
13	31.13437309	6.53375454	-20.36834258
6	34.67808775	8.21608786	-18.78731298
6	31.41569781	4.58292770	-20.34742434
1	34.70538089	7.31274546	-18.15904980
1	33.92553338	8.88680214	-18.35028014
1	35.66453311	8.69762714	-18.70610058
1	31.28749467	4.13597627	-21.34538519
1	30.71966060	4.07374305	-19.66333426
1	32.43129621	4.32988610	-20.00501783
8	32.08514090	8.82310513	-23.82993920
13	32.34870572	8.95174109	-22.12904042
8	29.73586519	7.15422552	-21.29417253
6	34.17028207	9.84057094	-21.67391127
1	34.08444461	10.50581457	-22.55314888
1	35.20429620	9.46625810	-21.79704059
1	34.15537996	10.48974467	-20.78699471
13	32.40889381	8.41884842	-25.46643822
6	30.99980274	8.52851760	-26.82470874
1	30.28818109	7.69559967	-26.71265577
1	31.40350163	8.47482364	-27.84624821
1	30.41851323	9.45847927	-26.74032266
13	35.07605886	8.40569986	-26.20817806
8	33.70354194	7.20351981	-25.74257981
13	34.28880450	5.52233839	-25.31126608
6	33.94560582	10.12175686	-26.28461219
6	32.93669508	4.32188393	-24.55758158
1	33.21289471	10.52609859	-25.55909336
1	33.54929202	10.30785863	-27.29366411
1	34.78742891	10.82413990	-26.14293797
1	32.53040022	4.70682254	-23.61012010
1	33.34591141	3.32094532	-24.35353716
1	32.08874859	4.18636981	-25.24635175
8	35.55567505	7.82037712	-27.88385508
13	34.99838022	6.12485506	-28.41940583
8	35.08697942	5.07718104	-26.88950095
6	33.51924383	5.91799408	-29.67481769
1	33.41701744	4.87295135	-30.00176787
1	33.66452241	6.53579725	-30.57283644
1	32.56169082	6.21532256	-29.22161445
13	36.31005379	5.80030463	-22.57103874
6	37.30937450	4.24368453	-21.93438269
1	37.90569098	4.48518718	-21.04259281

1	37.98753496	3.84074598	-22.70010339
1	36.61684259	3.43636119	-21.64988942
8	35.39492946	6.82112459	-21.55769835
13	36.93000872	7.15869656	-24.92060380
8	37.69547136	6.37614954	-26.39660798
13	37.34885838	7.30059224	-27.98235023
6	38.19107356	7.27351588	-23.32317841
6	38.68156756	8.52679404	-28.71153879
1	38.66910757	8.23980126	-23.56719891
1	38.99126760	6.51885287	-23.34916673
1	37.90605312	7.43271952	-22.26561297
1	38.82331083	9.40398619	-28.06231401
1	38.38380037	8.89795121	-29.70311009
1	39.66036194	8.03654468	-28.81745312
8	35.78657172	5.79551063	-24.29397722
13	36.91736793	4.82950371	-27.08268331
8	36.78388994	5.69879687	-28.72425357
6	37.72018175	3.08413345	-26.74501680
1	37.21169581	2.29189162	-27.31337317
1	37.65945117	2.81547234	-25.67970509
1	38.78270233	3.06903765	-27.02793379
6	30.82711354	10.12980758	-21.27133852
1	30.15201566	9.81642483	-22.06319076
1	31.23737125	11.13706820	-21.31373482
1	30.89364033	9.55927137	-20.34412404
17	30.95829462	7.41205195	-18.33665002
6	29.03298166	10.78189595	-20.28745032
6	28.03593874	9.75282867	-20.14015585
1	28.84448570	11.52095491	-21.07210317
1	27.99559523	9.36680090	-19.11596103
1	27.04994567	10.08872231	-20.49827778
6	29.66810635	11.36407433	-19.04237674
1	30.55411745	11.96425108	-19.29676986
1	29.99955083	10.54569779	-18.38373025
6	28.66832440	12.25904738	-18.28111944
1	28.28512188	13.04380195	-18.95650916
1	27.79689051	11.65838418	-17.97621772
6	29.29775719	12.91575372	-17.04643043
1	30.16736468	13.51805510	-17.35748289
1	29.69028234	12.12974352	-16.38093391
6	28.31046967	13.79778981	-16.27724392
1	27.44810032	13.21307716	-15.92452569
1	27.92556843	14.61017192	-16.91154486
1	28.78505813	14.25597662	-15.39841239

