

Cyclobutadiene nickel complexes as a catalyst for CH-activation reactions: computational study

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Computational methods

Preliminary geometry optimizations were carried out using Priroda 16^[S1] (2016.10.30) software at PBE0/3z level, which gave appropriate coordinates for further calculations. Additional geometry optimizations and single point energy calculations were carried out using Gaussian 09 package (revision D.01)^[S2] applying the M06-L functional^[S3] with TZVP basis set^[S4] and SMD solvation model^[S5]. The corresponding fitting basis set TZVPfit was employed. The optimized geometries were verified to have no negative frequencies for all intermediates and only one negative frequency for transition states.

Investigation of replacement of the cyclobutadiene ligand

In addition to a possible nucleophilic attack of acetate anion, we also investigated possible nucleophilic substitution of cyclobutadiene ligand (Figure S1). It was found that this side-reaction has very high energy barrier of 74.2 kcal mol⁻¹ with respect to starting materials.

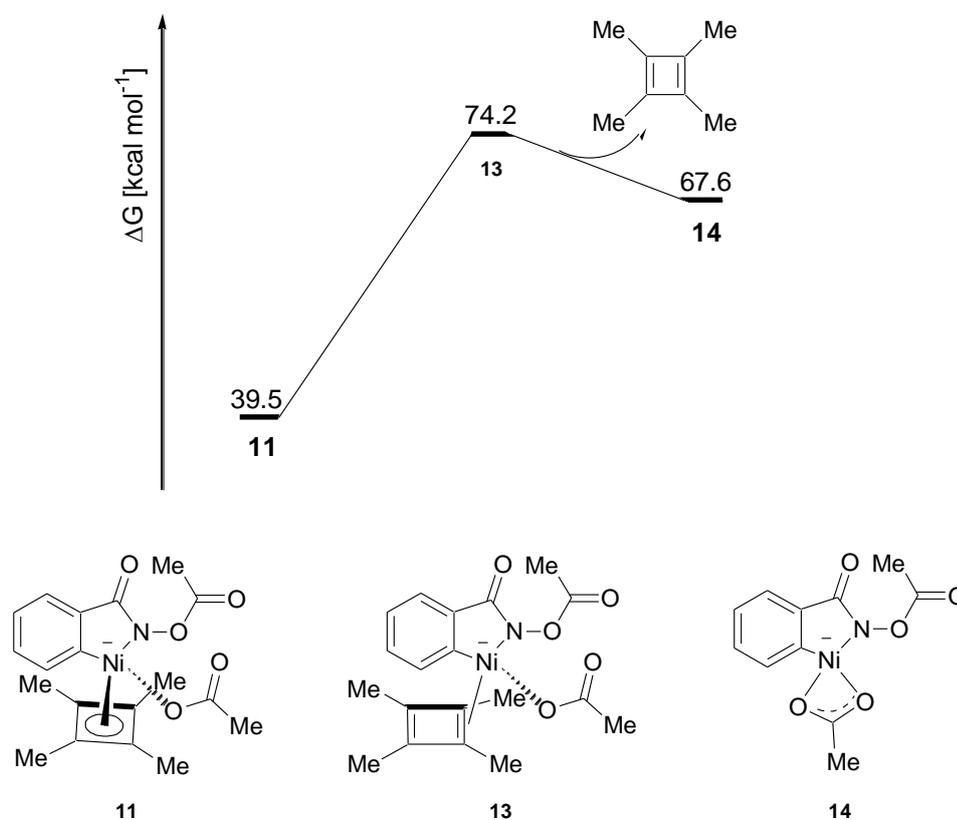


Figure S1. Proposed nucleophilic substitution mechanism, proceeding via thermodynamically unfavorable η^2 -cyclobutadiene species **13**.

Table S1. Gibbs free energies (kcal mol⁻¹) at 298 K in methanol (SMD) for Cb*Ni species, starting materials and product. CH-activation step highlighted in green, migratory insertion in red.

	G (kcal mol ⁻¹)	Δ, kcal mol ⁻¹
1_{Ni}	-1429064.13	0.00
N-acetoxybenzamide	-394572.084	-
AcOH	-143772.181	-
C ₂ H ₂	-48529.956	-
2_{Ni}	-1679861.03	3.00
TS1_{Ni}	-1679834.83	29.20
3_{Ni}	-1679841.13	22.90
4_{Ni}	-1536073.63	18.22
5_{Ni}	-1584599.32	22.48
TS2_{Ni}	-1584586.14	35.67
VI	-1584622.45	-0.65
1_{Ni} + product	-1728494.53	-100.54
Nucleophilic addition of the acetate anion		
AcO ⁻	-143483.75	-
TS-A	-1679516.80	58.80
10	-1679519.80	55.80
11	-1679536.14	39.46
TS-B	-1679515.39	60.21
12	-1679519.78	55.82
Nucleophilic substitution of the cyclobutadiene ring		
13	-1679501.36	74.24
14	-1483795.15	67.62
C ₄ Me ₄	-195712.83	-

Table S2. Gibbs free energies (kcal mol⁻¹) at 298 K in methanol (SMD) for Cp*Co species. CH-activation step highlighted in green, migratory insertion in red.

	G (kcal mol ⁻¹)	Δ, kcal mol ⁻¹
1_{Co}	-1399258.94	0.00
2_{Co}	-1650054.70	4.14
TS1_{Co}	-1650031.07	27.78
3_{Co}	-1650040.09	18.75
4_{Co}	-1506267.22	19.44
5_{Co}	-1554800.04	16.58
TS2_{Co}	-1554792.33	24.29
VI_{Co}	-1554816.05	0.57
1_{Co} + product	-1698689.34	-100.54

References

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- [S3] Y. Zhao and D. G. Truhlar, *J. Chem. Phys.*, 2006, **125**, 194101.
- [S4] A. Schäfer, C. Huber and R. Ahlrichs, *J. Chem. Phys.*, 1994, **100**, 5829.
- [S5] A. V. Marenich, C. J. Cramer and D. G. Truhlar, *J. Phys. Chem. B*, 2009, **113**, 6378.

Atomic coordinates for the optimized structures (Å)