TS(1_RS-5B_RS)

$\nu = 379.61 \text{ i cm}^{-1}$

6	27.08162692	14.49282635	-17.96767998
6	27.61677166	13.26961907	-18.43937954
6	27.63195406	12.34978927	-17.35756838

6 27.10168976 13.00142413 -16.21435862
6 26.75994923 14.33163036 -16.59439582
40 25.11636500 12.85755087 -17.81110760
6 23.52697490 11.96990986 -15.96413840
6 24.00539550 13.22031374 -15.51989211
6 23.52684239 14.21960770 -16.41696514
6 22.70847984 13.58125824 -17.38978706
6 22.73084575 12.19361014 -17.12935177
1 26.88926571 15.38610045 -18.55411363
1 27.95694145 13.08574184 -19.45386978
1 28.01080094 11.33243503 -17.38854697
1 27.00096325 12.56979438 -15.22297979
1 26.34785552 15.10216933 -15.95101709
1 23.72592166 11.01019480 -15.49646003
1 24.63079605 13.39021846 -14.64907523
1 23.72078429 15.28645135 -16.37291646
1 22.21688291 14.06530660 -18.23580907
1 22.21878213 11.43242483 -17.71194692
13 20.52038993 14.84864558 -20.81032005
8 22.09122957 14.75913346 -20.15940713
13 23.80260936 15.08129039 -20.29426672
6 19.01804992 14.22019715 -19.70540574
6 24.47198575 15.77872252 -22.01718162
1 19.23382693 14.32034768 -18.63208839
1 18.81151385 13.15506183 -19.89693828
1 18.09264078 14.77265132 -19.92253884
1 23.81859457 16.63328415 -22.26126285
1 24.40882889 15.07461065 -22.85733535
1 25.49879117 16.16545910 -21.96274363
8 24.19404214 12.40239014 -22.48713919
13 25.47387028 12.73657350 -21.34312858
8 24.72289585 13.47987444 -19.77153156
6 27.12537476 13.65534222 -21.97700886
1 27.39649151 14.53543843 -21.37556085
1 26.97682632 14.01279645 -23.00720846
1 27.99428955 12.97785463 -21.99342875
13 23.80366618 11.62854427 -23.95160566
6 25.02943811 10.40660728 -24.87741262
1 25.81368130 10.97510501 -25.40182061
1 24.52069516 9.78299220 -25.62566785
1 25.53897000 9.73722124 -24.16856713
13 21.04261275 11.06195585 -24.56102260
8 22.45340795 12.27903384 -24.92442066
13 21.94741822 13.78273528 -25.85564709
6 21.98433774 9.80673212 -23.27969156
6 23.30981000 15.17667363 -26.04579057
1 22.62217836 10.20348227 -22.46492786
1 22.52219629 8.98180101 -23.77022410
1 21.14523468 9.34903886 -22.72742793
1 23.57270859 15.64734971 -25.08710114

1 22.96067936 15.97589196 -26.71757017
1 24.24029179 14.78063748 -26.48109258
8 20.74756834 10.33825568 -26.23500453
13 21.47036042 11.17659097 -27.72944838
8 21.32707441 12.99271910 -27.37905847
6 23.05387083 10.46442201 -28.62185651
1 23.17555314 10.91307211 -29.61880727
1 22.98659885 9.37472351 -28.75357464
1 23.97338189 10.67315214 -28.05541920
13 19.59857010 15.47325496 -23.98632005
6 18.86969079 17.09438735 -24.80969529
1 18.23067752 17.65716416 -24.11360612
1 18.27888270 16.87277418 -25.71070397
1 19.68618882 17.76809365 -25.11292535
8 20.19671620 15.43669577 -22.38455063
13 19.18431701 12.85202034 -24.74682696
8 18.60116734 12.38974148 -26.43019404
13 19.01605352 10.62376316 -26.86989507
6 17.75321627 13.87441249 -23.69887297
6 17.66317556 9.22669428 -26.68859437
1 16.89397811 13.36799081 -24.17741622
1 17.42626766 14.93284308 -23.74315270
1 17.75330189 13.59388027 -22.63750897
1 17.39855408 9.05395937 -25.63444973
1 18.01909439 8.26990286 -27.09801696
1 16.73766737 9.49430219 -27.21919696
8 20.35663282 14.28217198 -25.10728490
13 19.54627549 13.02018939 -27.90252897
8 19.75625173 11.25269640 -28.44975930
6 18.85226116 14.49889788 -28.96982938
1 19.44594489 14.64695540 -29.88360139
1 18.87636909 15.44379753 -28.40641347
1 17.81003676 14.32293854 -29.27322013
6 26.04316341 10.84738656 -20.60770990
1 26.74932271 11.20660082 -19.86405508
1 26.48469703 10.21998374 -21.38398965
1 25.03222203 10.57711870 -20.31638464
17 24.37273522 16.55793500 -18.71963828
6 25.98300199 9.54408340 -18.67956774
6 25.27414422 10.33269242 -17.73073633
1 27.07377771 9.51897691 -18.60544313
1 25.79772168 10.45021043 -16.77240898
1 24.23370733 10.01870562 -17.60936862
6 25.38013907 8.29872414 -19.27449916
1 24.31736584 8.46823966 -19.50917098
1 25.88860136 8.02701805 -20.20965174
6 25.49657591 7.12038121 -18.28049120
1 26.55570808 6.97305707 -18.00857308
1 24.96667192 7.37313928 -17.34813584
6 24.93398972 5.81496506 -18.85673928

1	25.46656476	5.57080276	-19.79040798
1	23.87832636	5.96787574	-19.13494706
6	25.04496778	4.64306887	-17.87789240
1	24.49501620	4.84889465	-16.94781118
1	26.09363405	4.44775575	-17.60947308
1	24.63410294	3.72094570	-18.31148008

TS(1_SR-5B_SR)

$\nu = 340.96 \text{ i cm}^{-1}$

6	25.74697497	12.77621048	-17.01969790
6	27.09496892	12.33212545	-17.06479973
6	27.34655246	11.60237696	-15.87660184
6	26.14342750	11.53458098	-15.13017977
6	25.15369107	12.28039271	-15.83986839
40	25.66849076	10.17789895	-17.24677499
6	24.62228109	8.28575148	-15.86236240
6	23.79637179	9.42084553	-15.69620437
6	23.18932908	9.71300540	-16.94951510
6	23.62163638	8.72963610	-17.88126891
6	24.51787080	7.86257422	-17.22213278
1	25.25566349	13.37430716	-17.77659807
1	27.79155591	12.54356605	-17.86884769
1	28.30045231	11.17116477	-15.59034069
1	26.01420911	11.04449489	-14.16939412
1	24.12807405	12.45248772	-15.52748517
1	25.19459505	7.80099954	-15.08025073
1	23.63780134	9.96264797	-14.76992515
1	22.47657298	10.51262312	-17.13116511
1	23.35443751	8.69046114	-18.93186284
1	25.04002232	7.02459093	-17.67361851
13	23.18498172	14.56014249	-20.46791624
8	23.95472035	12.95938945	-20.76813383
13	23.19185470	11.78124853	-19.58800635
6	21.57044105	14.91259079	-21.53083540
6	21.70190127	10.61665864	-20.11826935
1	21.83602136	15.25169579	-22.54472446
1	20.95472001	15.70151779	-21.07389179
1	20.93981005	14.01884691	-21.64384409
1	21.19216001	10.12205314	-19.27928079
1	22.03048536	9.83603515	-20.82116602
1	20.94546701	11.22385898	-20.63837721
8	26.98779417	13.03269797	-20.25643708
13	25.60217980	12.06119744	-20.64054387
8	24.82510156	11.18051419	-19.15337694
6	25.77516984	10.92319634	-22.25376765
1	26.70468280	10.33329855	-22.26431489
1	25.77123220	11.54001619	-23.16769258
1	24.94151160	10.21085972	-22.35874945
13	28.49907813	13.71179776	-20.67787552
6	30.18465999	12.75469849	-20.35211734