				Reactant				
					8	-0.368805000	1.804769000	0.932556000
6	3.973596000	-0.645028000	0.192774000	6	-0.472753000	3.953914000	-0.141733000	
6	3.003907000	-1.494465000	-0.322350000	1	-1.511304000	4.086733000	-0.450981000	
6	1.701052000	-1.051199000	-0.476633000	1	-0.359198000	4.396757000	0.845085000	
6	1.360378000	0.253985000	-0.115931000	1	0.159193000	4.468794000	-0.861798000	
6	2.341390000	1.104542000	0.393204000	8	-1.688389000	0.015957000	-0.811777000	
6	3.640174000	0.655063000	0.550090000	6	-2.669694000	-0.209352000	-0.006824000	
1	4.991880000	-0.995516000	0.310690000	8	-2.559450000	-0.358024000	1.218888000	
1	3.264833000	-2.504653000	-0.612394000	6	-4.022326000	-0.256079000	-0.665792000	
1	0.958344000	-1.715916000	-0.900996000	1	-4.427026000	0.756864000	-0.711159000	
1	2.070336000	2.116311000	0.668293000	1	-3.964352000	-0.630935000	-1.686093000	
1	4.395593000	1.318914000	0.951901000	1	-4.712262000	-0.864761000	-0.084996000	
6	-0.010823000	0.800334000	-0.252650000	6	-0.777418000	-2.887177000	0.074493000	
8	-0.263706000	1.997572000	-0.243518000	1	-1.443878000	-2.704370000	-0.769096000	
7	-0.981443000	-0.150503000	-0.461563000	1	-0.358139000	-3.887240000	-0.063923000	
1	-0.950573000	-1.047042000	0.022027000	1	-1.369051000	-2.896396000	0.986975000	
8	-2.287779000	0.368542000	-0.449579000	6	0.856321000	-1.855200000	-2.415478000	
6	-3.170194000	-0.432343000	0.219566000	1	1.049189000	-1.043326000	-3.116763000	
8	-2.821482000	-1.455631000	0.758352000	1	1.540056000	-2.670984000	-2.667574000	
6	-4.539396000	0.122178000	0.135486000	1	-0.157500000	-2.216007000	-2.584521000	
1	-5.092293000	-0.430040000	-0.625859000	6	2.981606000	0.250096000	-1.405137000	
1	-5.046523000	-0.025521000	1.086073000	1	3.333353000	1.167166000	-0.936214000	
1	-4.538273000	1.174719000	-0.132161000	1	3.856492000	-0.371712000	-1.613149000	
		1_{co}		1	2.532468000	0.501631000	-2.365625000	
27	0.134871000	0.139139000	-0.120504000	6	2.603698000	0.597085000	1.744784000	
6	0.786500000	-1.201678000	1.274063000	1	3.441916000	0.079025000	2.218646000	
6	0.319891000	-1.896962000	0.128260000	1	3.011449000	1.446344000	1.197400000	
6	1.049638000	-1.420864000	-1.013976000	1	1.969168000	0.982076000	2.542842000	
6	2.038566000	-0.490630000	-0.541297000	6	0.287238000	-1.302350000	2.663016000	
6	1.859382000	-0.322937000	0.855854000	1	1.043551000	-1.765901000	3.302004000	
6	-0.168168000	2.502747000	-0.109862000	1	0.081460000	-0.315347000	3.080790000	
8	0.270346000	1.894485000	-1.137343000	1	-0.621604000	-1.896346000	2.730937000	

		2_{co}		1	2.279384000	-1.540841000	-1.601612000
27	-0.729088000	-0.525984000	0.048242000	6	-1.096593000	-3.625951000	-0.247786000
7	0.160723000	1.184124000	0.542775000	1	-1.925889000	-3.692231000	0.455738000
6	-1.047530000	-2.305698000	-0.913488000	1	-1.229948000	-4.418783000	-0.988784000
6	-2.137353000	-1.435180000	-1.144451000	1	-0.173854000	-3.838881000	0.290419000
6	-1.631729000	-0.227364000	-1.743643000	6	0.666216000	0.560020000	-2.632433000
6	-0.227513000	-0.409171000	-1.965588000	1	1.715330000	0.319088000	-2.475807000
6	0.148872000	-1.664939000	-1.416849000	1	0.477997000	0.536354000	-3.709434000
8	-2.064430000	-0.227584000	1.534426000	1	0.482587000	1.578775000	-2.292904000
8	-0.277592000	-1.409813000	1.847343000	6	-2.467197000	0.928498000	-2.145409000
6	-1.339223000	-0.907145000	2.327982000	1	-3.183449000	0.628906000	-2.915151000
6	-1.703893000	-1.072509000	3.755738000	1	-3.050317000	1.311958000	-1.304583000
1	-2.780587000	-1.005535000	3.892692000	1	-1.866791000	1.743650000	-2.541965000
1	-1.333289000	-2.018610000	4.143486000	6	-3.546975000	-1.659926000	-0.764186000
1	-1.239648000	-0.269818000	4.331599000	1	-4.102842000	-2.024298000	-1.632685000
8	-0.824090000	2.181632000	0.911771000	1	-3.647152000	-2.403654000	0.024332000
6	1.401902000	1.684378000	0.614861000	1	-4.029758000	-0.738946000	-0.439281000
6	2.500955000	0.690325000	0.424715000	6	-2.093029000	4.096750000	0.539592000
6	2.604306000	-0.434650000	1.237795000	1	-2.782908000	4.355355000	-0.261382000
6	3.512265000	0.963912000	-0.497349000	1	-2.637120000	3.677569000	1.381730000
6	3.699861000	-1.279573000	1.125376000	1	-1.603638000	5.016375000	0.863244000
1	1.832823000	-0.638399000	1.968278000				
					TS1_{co} (one imaginary frequency at 1312i cm ⁻¹)		
6	4.591196000	0.103882000	-0.625209000	27	0.147277000	-0.581187000	-0.060745000
1	3.442627000	1.852789000	-1.114524000	7	-1.001399000	0.965097000	0.245891000
6	4.688489000	-1.019341000	0.188310000	6	1.157038000	-0.927485000	-1.858117000
1	3.777794000	-2.146814000	1.770427000	6	1.273067000	-2.053131000	-0.970764000
1	5.363932000	0.314596000	-1.354873000	6	-0.046513000	-2.542441000	-0.737547000
1	5.539290000	-1.683679000	0.094691000	6	-0.982558000	-1.678864000	-1.379320000
8	1.686855000	2.876178000	0.844574000	6	-0.222082000	-0.687120000	-2.095296000
6	-1.055515000	3.165912000	0.014293000	8	-0.450819000	-1.312043000	1.698169000
8	-0.498175000	3.271771000	-1.054063000	8	1.188538000	-0.259640000	2.762589000
6	1.496456000	-2.274214000	-1.414393000	6	0.187674000	-1.046260000	2.749757000
1	1.712131000	-2.771709000	-0.468228000	6	-0.245325000	-1.656003000	4.037099000
1	1.559262000	-3.036086000	-2.197078000	1	0.618640000	-2.002729000	4.600789000

1	-0.739887000	-0.892458000	4.639216000	6	-0.382048000	-3.714927000	0.097024000
1	-0.938969000	-2.475320000	3.870005000	1	-1.395999000	-3.663789000	0.489508000
8	-2.364214000	0.787005000	0.636148000	1	-0.311969000	-4.620028000	-0.513439000
6	-0.504956000	2.179968000	0.516009000	1	0.311131000	-3.835457000	0.928950000
6	0.967647000	2.134164000	0.336876000	6	-4.656107000	1.103078000	0.353618000
6	1.582183000	0.869223000	0.441064000	1	-5.364652000	1.062183000	-0.469916000
6	1.704891000	3.285559000	0.098768000	1	-4.702283000	0.188510000	0.939758000
6	2.976792000	0.823126000	0.325842000	1	-4.940516000	1.934738000	1.000495000
1	1.290120000	0.163749000	1.566446000				
6	3.083439000	3.200884000	-0.035596000	27	0.260257000	-0.552112000	-0.049091000
1	1.195644000	4.240298000	0.020666000	7	-1.026409000	0.907171000	0.367037000
6	3.719334000	1.970619000	0.089406000	6	-0.494865000	-1.251246000	-1.814039000
1	3.494196000	-0.122118000	0.456633000	6	0.916959000	-1.483477000	-1.792087000
1	3.665039000	4.094855000	-0.226900000	6	1.211085000	-2.275524000	-0.654052000
1	4.798724000	1.910189000	0.010496000	6	-0.048766000	-2.633092000	-0.028357000
8	-1.142041000	3.186309000	0.875329000	6	-1.090432000	-2.024023000	-0.743335000
6	-3.289769000	1.362140000	-0.174881000	8	1.084513000	-0.748812000	1.809796000
8	-3.022594000	2.001856000	-1.164581000	8	0.141823000	0.928338000	2.954204000
6	2.256627000	-0.185480000	-2.516168000	6	0.971810000	-0.086796000	2.844304000
1	3.224826000	-0.386741000	-2.063078000	6	1.781262000	-0.364176000	4.050835000
1	2.313190000	-0.490728000	-3.564875000	1	2.557544000	0.398294000	4.135342000
1	2.088323000	0.891816000	-2.506452000	1	1.169177000	-0.304346000	4.948553000
6	2.521002000	-2.682838000	-0.473191000	1	2.253855000	-1.338613000	3.975207000
1	2.487190000	-2.846496000	0.606008000	8	-2.348168000	0.734393000	0.895967000
1	2.676938000	-3.659887000	-0.937864000	6	-0.735301000	2.188241000	0.010845000
1	3.395343000	-2.072898000	-0.691901000	6	0.689312000	2.233300000	-0.386638000
6	-0.745809000	0.391174000	-2.963575000	6	1.375032000	1.010880000	-0.393434000
1	-0.516644000	0.169152000	-4.009414000	6	1.339299000	3.441153000	-0.626130000
1	-1.823007000	0.504721000	-2.874610000	6	2.754551000	1.044784000	-0.575789000
1	-0.284321000	1.352893000	-2.733637000	1	-0.327220000	1.023084000	2.085531000
6	-2.457813000	-1.828971000	-1.348919000	6	2.706632000	3.446523000	-0.850761000
1	-2.774718000	-2.671986000	-1.968524000	1	0.770411000	4.365575000	-0.615825000
1	-2.819890000	-2.021338000	-0.337527000	6	3.413789000	2.249629000	-0.804761000
1	-2.964374000	-0.941177000	-1.725724000	1	3.335222000	0.127709000	-0.542541000