1 30.39143764 12.68873064 -19.27182034
1 31.04752520 13.25644056 -20.81366538
1 30.14810269 11.72509943 -20.73872789
13 28.31643633 15.87926868 -22.37305135
8 28.57516962 15.50603295 -20.54725525
13 28.12845167 16.87522880 -19.42058099
6 28.58748845 13.97738500 -23.09412224
6 28.10400431 16.44719112 -17.50723845
1 28.10197969 13.02736291 -22.79558805
1 29.64522075 13.75830931 -23.30233004
1 28.10259681 14.15071005 -24.07224366
1 27.35037911 15.68284423 -17.26416669
1 27.87656393 17.33472304 -16.89729066
1 29.07805934 16.06497943 -17.16530801
8 29.72219562 17.00693818 -22.73297044
13 30.61539748 17.77793664 -21.29165662
8 29.30703859 18.13155375 -20.02246467
6 32.36471882 17.10806921 -20.74390002
1 32.81702073 17.74967811 -19.97379611
1 33.06184670 17.06324793 -21.59318816
1 32.29030459 16.09326899 -20.32494582
13 24.80006895 17.44890662 -19.86781101
6 23.96517991 18.84540006 -18.77522656
1 22.87065310 18.85269220 -18.88332348
1 24.33944710 19.84844406 -19.02734042
1 24.18207776 18.67523371 -17.70905825
8 24.20390674 15.85235829 -19.98858836
13 26.55531658 17.71333003 -21.98384553
8 27.68032634 19.14114416 -22.27159170
13 29.15551066 18.68718887 -23.32706458
6 24.57272331 18.13598504 -22.24061281
6 29.15246525 19.09663135 -25.23623692
1 24.71109227 18.95509846 -22.97100827
1 23.82802543 18.58719342 -21.55430836
1 24.06005387 17.31544882 -22.75967794
1 28.40222542 18.50022040 -25.77702383
1 30.13045048 18.88462640 -25.69259827
1 28.92100215 20.15647963 -25.41750738
8 26.58060380 17.57058861 -20.10511292
13 28.79296537 19.69217061 -20.88547400
8 30.24145923 19.44558130 -22.02946345
6 28.37569975 21.29853131 -19.85920658
1 29.22029639 21.59876603 -19.22208165
1 27.50869242 21.13723393 -19.20110889
1 28.13562751 22.14565546 -20.51792072
6 26.82124678 9.14875284 -19.23701952
1 27.60178094 9.69401608 -19.77840099
1 25.85318153 9.43131961 -19.67380892
1 26.94232856 8.07229008 -19.37292998
17 22.33940861 13.52020252 -18.33842314

6	28.18678582	8.92154034	-17.44755143
6	27.46669915	8.65444397	-16.27643797
1	28.65695071	9.90553196	-17.53484775
1	27.63338994	9.23588947	-15.37471629
1	27.18974128	7.61310619	-16.10537572
6	28.95937001	7.83127045	-18.15590689
1	28.37485946	6.89775800	-18.16031323
1	29.16747697	8.09829327	-19.20126105
6	30.29736482	7.58688874	-17.42827799
1	30.86680781	8.53084742	-17.37950552
1	30.09997914	7.28877980	-16.38599109
6	31.15173293	6.51693718	-18.11883371
1	31.34311356	6.82122081	-19.16095728
1	30.57957055	5.57586059	-18.17338388
6	32.48220419	6.26900129	-17.40275313
1	32.31943503	5.93366429	-16.36779017
1	33.08854443	7.18596106	-17.36440648
1	33.07426914	5.49800206	-17.91506249

TS(1_SS-5B_SS)

$\nu = 289.20 \text{ i cm}^{-1}$

6	32.78935533	6.75126923	-4.38617155
6	33.34599801	7.79488753	-5.16751861
6	34.05116793	7.20297527	-6.24561962
6	33.91010193	5.79498335	-6.14989291
6	33.13012973	5.51697688	-4.98812481
40	31.55850425	6.59556416	-6.64996484
6	31.33109555	4.68497165	-8.37748567
6	31.38787490	4.04148266	-7.12332257
6	30.22633081	4.39332674	-6.39061215
6	29.42170271	5.22441740	-7.22216008
6	30.10367538	5.41957652	-8.43831857
1	32.17342526	6.86053473	-3.50164123
1	33.25840444	8.85765955	-4.96637662
1	34.60829056	7.74051715	-7.00629293
1	34.34238336	5.06220349	-6.82479925
1	32.84896315	4.54098181	-4.60653577
1	32.06318021	4.58407785	-9.17028456
1	32.18503047	3.39074399	-6.77860135
1	29.98880426	4.03781607	-5.39208591
1	28.47514147	5.67351342	-6.94199315
1	29.75227474	6.01465971	-9.27639679
13	27.77160892	7.87418809	-1.44592899
8	28.59838440	7.58549601	-2.95787150
13	29.02991151	6.05103970	-3.89800813
6	27.11526134	6.33043631	-0.44270464
6	27.39395909	5.08395199	-4.44058667
1	27.81892029	5.48820465	-0.50572931
1	26.15354013	5.98161717	-0.84971958
1	26.95806229	6.57797162	0.61603737