3co

1	3.225735000	4.378771000	-1.039422000	6	0.645533000	-2.228004000	0.797026000
1	4.489187000	2.254438000	-0.948297000	6	-0.664292000	-1.803393000	1.212526000
8	-1.490222000	3.165889000	0.099003000	6	-1.531039000	-1.772133000	0.071703000
6	-3.383990000	0.926976000	0.037021000	8	-1.987181000	1.470253000	-0.799639000
8	-3.256185000	1.214802000	-1.128463000	6	0.131402000	2.321100000	-0.368674000
6	-2.539119000	-2.174801000	-0.458167000	6	1.541403000	1.924040000	-0.148828000
1	-3.145225000	-1.487184000	-1.044603000	6	1.771907000	0.543457000	-0.037100000
1	-2.867301000	-3.185992000	-0.713169000	6	2.559692000	2.863226000	-0.089785000
1	-2.772765000	-2.025600000	0.597097000	6	3.095653000	0.138282000	0.105316000
6	-1.197630000	-0.507163000	-2.888825000	6	3.870903000	2.430103000	0.062995000
1	-0.856589000	0.527468000	-2.961502000	1	2.325422000	3.920267000	-0.168245000
1	-1.004553000	-0.973914000	-3.858553000	6	4.133995000	1.070626000	0.149644000
1	-2.274263000	-0.490371000	-2.738868000	1	3.347319000	-0.913872000	0.184166000
6	1.858947000	-1.014147000	-2.833267000	1	4.681357000	3.147753000	0.108365000
1	2.890601000	-0.996417000	-2.488483000	1	5.157670000	0.726974000	0.254663000
1	1.813374000	-1.696939000	-3.686919000	8	-0.300054000	3.473475000	-0.415843000
1	1.601006000	-0.022143000	-3.203189000	6	-2.726779000	1.807258000	0.292909000
6	2.543000000	-2.748700000	-0.208120000	8	-2.280598000	1.854636000	1.414932000
1	2.694451000	-2.576945000	0.859279000	6	-4.127845000	2.105171000	-0.105144000
1	2.646954000	-3.824473000	-0.374519000	1	-4.351705000	1.768199000	-1.113609000
1	3.349709000	-2.254387000	-0.747433000	1	-4.812301000	1.646363000	0.605435000
6	-0.186580000	-3.484618000	1.175475000	1	-4.278622000	3.184492000	-0.056854000
1	-1.096278000	-3.258126000	1.731646000	6	-1.027091000	-1.449403000	2.600648000
1	-0.233622000	-4.539718000	0.890678000	1	-1.936967000	-0.854296000	2.651016000
1	0.663200000	-3.374289000	1.849483000	1	-1.193824000	-2.358423000	3.186989000
6	-4.675781000	0.733659000	0.749435000	1	-0.225270000	-0.898997000	3.093737000
1	-5.347889000	0.151541000	0.121860000	6	1.773999000	-2.487658000	1.721312000
1	-4.549987000	0.248374000	1.713435000	1	1.559861000	-3.371601000	2.327864000
1	-5.136183000	1.709855000	0.906448000	1	2.705324000	-2.676429000	1.191337000
		4c_o		1	1.937599000	-1.660290000	2.412814000
27	0.093040000	-0.493704000	-0.121790000	6	1.721067000	-2.795497000	-1.503505000
7	-0.616579000	1.187160000	-0.525478000	1	2.679260000	-2.800190000	-0.987301000
6	-0.736913000	-2.090978000	-1.056732000	1	1.543868000	-3.805701000	-1.883068000
6	0.613238000	-2.382290000	-0.612802000	1	1.806709000	-2.141803000	-2.372613000

6	-1.170492000	-2.058626000	-2.469663000	1	5.241811000	1.486808000	0.370497000
1	-0.358829000	-1.752259000	-3.129514000	6	0.145896000	-3.581982000	-1.286362000
1	-1.487546000	-3.054757000	-2.792902000	1	1.213687000	-3.550411000	-1.499690000
1	-2.011945000	-1.382475000	-2.618661000	1	-0.096703000	-4.605242000	-0.985807000
6	-2.978653000	-1.456295000	0.080557000	1	-0.399250000	-3.385150000	-2.209595000
1	-3.308099000	-1.007634000	-0.855896000	6	-2.748501000	-2.479164000	-0.810801000
1	-3.563610000	-2.369511000	0.220536000	1	-3.056263000	-3.504458000	-0.587793000
1	-3.243151000	-0.786762000	0.898398000	1	-3.597410000	-1.831323000	-0.599539000
		5_{co}		1	-2.546467000	-2.436654000	-1.882121000
27	-0.234435000	-0.534133000	-0.292220000	6	-2.678493000	-0.691391000	1.861685000
7	1.103722000	0.835708000	0.099031000	1	-3.531471000	-0.559121000	1.199087000
6	-0.174412000	-1.269290000	1.634824000	1	-2.996868000	-1.340693000	2.682156000
6	-1.522619000	-1.309529000	1.172870000	1	-2.429928000	0.276738000	2.296558000
6	-1.556080000	-2.112363000	-0.008429000	6	0.301696000	-0.515552000	2.817498000
6	-0.235605000	-2.644857000	-0.207692000	1	-0.249206000	0.416547000	2.945528000
6	0.621472000	-2.119259000	0.786649000	1	0.154156000	-1.104090000	3.727390000
8	2.452371000	0.522357000	0.419739000	1	1.362124000	-0.277963000	2.748856000
6	0.755344000	2.101441000	0.374113000	6	2.055693000	-2.459326000	0.961159000
6	-0.683405000	2.246506000	0.073649000	1	2.545227000	-1.800595000	1.674799000
6	-1.357227000	1.090836000	-0.337492000	1	2.155333000	-3.482231000	1.334204000
6	-1.336280000	3.472848000	0.171477000	1	2.608158000	-2.408898000	0.021379000
6	-2.696710000	1.205816000	-0.694997000	6	-0.502135000	-0.348182000	-2.332594000
6	-2.678773000	3.562134000	-0.156971000	6	0.674608000	-0.668615000	-2.142397000
1	-0.780054000	4.345441000	0.499267000	1	1.708903000	-0.920568000	-2.264100000
6	-3.353291000	2.428245000	-0.597766000	1	-1.412257000	-0.092658000	-2.836555000
1	-3.247599000	0.341356000	-1.052268000				
1	-3.197828000	4.510282000	-0.082892000				
1	-4.400262000	2.495717000	-0.873402000				
8	1.508182000	3.004708000	0.783491000				
6	3.378891000	0.974737000	-0.466729000				
8	3.111017000	1.602569000	-1.463785000				
6	4.745100000	0.596481000	-0.017371000				
1	4.730861000	-0.162118000	0.760736000				
1	5.321429000	0.246646000	-0.871455000				
					TS2_{co} (one imaginary frequency at 316i cm ⁻¹)		
				27	-0.279041000	-0.561429000	-0.331311000
				7	1.091984000	0.854532000	-0.252334000
				6	-1.237346000	-1.374743000	1.363079000
				6	-1.501425000	-2.153372000	0.184522000
				6	-0.252105000	-2.641664000	-0.311657000
				6	0.786948000	-2.107300000	0.497337000
				6	0.164514000	-1.326771000	1.545450000
				8	2.434441000	0.571647000	-0.670434000