1	26.71276200	5.72668806	-5.02042487
1	26.85049591	4.77280304	-3.53372012
1	27.56972300	4.16906681	-5.02401375
8	28.08040468	9.46733137	-5.13383604
13	29.38539569	8.69308606	-4.27247531
8	29.96209511	7.10464761	-5.06078860
6	30.70983632	9.87339651	-3.38552032
1	31.56635641	9.32595402	-2.96241813
1	30.21557616	10.37617527	-2.53759775
1	31.10989989	10.66853898	-4.03271102
13	27.01701913	10.59549387	-5.80347710
6	26.99424393	11.12077249	-7.68984695
1	27.83120325	11.80439127	-7.90257364
1	26.06679308	11.63821831	-7.97178694
1	27.11365228	10.24777332	-8.34770422
13	24.43651614	10.75747923	-4.40239650
8	26.10653901	11.62895423	-4.66090277
13	26.60106326	12.79026601	-3.32180211
6	24.51938810	9.33422989	-5.81693285
6	28.43296465	13.47483374	-3.46205692
1	25.43043406	8.70671185	-5.87711871
1	24.28900438	9.69907779	-6.82943910
1	23.73171157	8.60652125	-5.55858633
1	29.18812185	12.67582778	-3.41793660
1	28.65773937	14.17836426	-2.64587399
1	28.58834185	14.02214070	-4.40467014
8	23.27072318	12.15469492	-4.71102291
13	23.92860991	13.89100609	-4.77046679
8	25.22409292	13.97565813	-3.44082588
6	24.21968230	14.78771947	-6.47931152
1	24.47190595	15.84868021	-6.33755698
1	23.32469364	14.73931003	-7.11637287
1	25.04694785	14.32505018	-7.03831518
13	26.78285873	10.92848559	-0.41658113
6	27.39774018	11.88249026	1.18089990
1	27.59366555	11.19980991	2.02108254
1	26.66973288	12.63462188	1.51969123
1	28.33959715	12.41348670	0.97286747
8	27.56034887	9.48460361	-0.95103106
13	24.47319796	11.09887241	-1.83953183
8	23.30371158	12.51330460	-1.75142715
13	22.18597769	12.57324789	-3.25247860
6	24.61469989	10.09238510	-0.03258271
6	20.36842640	11.86961611	-3.13962189
1	23.59701924	10.40967393	0.26513173
1	25.15436463	10.22169481	0.92737631
1	24.58127927	9.01026792	-0.21750389
1	20.36452485	10.77735491	-3.00588728
1	19.79763660	12.08924906	-4.05373861
1	19.82218266	12.30612946	-2.29064650

8	26.15260834	11.94531780	-1.76791903
13	23.94623863	14.22162264	-2.11740010
8	22.67646706	14.34925344	-3.47036291
6	24.25132170	15.49733064	-0.67299814
1	24.48809725	16.49716271	-1.06493120
1	25.09300492	15.18647474	-0.03602077
1	23.36714702	15.59298531	-0.02624393
6	30.84520076	8.97053750	-6.92005638
1	31.08833780	9.06965694	-5.85331266
1	31.08054126	9.94597434	-7.34593405
1	29.77383624	8.77819732	-7.06069249
17	30.32444969	4.80544581	-2.62823849
6	32.19040627	8.53481808	-8.71542010
6	32.59746251	7.21441816	-8.91062537
1	32.89538951	9.22053102	-8.24182871
1	32.09556259	6.66636472	-9.70449688
1	33.62885815	6.92356725	-8.72931411
6	31.23740560	9.16465251	-9.70803559
1	30.74972284	10.05770943	-9.29433674
1	30.43714368	8.44968781	-9.95693132
6	31.98235225	9.56232268	-10.99863333
1	32.81238421	10.24445794	-10.74600069
1	32.44309939	8.66910347	-11.45006205
6	31.06367520	10.24144843	-12.02120259
1	30.60516068	11.13304780	-11.56274797
1	30.23173817	9.56119336	-12.26858768
6	31.79789373	10.64293377	-13.30343718
1	32.23933674	9.76576899	-13.79923089
1	32.61332449	11.34936352	-13.08864504
1	31.11797272	11.12497127	-14.01945970