6	0.746158000	2.137974000	-0.453000000	6	-2.233366000	-0.752702000	2.266435000
6	-0.711085000	2.246569000	-0.272105000	1	-3.215907000	-0.673561000	1.805419000
6	-1.459849000	1.066421000	-0.432138000	1	-2.342564000	-1.358044000	3.170491000
6	-1.326050000	3.450589000	0.059067000	1	-1.926243000	0.244609000	2.584868000
6	-2.843835000	1.136266000	-0.226654000	6	-2.825806000	-2.502457000	-0.384370000
6	-2.691656000	3.493771000	0.271608000	1	-2.857560000	-2.337342000	-1.462618000
1	-0.714531000	4.340394000	0.166406000	1	-3.041394000	-3.561902000	-0.221622000
6	-3.445035000	2.327873000	0.134316000	1	-3.633093000	-1.932312000	0.071735000
1	-3.456683000	0.255943000	-0.384207000			6co	
1	-3.174642000	4.425219000	0.540712000	27	0.785628000	-0.378812000	-0.316753000
1	-4.516644000	2.356266000	0.296422000	7	-0.100825000	1.295937000	-0.076290000
8	1.508728000	3.081285000	-0.732737000	8	0.866824000	2.309497000	0.321860000
6	-0.027936000	-0.524175000	-2.251417000	6	-1.344034000	1.773016000	0.086252000
1	0.670280000	-0.981179000	-2.930504000	6	-2.469273000	0.788855000	-0.023348000
6	-1.114438000	0.113528000	-2.087044000	6	-2.625498000	-0.224473000	-0.992646000
1	-2.019068000	0.407383000	-2.591281000	6	-3.494247000	1.003817000	0.905575000
6	3.399232000	0.940120000	0.205841000	6	-3.840140000	-0.929347000	-1.009895000
8	3.185334000	1.487956000	1.263019000	6	-4.649769000	0.246782000	0.909543000
6	4.741674000	0.581375000	-0.327640000	1	-3.363511000	1.792542000	1.636499000
1	5.334148000	0.131239000	0.466854000	6	-4.830724000	-0.719906000	-0.071708000
1	4.682816000	-0.094023000	-1.176899000	1	-3.980510000	-1.680065000	-1.779941000
1	5.250528000	1.494526000	-0.638297000	1	-5.412486000	0.423909000	1.657597000
6	-0.089647000	-3.536412000	-1.480707000	1	-5.741947000	-1.305020000	-0.105660000
1	0.924656000	-3.509963000	-1.876545000	8	-1.599501000	2.955366000	0.384837000
1	-0.304333000	-4.569071000	-1.192853000	6	-0.320287000	-0.773070000	-1.809589000
1	-0.780065000	-3.282600000	-2.286462000	1	0.250884000	-1.190230000	-2.648002000
6	2.233938000	-2.397023000	0.348481000	6	-1.636259000	-0.625663000	-1.992854000
1	2.849388000	-1.719864000	0.938625000	1	-2.079498000	-0.963203000	-2.932448000
1	2.451224000	-3.412028000	0.692287000	6	1.705015000	2.755322000	-0.646410000
1	2.556735000	-2.335042000	-0.691399000	8	2.575721000	3.517352000	-0.283033000
6	0.857370000	-0.607212000	2.638993000	6	1.504421000	2.291546000	-2.044182000
1	0.431468000	0.384087000	2.800562000	1	2.141355000	2.872841000	-2.704193000
1	0.751148000	-1.158069000	3.577867000	1	1.772049000	1.235274000	-2.143760000
1	1.921014000	-0.488839000	2.443013000	1	0.461159000	2.381509000	-2.344114000

6	2.306345000	-1.737497000	-0.083170000	6	3.990989000	0.473451000	-0.539213000
6	1.055148000	-2.361343000	0.114142000	1	3.993346000	1.227776000	-1.323397000
6	0.378604000	-1.633244000	1.159866000	1	4.686780000	0.752930000	0.248342000
6	1.306337000	-0.651314000	1.696021000	1	4.341926000	-0.460571000	-0.983592000
6	2.467786000	-0.689260000	0.917870000	8	-0.228223000	1.792122000	0.998677000
6	0.988524000	0.261639000	2.818164000	8	-0.878228000	1.763637000	-1.084348000
1	-0.001024000	0.708628000	2.706927000	6	-0.654546000	2.417990000	-0.021549000
1	0.980532000	-0.292767000	3.760416000	6	-0.883739000	3.888743000	0.020831000
1	1.714994000	1.066049000	2.913776000	1	-0.059881000	4.395795000	-0.482131000
6	-0.961609000	-1.933020000	1.709812000	1	-1.795528000	4.151287000	-0.512473000
1	-1.626599000	-2.355523000	0.956785000	1	-0.930991000	4.254579000	1.043232000
1	-0.883931000	-2.665229000	2.520130000	6	-0.431678000	-1.421416000	2.529435000
1	-1.434741000	-1.042826000	2.124328000	1	0.595714000	-1.719331000	2.722443000
6	0.513597000	-3.528211000	-0.619330000	1	-0.603967000	-0.438420000	2.968256000
1	0.872598000	-3.570673000	-1.647025000	1	-1.095805000	-2.123722000	3.041117000
1	0.827193000	-4.453467000	-0.128419000	6	1.085309000	-2.779085000	-0.340539000
1	-0.575526000	-3.524636000	-0.638924000	1	1.520625000	-2.543240000	-1.312247000
6	3.308950000	-2.061550000	-1.122567000	1	1.835592000	-2.646032000	0.436468000
1	4.152586000	-2.605334000	-0.687965000	1	0.810345000	-3.836971000	-0.358014000
1	2.889764000	-2.681709000	-1.913352000	6	-1.553658000	-1.555864000	-2.311215000
1	3.720539000	-1.158779000	-1.577703000	1	-2.169865000	-2.445344000	-2.474369000
6	3.656199000	0.190010000	1.020548000	1	-2.139644000	-0.691647000	-2.622676000
1	3.462679000	1.068391000	1.634107000	1	-0.675415000	-1.649926000	-2.948429000
1	4.496664000	-0.349485000	1.466245000	6	-3.111038000	-0.254574000	0.588484000
1	3.991714000	0.529917000	0.039203000	1	-3.868408000	-1.007687000	0.824867000
		1Ni		1	-3.028303000	0.402552000	1.454561000
28	-0.183209000	0.041674000	-0.142483000	1	-3.474632000	0.320374000	-0.262456000
6	-1.188346000	-1.458278000	-0.898802000			2Ni	
6	-1.823621000	-0.892539000	0.290062000	28	-0.804712000	-0.513657000	-0.027051000
6	-0.108155000	-1.966255000	-0.082129000	7	0.151196000	1.144670000	0.549453000
6	-0.731616000	-1.419088000	1.096349000	6	-1.677239000	-1.805291000	-1.199004000
8	1.649427000	0.383428000	-0.825261000	6	-1.438094000	-0.527272000	-1.879216000
8	2.455554000	-0.045337000	1.214743000	6	-0.011589000	-0.795491000	-1.861806000
6	2.610052000	0.256904000	0.018208000	6	-0.254578000	-2.064695000	-1.223712000

8	-2.453703000	-0.123959000	1.183195000	1	1.639462000	-2.944771000	-0.846291000
8	-0.854062000	-1.432435000	1.887883000	6	-2.860579000	-2.608419000	-0.867714000
6	-1.957868000	-0.846556000	2.102053000	1	-3.129069000	-3.245536000	-1.715270000
6	-2.651151000	-0.972991000	3.413616000	1	-2.665505000	-3.263175000	-0.017952000
1	-3.731316000	-0.979972000	3.282076000	1	-3.720555000	-1.978353000	-0.644405000
1	-2.333264000	-1.867233000	3.944023000	6	-2.308660000	0.483697000	-2.484477000
1	-2.401506000	-0.106277000	4.028195000	1	-2.853528000	0.044954000	-3.325399000
8	-0.796751000	2.215223000	0.756875000	1	-3.061033000	0.830945000	-1.772318000
6	1.405595000	1.603624000	0.670924000	1	-1.740867000	1.335881000	-2.850985000
6	2.465768000	0.559494000	0.576360000	TS1_{ni} (one imaginary frequency at 1096i cm ⁻¹)			
6	2.296307000	-0.739254000	1.050927000	28	0.189001000	-0.699641000	-0.090763000
6	3.689029000	0.926013000	0.013747000	7	-1.004156000	0.836307000	0.318982000
6	3.336062000	-1.654655000	0.961989000	6	1.217057000	-1.731211000	-1.475111000
1	1.361086000	-1.027260000	1.516446000	6	0.095947000	-2.524055000	-1.042170000
6	4.717175000	0.005162000	-0.091588000	6	-0.831957000	-1.561444000	-1.568154000
1	3.817739000	1.940104000	-0.346366000	6	0.295443000	-0.740509000	-2.028106000
6	4.543452000	-1.289119000	0.384351000	8	-0.251059000	-1.631477000	1.687428000
1	3.200682000	-2.658118000	1.348371000	8	1.175011000	-0.275153000	2.725817000
1	5.659013000	0.296556000	-0.541171000	6	0.309101000	-1.218757000	2.730085000
1	5.351046000	-2.007880000	0.312637000	6	-0.038326000	-1.814422000	4.050553000
8	1.720284000	2.797665000	0.849068000	1	0.857336000	-1.968610000	4.649222000
6	-0.939174000	3.065845000	-0.285753000	1	-0.673768000	-1.113795000	4.594527000
8	-0.347109000	2.960814000	-1.336526000	1	-0.575959000	-2.750618000	3.929561000
6	-1.907398000	4.142416000	0.057125000	8	-2.386954000	0.723446000	0.660269000
1	-2.549119000	3.870005000	0.890883000	6	-0.495582000	2.060311000	0.510216000
1	-1.344275000	5.034973000	0.334409000	6	0.972135000	2.019105000	0.265974000
1	-2.506900000	4.388100000	-0.816436000	6	1.623957000	0.772092000	0.366049000
6	1.169697000	-0.143194000	-2.434692000	6	1.663217000	3.180393000	-0.054041000
1	2.089191000	-0.569872000	-2.036829000	6	3.004260000	0.756547000	0.142350000
1	1.171355000	-0.291379000	-3.518416000	1	1.321821000	0.085817000	1.559583000
1	1.160452000	0.932354000	-2.255203000	6	3.027809000	3.122688000	-0.296929000
6	0.581308000	-3.193928000	-0.815295000	1	1.127357000	4.121568000	-0.118570000
1	0.316441000	-3.541775000	0.184839000	6	3.700034000	1.910875000	-0.191515000
1	0.406390000	-4.033359000	-1.494562000	1	3.558038000	-0.169021000	0.262995000

1	3.570698000	4.023448000	-0.558100000	6	-1.273695000	0.664292000	2.700829000
1	4.770786000	1.871374000	-0.357542000	6	-2.155169000	1.111119000	3.803926000
8	-1.115512000	3.088230000	0.842350000	1	-2.966389000	0.392133000	3.926143000
6	-3.249763000	1.280505000	-0.227265000	1	-1.603420000	1.134215000	4.742598000
8	-2.908137000	1.864557000	-1.230085000	1	-2.572918000	2.089624000	3.590269000
6	-4.655741000	1.046837000	0.198586000	8	2.175792000	-0.970435000	1.096768000
1	-5.169695000	0.494606000	-0.588383000	6	0.389955000	-2.165683000	0.200684000
1	-4.723254000	0.495145000	1.131954000	6	-0.981371000	-2.037753000	-0.345803000
1	-5.160171000	2.006550000	0.304203000	6	-1.485415000	-0.744408000	-0.551511000
6	-2.289646000	-1.541916000	-1.751961000	6	-1.751384000	-3.173656000	-0.584694000
1	-2.634041000	-0.567431000	-2.092284000	6	-2.813885000	-0.632033000	-0.953118000
1	-2.580274000	-2.278767000	-2.505953000	1	-0.059331000	-0.675819000	2.153681000
1	-2.813367000	-1.805622000	-0.830816000	6	-3.060414000	-3.035641000	-1.016894000
6	0.438635000	0.421641000	-2.912663000	1	-1.318293000	-4.155027000	-0.419533000
1	1.384521000	0.935972000	-2.738358000	6	-3.593545000	-1.763267000	-1.185227000
1	0.423481000	0.104227000	-3.959558000	1	-3.268837000	0.343374000	-1.092349000
1	-0.380607000	1.127922000	-2.772587000	1	-3.667873000	-3.911842000	-1.210027000
6	2.656560000	-1.997443000	-1.597887000	1	-4.624707000	-1.649631000	-1.503615000
1	3.083995000	-2.368632000	-0.665758000	8	0.997736000	-3.236235000	0.336178000
1	2.817129000	-2.773076000	-2.352497000	6	3.143403000	-1.283065000	0.196316000
1	3.204511000	-1.111082000	-1.911125000	6	4.475181000	-1.298596000	0.858511000
6	-0.037691000	-3.819149000	-0.371220000	1	4.450076000	-0.855047000	1.850254000
1	-0.982318000	-3.899266000	0.164643000	1	4.807894000	-2.333820000	0.945213000
1	-0.015585000	-4.615042000	-1.121524000	1	5.195175000	-0.774796000	0.232088000
1	0.786917000	-3.999226000	0.317871000	8	2.933424000	-1.514050000	-0.971925000
		3Ni		6	0.662002000	0.396807000	-3.062099000
28	-0.180850000	0.665956000	-0.129448000	1	-0.281815000	0.012177000	-3.447695000
7	0.834819000	-0.936729000	0.586511000	1	1.131639000	0.985431000	-3.856432000
6	0.452006000	1.228243000	-1.869569000	1	1.322922000	-0.444583000	-2.851585000
6	-0.627275000	2.077561000	-1.388845000	6	-1.926025000	2.513805000	-1.923856000
6	0.312452000	2.675025000	-0.426154000	1	-2.651547000	2.691934000	-1.127749000
6	1.356883000	1.846920000	-0.873992000	1	-1.812583000	3.455966000	-2.469108000
8	-1.179670000	1.267747000	1.630953000	1	-2.340355000	1.783529000	-2.616986000
8	-0.606420000	-0.443170000	2.955919000	6	0.207230000	3.750441000	0.567495000