The 3 ζ basis set

	basis	basis2
H	{5s2p}/[3s1p]	{5s2p}
C	{11s6p2d}/[6s3p2d]	{10s3p3d1f}
O	{11s6p2d}/[6s3p2d]	{10s3p3d1f}
Al	{15s11p2d}/[10s6p2d]	{14s3p3d1f1g}
Cl	{15s11p2d}/[10s6p2d]	{14s3p3d1f1g}
Zr	{20s16p11d}/[14s11p7d]	{22s5p5d4f4g}

\$BASIS

default=3z

set=3z

1 4			
0	3	2.951830e+1	2.663542e-2
		4.459397e+0	1.992677e-1
		1.020214e+0	8.443136e-1
0	1	2.789184e-1	1.0
0	1	8.185002e-2	1.0
1	1	1.020214e+0	1.0

6 11			
0	6	2.192464e+4	4.524117e-4
		3.285791e+3	3.511161e-3
		7.474901e+2	1.834054e-2
		2.109105e+2	7.595411e-2
		6.756323e+1	2.620972e-1
		2.308674e+1	7.228794e-1
0	1	8.151221e+0	1.0
0	1	2.947252e+0	1.0
0	1	9.660187e-1	1.0
0	1	3.231446e-1	1.0
0	1	1.010825e-1	1.0
1	4	2.308674e+1	2.068355e-2
		8.151221e+0	6.066722e-2
		2.947252e+0	2.747077e-1
		9.660187e-1	7.569660e-1
1	1	3.231446e-1	1.0
1	1	1.010825e-1	1.0
2	1	9.660187e-1	1.0
2	1	3.231446e-1	1.0

8 11			
0	6	4.329613e+4	4.072680e-4

		6.488002e+3	3.161859e-3
		1.475115e+3	1.655825e-2
		4.145497e+2	6.955296e-2
		1.307826e+2	2.509878e-1
		4.335636e+1	7.406456e-1
0	1	1.483471e+1	1.0
0	1	5.267952e+0	1.0
0	1	1.749247e+0	1.0
0	1	5.715713e-1	1.0
0	1	1.709446e-1	1.0
1	4	4.335636e+1	2.013959e-2
		1.483471e+1	6.777478e-2
		5.267952e+0	2.935987e-1
		1.749247e+0	7.357518e-1
1	1	5.715713e-1	1.0
1	1	1.709446e-1	1.0
2	1	1.749247e+0	1.0
2	1	5.715713e-1	1.0

13 18

0	6	2.382966e+5	3.811725e-4
		3.569645e+4	2.962297e-3
		8.116019e+3	1.557456e-2
		2.284096e+3	6.609540e-2
		7.300537e+2	2.418684e-1
		2.546557e+2	7.476854e-1
0	1	9.502825e+1	1.0
0	1	3.741167e+1	1.0
0	1	1.536696e+1	1.0
0	1	6.290235e+0	1.0
0	1	2.543955e+0	1.0
0	1	1.012528e+0	1.0
0	1	3.453793e-1	1.0
0	1	1.253362e-1	1.0
0	1	4.096564e-2	1.0
1	6	7.300537e+2	1.232426e-3
		2.546557e+2	5.132843e-3
		9.502825e+1	2.674667e-2
		3.741167e+1	9.921941e-2
		1.536696e+1	3.081204e-1
		6.290235e+0	6.701420e-1
1	1	2.543955e+0	1.0
1	1	1.012528e+0	1.0
1	1	3.453793e-1	1.0
1	1	1.253362e-1	1.0
1	1	4.096564e-2	1.0
2	1	3.453793e-1	1.0
2	1	1.253362e-1	1.0