1	0.868334000	3.579670000	1.417610000	1	3.197732000	1.231736000	0.898241000
1	0.504994000	4.699071000	0.110716000	1	2.742282000	2.549317000	1.979082000
1	-0.814019000	3.871108000	0.926173000	1	2.075561000	0.949121000	2.246813000
6	2.800644000	1.783880000	-0.584701000	6	1.880314000	2.105407000	-1.977901000
1	3.296191000	1.023530000	-1.184094000	1	1.363803000	1.589044000	-2.788732000
1	3.265419000	2.745262000	-0.818206000	1	2.115849000	3.109896000	-2.340986000
1	3.003123000	1.589082000	0.470654000	1	2.820969000	1.594830000	-1.774711000
		4Ni		6	-1.468151000	3.046990000	-1.387722000
28	-0.076652000	0.623991000	-0.107162000	1	-2.439887000	2.967915000	-0.902752000
7	0.640449000	-1.083964000	-0.458036000	1	-1.287720000	4.105467000	-1.598835000
6	-0.396504000	2.514874000	-0.537263000	1	-1.508248000	2.531597000	-2.348220000
6	-0.198567000	2.327982000	0.860080000	6	-0.975072000	2.585589000	2.079151000
6	1.237034000	1.996624000	0.602167000	1	-0.776624000	1.834539000	2.844567000
6	1.040736000	2.179534000	-0.776143000	1	-0.696660000	3.555997000	2.501290000
8	2.011772000	-1.379392000	-0.713497000	1	-2.044702000	2.608138000	1.876050000
6	-0.161594000	-2.175273000	-0.422686000			5Ni	
6	-1.561616000	-1.730338000	-0.178382000	28	0.310565000	0.668520000	-0.333469000
6	-1.759830000	-0.352754000	0.010184000	7	-0.974253000	-0.864326000	-0.264743000
6	-2.609066000	-2.639371000	-0.129874000	6	1.192698000	2.220973000	0.501142000
6	-3.058859000	0.082320000	0.247435000	6	-0.065785000	2.713016000	-0.080746000
6	-3.898567000	-2.179566000	0.108241000	6	-0.819054000	1.952890000	0.837577000
1	-2.411681000	-3.696861000	-0.275849000	6	0.420720000	1.446215000	1.455435000
6	-4.120327000	-0.822430000	0.295654000	8	-2.346345000	-0.787395000	-0.671801000
1	-3.270548000	1.136763000	0.400855000	6	-0.478663000	-2.112128000	-0.320108000
1	-4.726093000	-2.877818000	0.149349000	6	0.987211000	-2.061387000	-0.097873000
1	-5.126644000	-0.462622000	0.482183000	6	1.605535000	-0.803021000	-0.090092000
8	0.199549000	-3.349433000	-0.565865000	6	1.725249000	-3.234194000	0.045548000
6	2.700681000	-1.846495000	0.362504000	6	2.988891000	-0.760399000	0.047732000
6	4.122411000	-2.085062000	-0.001966000	6	3.099784000	-3.168763000	0.203580000
1	4.302877000	-3.160496000	-0.025649000	1	1.209742000	-4.189206000	0.023266000
1	4.375803000	-1.663267000	-0.970862000	6	3.729757000	-1.930044000	0.199197000
1	4.765471000	-1.662808000	0.768509000	1	3.519839000	0.185502000	0.023908000
8	2.204317000	-2.034124000	1.447971000	1	3.680296000	-4.076430000	0.319452000
6	2.371389000	1.655153000	1.469450000	1	4.807513000	-1.872130000	0.307836000

8	-1.120544000	-3.158198000	-0.534204000	8	-2.393539000	-0.695033000	-0.666837000
6	-0.150150000	0.865315000	-2.481610000	6	-0.561857000	-2.071506000	-0.402031000
1	-1.185181000	0.982255000	-2.722239000	6	0.900268000	-2.060629000	-0.186263000
6	1.058924000	0.732472000	-2.388350000	6	1.592768000	-0.851024000	-0.362689000
1	2.112801000	0.637627000	-2.539685000	6	1.571585000	-3.214575000	0.214493000
6	-3.249920000	-1.193386000	0.251609000	6	2.963871000	-0.830329000	-0.093220000
8	-2.959717000	-1.626098000	1.344456000	6	2.925124000	-3.170132000	0.492225000
6	-4.634397000	-1.024584000	-0.267618000	1	1.008442000	-4.135685000	0.323166000
1	-5.222389000	-0.472287000	0.464432000	6	3.616352000	-1.968730000	0.347778000
1	-4.660923000	-0.510126000	-1.224303000	1	3.538291000	0.072420000	-0.267903000
1	-5.092103000	-2.007778000	-0.376816000	1	3.446378000	-4.062613000	0.816489000
6	0.708805000	0.744119000	2.714002000	1	4.678243000	-1.927693000	0.562588000
1	1.737150000	0.386564000	2.744879000	8	-1.227222000	-3.092311000	-0.667229000
1	0.562961000	1.417918000	3.563556000	6	0.182193000	0.704012000	-2.344165000
1	0.037455000	-0.104190000	2.857382000	1	-0.419217000	1.176840000	-3.100837000
6	2.581611000	2.698852000	0.421648000	6	1.271169000	0.104558000	-2.099619000
1	2.932730000	2.763351000	-0.609759000	1	2.222850000	-0.181874000	-2.512745000
1	2.652325000	3.705832000	0.844206000	6	-3.310710000	-1.058564000	0.257493000
1	3.260790000	2.062629000	0.986280000	8	-3.035280000	-1.514236000	1.345554000
6	-0.378873000	3.696849000	-1.124011000	6	-4.687796000	-0.790599000	-0.239676000
1	-1.380230000	3.556498000	-1.530149000	1	-5.136603000	-0.018468000	0.386648000
1	-0.334000000	4.703932000	-0.698925000	1	-4.700273000	-0.462400000	-1.275056000
1	0.345977000	3.662835000	-1.937768000	1	-5.292026000	-1.689356000	-0.129071000
6	-2.249245000	1.825257000	1.149639000	6	0.459468000	0.658795000	2.705930000
1	-2.570602000	2.674443000	1.759501000	1	1.440071000	0.190465000	2.794871000
1	-2.862048000	1.828798000	0.247009000	1	0.315701000	1.292685000	3.585781000
1	-2.453898000	0.920920000	1.720453000	1	-0.301685000	-0.122533000	2.741259000
	TS_{Ni} (one imaginary frequency at 357i cm⁻¹)			6	2.697441000	2.474438000	0.635939000
28	0.288282000	0.712365000	-0.369591000	1	3.117875000	2.476115000	-0.371334000
7	-1.026575000	-0.823149000	-0.242673000	1	2.857684000	3.476293000	1.045318000
6	1.259249000	2.178283000	0.623570000	1	3.252008000	1.772487000	1.255616000
6	0.136541000	2.720664000	-0.137760000	6	0.017194000	3.722157000	-1.207190000
6	-0.777772000	2.018726000	0.710770000	1	-0.948432000	3.660543000	-1.707451000
6	0.350276000	1.444509000	1.467587000	1	0.110504000	4.727812000	-0.787288000