17 18

0	6	4.886680e+5	3.683119e-4
		7.319565e+4	2.862919e-3
		1.663917e+4	1.506844e-2
		4.678381e+3	6.424228e-2
		1.491358e+3	2.379472e-1
		5.186839e+2	7.529444e-1
0	1	1.935542e+2	1.0
0	1	7.648497e+1	1.0
0	1	3.167528e+1	1.0
0	1	1.322806e+1	1.0
0	1	5.558031e+0	1.0
0	1	2.335902e+0	1.0
0	1	8.433804e-1	1.0
0	1	3.183365e-1	1.0
0	1	1.082213e-1	1.0
1	6	1.491358e+3	1.074090e-3
		5.186839e+2	4.581779e-3
		1.935542e+2	2.412967e-2
		7.648497e+1	9.277696e-2
		3.167528e+1	2.982536e-1
		1.322806e+1	6.822171e-1
1	1	5.558031e+0	1.0
1	1	2.335902e+0	1.0
1	1	8.433804e-1	1.0
1	1	3.183365e-1	1.0
1	1	1.082213e-1	1.0
2	1	8.433804e-1	1.0
2	1	3.183365e-1	1.0

40 32

0	7	8.630368e+6	1.121190e-4
		1.292334e+6	8.718985e-4
		2.938924e+5	4.593228e-3
		8.285723e+4	1.959568e-2
		2.662709e+4	7.312057e-2
		9.366428e+3	2.438635e-1
		3.521342e+3	7.312777e-1
0	1	1.384408e+3	1.0
0	1	5.653707e+2	1.0
0	1	2.398940e+2	1.0
0	1	1.041929e+2	1.0
0	1	4.656738e+1	1.0
0	1	2.141357e+1	1.0
0	1	9.766987e+0	1.0
0	1	4.396453e+0	1.0
0	1	1.944582e+0	1.0
0	1	7.892078e-1	1.0
0	1	2.964932e-1	1.0
0	1	9.504214e-2	1.0

0	1	3.384268e-2	1.0
1	6	2.662709e+4	5.110416e-4
		9.366428e+3	2.265163e-3
		3.521342e+3	1.217301e-2
		1.384408e+3	5.670463e-2
		5.653707e+2	2.292390e-1
		2.398940e+2	7.722212e-1
1	1	1.041929e+2	1.0
1	1	4.656738e+1	1.0
1	1	2.141357e+1	1.0
1	1	9.766987e+0	1.0
1	1	4.396453e+0	1.0
1	1	1.944582e+0	1.0
1	1	7.892078e-1	1.0
1	1	2.964932e-1	1.0
1	1	9.504214e-2	1.0
1	1	3.384268e-2	1.0
2	5	5.653707e+2	3.659557e-3
		2.398940e+2	1.570457e-2
		1.041929e+2	8.107027e-2
		4.656738e+1	2.819669e-1
		2.141357e+1	7.175838e-1
2	1	9.766987e+0	1.0
2	1	4.396453e+0	1.0
2	1	1.944582e+0	1.0
2	1	7.892078e-1	1.0
2	1	2.964932e-1	1.0
2	1	9.504214e-2	1.0

\$END

\$Basis2

default=3z

set=3z

1 7

0	1	2.04937577e-01	1.0
0	1	5.52861763e-01	1.0
1	1	5.52861763e-01	1.0
0	1	1.49145966e+00	1.0
1	1	1.49145966e+00	1.0
0	1	4.02352281e+00	1.0
0	1	1.08542901e+01	1.0

6 17

0	1	1.75774940e-01	1.0
0	1	4.40360864e-01	1.0
1	1	4.40360864e-01	1.0
2	1	4.40360864e-01	1.0
0	1	1.10321580e+00	1.0
1	1	1.10321580e+00	1.0
2	1	1.10321580e+00	1.0
3	1	1.10321580e+00	1.0
0	1	2.76383573e+00	1.0
1	1	2.76383573e+00	1.0
2	1	2.76383573e+00	1.0
0	1	6.92411041e+00	1.0
0	1	1.73466550e+01	1.0
0	1	4.34577760e+01	1.0
0	1	1.08872765e+02	1.0
0	1	2.72753926e+02	1.0
0	1	6.83317851e+02	1.0

8 17

0	1	2.78763508e-01	1.0
0	1	7.06097473e-01	1.0
1	1	7.06097473e-01	1.0
2	1	7.06097473e-01	1.0
0	1	1.78851832e+00	1.0
1	1	1.78851832e+00	1.0
2	1	1.78851832e+00	1.0
3	1	1.78851832e+00	1.0
0	1	4.53024959e+00	1.0
1	1	4.53024959e+00	1.0
2	1	4.53024959e+00	1.0
0	1	1.14749517e+01	1.0
0	1	2.90656207e+01	1.0
0	1	7.36221232e+01	1.0
0	1	1.86482067e+02	1.0
0	1	4.72352057e+02	1.0
0	1	1.19644998e+03	1.0

13 22

0	1	6.36338538e-02	1.0
0	1	1.46064791e-01	1.0
1	1	1.46064791e-01	1.0
2	1	1.46064791e-01	1.0
0	1	3.35276303e-01	1.0
1	1	3.35276303e-01	1.0
2	1	3.35276303e-01	1.0
3	1	3.35276303e-01	1.0
4	1	3.35276303e-01	1.0
0	1	7.69591345e-01	1.0
1	1	7.69591345e-01	1.0

2	1	7.69591345e-01	1.0
0	1	1.76651566e+00	1.0
0	1	4.05485013e+00	1.0
0	1	9.30748025e+00	1.0
0	1	2.13643380e+01	1.0
0	1	4.90395816e+01	1.0
0	1	1.12565181e+02	1.0
0	1	2.58381484e+02	1.0
0	1	5.93087410e+02	1.0
0	1	1.36136951e+03	1.0
0	1	3.12487995e+03	1.0

17 22

0	1	2.01070734e-01	1.0
0	1	4.40284706e-01	1.0
1	1	4.40284706e-01	1.0
2	1	4.40284706e-01	1.0
0	1	9.64091681e-01	1.0
1	1	9.64091681e-01	1.0
2	1	9.64091681e-01	1.0
3	1	9.64091681e-01	1.0
4	1	9.64091681e-01	1.0
0	1	2.11107213e+00	1.0
1	1	2.11107213e+00	1.0
2	1	2.11107213e+00	1.0
0	1	4.62261589e+00	1.0
0	1	1.01221448e+01	1.0
0	1	2.21644664e+01	1.0
0	1	4.85335452e+01	1.0
0	1	1.06273933e+02	1.0
0	1	2.32708094e+02	1.0
0	1	5.09561051e+02	1.0
0	1	1.11578613e+03	1.0
0	1	2.44323756e+03	1.0
0	1	5.34995874e+03	1.0

40 40

0	1	7.10328641e-02	1.0
0	1	1.33323632e-01	1.0
1	1	1.33323632e-01	1.0
2	1	1.33323632e-01	1.0
0	1	2.50238971e-01	1.0
1	1	2.50238971e-01	1.0
2	1	2.50238971e-01	1.0
3	1	2.50238971e-01	1.0
4	1	2.50238971e-01	1.0
0	1	4.69680744e-01	1.0
1	1	4.69680744e-01	1.0
2	1	4.69680744e-01	1.0

3	1	4.69680744e-01	1.0
4	1	4.69680744e-01	1.0
0	1	8.81557338e-01	1.0
1	1	8.81557338e-01	1.0
2	1	8.81557338e-01	1.0
3	1	8.81557338e-01	1.0
4	1	8.81557338e-01	1.0
0	1	1.65462040e+00	1.0
1	1	1.65462040e+00	1.0
2	1	1.65462040e+00	1.0
3	1	1.65462040e+00	1.0
4	1	1.65462040e+00	1.0
0	1	3.10560476e+00	1.0
0	1	5.82899917e+00	1.0
0	1	1.09406167e+01	1.0
0	1	2.05347591e+01	1.0
0	1	3.85422818e+01	1.0
0	1	7.23411207e+01	1.0
0	1	1.35779136e+02	1.0
0	1	2.54847778e+02	1.0
0	1	4.78331147e+02	1.0
0	1	8.97793530e+02	1.0
0	1	1.68509458e+03	1.0
0	1	3.16280262e+03	1.0
0	1	5.93635549e+03	1.0
0	1	1.11421169e+04	1.0
0	1	2.09129606e+04	1.0
0	1	3.92521391e+04	1.0