6	-1.877034000	-1.441701000	-0.081144000	7	-1.493212000	1.038370000	-0.597974000
6	-4.296866000	-1.248734000	-0.470655000	6	1.174072000	-0.170821000	1.424223000
6	-2.073420000	-2.812690000	0.092157000	6	1.237399000	-1.390728000	0.658445000
6	-4.452008000	-2.616791000	-0.289975000	6	2.048234000	-0.665896000	-0.409816000
1	-5.151560000	-0.614772000	-0.686964000	6	1.545779000	0.594749000	0.277795000
6	-3.336456000	-3.395711000	-0.014327000	8	3.503800000	-0.960924000	-0.082266000
1	-1.234473000	-3.464388000	0.316605000	8	4.282163000	0.695489000	-1.404388000
1	-5.432942000	-3.071479000	-0.365256000	6	4.469588000	-0.241209000	-0.648274000
1	-3.449358000	-4.466533000	0.121762000	6	5.819413000	-0.737679000	-0.245425000
8	-3.757951000	1.601731000	-0.688742000	1	5.975779000	-1.739170000	-0.647539000
6	-1.317680000	3.179582000	0.317641000	1	6.594749000	-0.077180000	-0.622701000
6	-1.023213000	4.608495000	0.021594000	1	5.893740000	-0.813305000	0.838516000
1	-0.446965000	4.725504000	-0.893030000	8	-1.233959000	2.440709000	-0.800441000
1	-1.968661000	5.139848000	-0.098810000	6	-2.809696000	0.761992000	-0.611464000
1	-0.494404000	5.056126000	0.859862000	6	-2.998767000	-0.698416000	-0.396693000
8	-1.589038000	2.726403000	1.407906000	6	-1.845891000	-1.440062000	-0.059136000
6	0.824193000	0.059960000	2.817865000	6	-4.257616000	-1.273279000	-0.525392000
1	0.137219000	-0.678761000	3.232427000	6	-2.040986000	-2.812506000	0.119451000
1	1.745449000	0.014565000	3.407097000	6	-4.408569000	-2.640896000	-0.336027000
1	0.397881000	1.054429000	2.955291000	1	-5.110563000	-0.648384000	-0.773582000
6	1.279491000	-2.848382000	0.925062000	6	-3.294960000	-3.407742000	-0.019733000
1	1.062817000	-3.475276000	0.058351000	1	-1.203700000	-3.455301000	0.376363000
1	2.285157000	-3.111410000	1.268548000	1	-5.383330000	-3.104151000	-0.435917000
1	0.583477000	-3.117665000	1.720149000	1	-3.403563000	-4.478340000	0.123365000
6	1.877789000	-0.888424000	-1.922907000	8	-3.738782000	1.576234000	-0.782733000
1	2.383614000	-0.103260000	-2.479561000	6	-1.298133000	3.196003000	0.317177000
1	2.344886000	-1.846662000	-2.149272000	6	-0.981394000	4.616950000	0.002895000
1	0.840886000	-0.940416000	-2.272980000	1	-0.422765000	4.716843000	-0.924515000
6	1.847359000	2.025661000	0.128504000	1	-1.917599000	5.167945000	-0.098748000
1	1.221111000	2.648157000	0.769021000	1	-0.424805000	5.059322000	0.826118000
1	2.885055000	2.215322000	0.420037000	8	-1.583513000	2.766250000	1.414104000
1	1.734971000	2.369818000	-0.900965000	6	0.873578000	0.154901000	2.830719000
		10		1	0.162263000	-0.551102000	3.261760000
28	-0.263861000	-0.279167000	0.072291000	1	1.784120000	0.108988000	3.436313000

1	0.466252000	1.162021000	2.930618000	1	2.696539000	3.500302000	0.865203000
6	1.327136000	-2.813047000	1.059627000	6	4.300571000	0.594532000	0.185985000
1	1.099050000	-3.486065000	0.230242000	1	3.366310000	-1.267882000	-0.262435000
1	2.336022000	-3.064925000	1.405916000	1	4.999384000	2.569319000	0.671738000
1	0.639045000	-3.042752000	1.874743000	1	5.298954000	0.174058000	0.121690000
6	1.824397000	-0.964652000	-1.868512000	8	0.121461000	3.343312000	0.900662000
1	2.330486000	-0.254715000	-2.519792000	6	-2.430424000	2.406815000	-0.369602000
1	2.171289000	-1.970332000	-2.114165000	6	-3.846610000	2.692540000	-0.008587000
1	0.753506000	-0.921870000	-2.085240000	1	-4.172057000	2.138882000	0.867844000
6	1.896614000	2.024955000	0.112912000	1	-3.956055000	3.760503000	0.179800000
1	1.287724000	2.649900000	0.769377000	1	-4.484320000	2.445799000	-0.856838000
1	2.942041000	2.221204000	0.372208000	8	-1.863581000	2.827913000	-1.355167000
1	1.751987000	2.371681000	-0.912486000	6	0.449228000	0.014916000	-3.121526000
		11		1	1.535468000	0.101603000	-3.145532000
28	0.165756000	-0.639313000	-0.144825000	1	0.124290000	-0.348404000	-4.101657000
7	-0.509742000	1.204405000	0.277618000	1	0.026477000	1.013067000	-2.992261000
6	0.007240000	-0.895986000	-2.053490000	6	1.763822000	-2.903358000	-1.594310000
6	0.561383000	-2.076058000	-1.401863000	1	2.111614000	-3.339377000	-0.655672000
6	-0.772269000	-2.365056000	-0.854999000	1	1.549938000	-3.735871000	-2.272223000
6	-1.311984000	-1.221299000	-1.474836000	1	2.579512000	-2.329411000	-2.032089000
8	0.257310000	-1.354766000	1.773089000	6	-1.313112000	-3.472651000	-0.054079000
8	-1.947449000	-1.091653000	2.097314000	1	-2.281899000	-3.225083000	0.376794000
6	-0.811621000	-1.438803000	2.473446000	1	-1.444622000	-4.353415000	-0.690025000
6	-0.650413000	-2.028868000	3.853089000	1	-0.630905000	-3.764587000	0.746308000
1	-1.095485000	-1.368613000	4.597589000	6	-2.662366000	-0.645856000	-1.598514000
1	-1.196696000	-2.972985000	3.900140000	1	-2.627253000	0.348947000	-2.040718000
1	0.389781000	-2.214703000	4.111599000	1	-3.281025000	-1.268708000	-2.250704000
8	-1.862584000	1.596612000	0.548961000	1	-3.172885000	-0.587148000	-0.635444000
6	0.376231000	2.173846000	0.541979000		TS-B (one imaginary frequency at 218i cm ⁻¹)		
6	1.752659000	1.640250000	0.371233000	28	-0.260722000	-0.223930000	-0.078979000
6	1.896399000	0.284593000	0.031161000	7	1.280024000	0.852659000	0.470225000
6	2.855199000	2.459880000	0.597855000	6	-1.072186000	0.318229000	-1.714622000
6	3.191926000	-0.220341000	-0.038628000	6	-1.726154000	-0.891223000	-1.214485000
6	4.135927000	1.937954000	0.497315000	6	-2.658277000	0.029725000	-0.550534000

6	-1.673364000	1.098613000	-0.633525000	1	-1.140781000	-2.548172000	-2.423409000
8	-3.059913000	-0.533751000	1.274706000	6	-4.107463000	0.152785000	-0.851209000
8	-0.919247000	-0.524081000	1.944766000	1	-4.588373000	0.910152000	-0.234549000
6	-2.145125000	-0.648687000	2.157658000	1	-4.204222000	0.456611000	-1.897117000
6	-2.617738000	-0.992286000	3.542474000	1	-4.628513000	-0.795004000	-0.725325000
1	-2.851154000	-2.057824000	3.579327000	6	-1.812681000	2.552416000	-0.395245000
1	-1.848216000	-0.786373000	4.282788000	1	-0.975474000	3.105009000	-0.823500000
1	-3.528916000	-0.452744000	3.794821000	1	-2.727410000	2.950482000	-0.847899000
8	1.244034000	2.219861000	0.909967000	1	-1.853063000	2.788799000	0.671142000
6	2.500275000	0.307109000	0.542223000			12	
6	2.398492000	-1.131269000	0.181631000	28	-0.193329000	-0.224899000	-0.111541000
6	1.116401000	-1.625625000	-0.144487000	7	1.292664000	0.889734000	0.500151000
6	3.529721000	-1.941126000	0.198571000	6	-1.219221000	0.291117000	-1.662879000
6	1.039233000	-2.993189000	-0.421161000	6	-1.714937000	-0.955570000	-1.109954000
6	3.415742000	-3.291670000	-0.098991000	6	-2.696091000	-0.134847000	-0.291597000
1	4.491999000	-1.506623000	0.454106000	6	-1.729705000	1.004466000	-0.522268000
6	2.164805000	-3.815487000	-0.401775000	8	-3.043215000	-0.582171000	1.105999000
1	0.081022000	-3.448220000	-0.657880000	8	-0.949551000	-0.517332000	1.948622000
1	4.290478000	-3.931347000	-0.088901000	6	-2.152642000	-0.708797000	2.072225000
1	2.064745000	-4.873370000	-0.624485000	6	-2.778887000	-1.131723000	3.356829000
8	3.560838000	0.884364000	0.872142000	1	-3.179093000	-2.140904000	3.253128000
6	1.661248000	3.127487000	0.000396000	1	-2.045201000	-1.120567000	4.157317000
6	1.547479000	4.505495000	0.553459000	1	-3.613858000	-0.479827000	3.609796000
1	0.802163000	4.567296000	1.342708000	8	1.219487000	2.267364000	0.913261000
1	2.512349000	4.796830000	0.971395000	6	2.535367000	0.397511000	0.565889000
1	1.307118000	5.201618000	-0.246784000	6	2.494867000	-1.044419000	0.206581000
8	2.071424000	2.845183000	-1.104489000	6	1.238250000	-1.579258000	-0.163651000
6	-0.517630000	0.680368000	-3.031950000	6	3.655932000	-1.809233000	0.249775000
1	0.081737000	-0.133289000	-3.443151000	6	1.232183000	-2.944467000	-0.470592000
1	-1.321977000	0.888367000	-3.745137000	6	3.605822000	-3.159036000	-0.069871000
1	0.105416000	1.573137000	-2.971608000	1	4.592730000	-1.341394000	0.539626000
6	-2.007080000	-2.187904000	-1.868347000	6	2.387487000	-3.723932000	-0.427752000
1	-2.283860000	-2.957414000	-1.144477000	1	0.303148000	-3.433656000	-0.753471000
1	-2.836292000	-2.101652000	-2.579417000	1	4.504325000	-3.764418000	-0.038262000

1	2.337045000	-4.779892000	-0.675343000	6	1.466540000	1.310327000	0.142326000
8	3.574028000	1.022403000	0.882492000	6	1.209325000	3.744616000	0.175630000
6	1.534341000	3.163562000	-0.043842000	6	2.763445000	1.477083000	0.625411000
6	1.391056000	4.553916000	0.470565000	6	2.502127000	3.882327000	0.661470000
1	0.822765000	4.595362000	1.396214000	1	0.588583000	4.614847000	-0.014936000
1	2.385586000	4.963373000	0.652202000	6	3.272756000	2.748401000	0.889964000
1	0.915716000	5.173421000	-0.287586000	1	3.396193000	0.613866000	0.808787000
8	1.886156000	2.867000000	-1.165667000	1	2.908298000	4.867182000	0.860901000
6	-0.704728000	0.685561000	-2.989335000	1	4.282737000	2.854524000	1.273107000
1	-0.073080000	-0.092316000	-3.421709000	8	-1.421810000	3.141120000	-0.998969000
1	-1.531046000	0.858522000	-3.687906000	6	-3.292510000	0.979006000	-0.481383000
1	-0.123062000	1.607174000	-2.941120000	6	-4.508252000	0.729397000	-1.303710000
6	-1.956281000	-2.266203000	-1.760671000	1	-4.878130000	1.693404000	-1.656429000
1	-2.114103000	-3.065593000	-1.032922000	1	-4.309618000	0.099121000	-2.165987000
1	-2.847495000	-2.235295000	-2.398690000	1	-5.286489000	0.288310000	-0.684082000
1	-1.117462000	-2.556265000	-2.395101000	8	-3.283171000	1.477954000	0.619296000
6	-4.082197000	0.026909000	-0.878570000	8	3.591456000	-1.792636000	0.511430000
1	-4.652336000	0.787651000	-0.343032000	8	2.018361000	-1.252276000	-1.001899000
1	-4.009258000	0.326510000	-1.923985000	6	3.176795000	-1.677978000	-0.653170000
1	-4.640610000	-0.909364000	-0.827477000	6	4.078463000	-2.033940000	-1.807908000
6	-1.903956000	2.448791000	-0.238045000	1	4.784663000	-2.811557000	-1.522662000
1	-1.136076000	3.046132000	-0.732449000	1	3.517224000	-2.346827000	-2.686343000
1	-2.873340000	2.817499000	-0.594094000	1	4.654824000	-1.147896000	-2.082783000
1	-1.855931000	2.668685000	0.832303000	6	-0.071346000	-3.373225000	-0.741147000
		13		1	1.013155000	-3.464310000	-0.679106000
28	0.478267000	-0.344394000	-0.315942000	1	-0.499805000	-4.236240000	-0.214540000
7	-0.933106000	0.926350000	-0.539544000	1	-0.344210000	-3.478722000	-1.794242000
6	-0.556729000	-2.083908000	-0.159054000	6	0.800206000	-1.953954000	2.164708000
6	-0.241578000	-1.610077000	1.183920000	1	0.893211000	-1.179129000	2.929625000
6	-1.652875000	-1.314724000	1.473664000	1	0.495593000	-2.869571000	2.687583000
6	-2.000643000	-1.898641000	0.297416000	1	1.772973000	-2.123629000	1.707648000
8	-2.177995000	0.603385000	-1.164364000	6	-2.321678000	-0.714063000	2.639357000
6	-0.658014000	2.251288000	-0.587190000	1	-3.405045000	-0.698673000	2.521565000
6	0.710678000	2.470271000	-0.070268000	1	-2.091790000	-1.265228000	3.556394000

