

The fundamental nature and importance of electrostatic potential in hydrogen bond formation: A case study of heterocycles frequently observed in drugs

Mambatta Haritha^{a,b} and Cherumuttathu H. Suresh^{*a,b}

^aChemical Sciences and Technology Division, CSIR– National Institute for Interdisciplinary Science and Technology, Thiruvananthapuram Kerala, 695 019, India.

^bAcademy of Scientific and Innovative Research (AcSIR), Ghaziabad 201002, India.
Tel: +91-471-2515472, E-mail: sureshch@niist.res.in, sureshch@gmail.com

Supporting Information

Table of Contents

1. Figure S1. Dataset of ring systems in r_b category (CN [—] HN motif) and their ring...H ₂ O complex	–S2
2. Figure S2. Dataset of ring systems in r_c category (CN [—] HC motif) and their ring...H ₂ O complex	–S3
3. Figure S3. Dataset of ring systems in r_d category (CF [—] HC motif) and their ring...H ₂ O complex	–S4
4. Figure S4. Dataset of ring systems in r_e category (CN [—] OC motif) and their ring...H ₂ O complex	–S5
5. Table S1. MESP topology data and hydrogen bond energy data in kcal/mol for ring molecules in category r_b .	–S6
6. Table S2. MESP topology data and hydrogen bond energy data in kcal/mol for ring molecules in category r_c .	–S6
7. Table S3. MESP topology data and hydrogen bond energy data in kcal/mol for ring molecules in category r_d .	–S7
8. Table S4. MESP topology data and hydrogen bond energy data in kcal/mol for ring molecules in category r_e .	–S8
9. Table S5. Cartesian coordinates of optimized geometry of rings at M06L/6-311++G(d,p) level. Atomic number followed by X, Y, Z coordinates in Å.	–S8

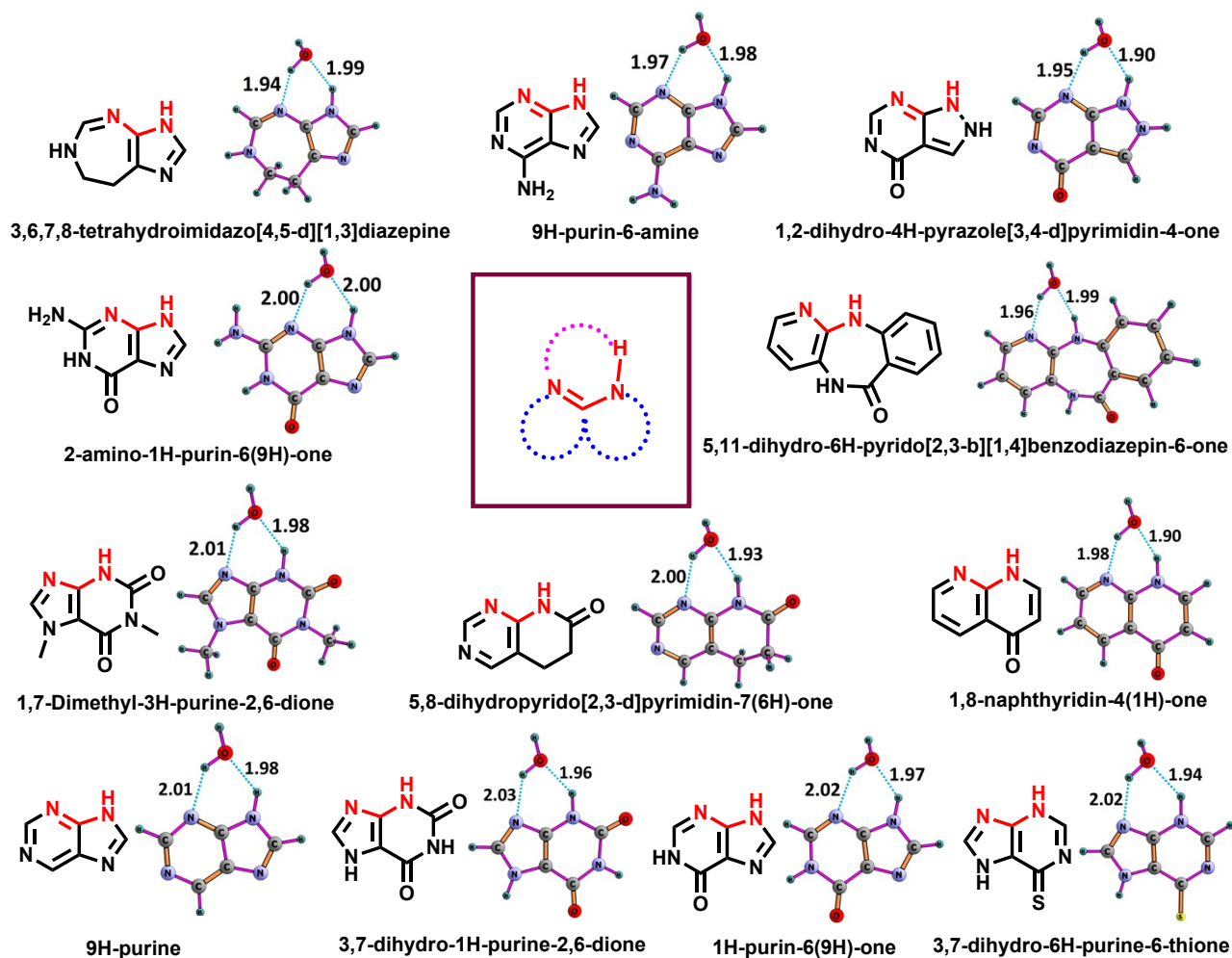
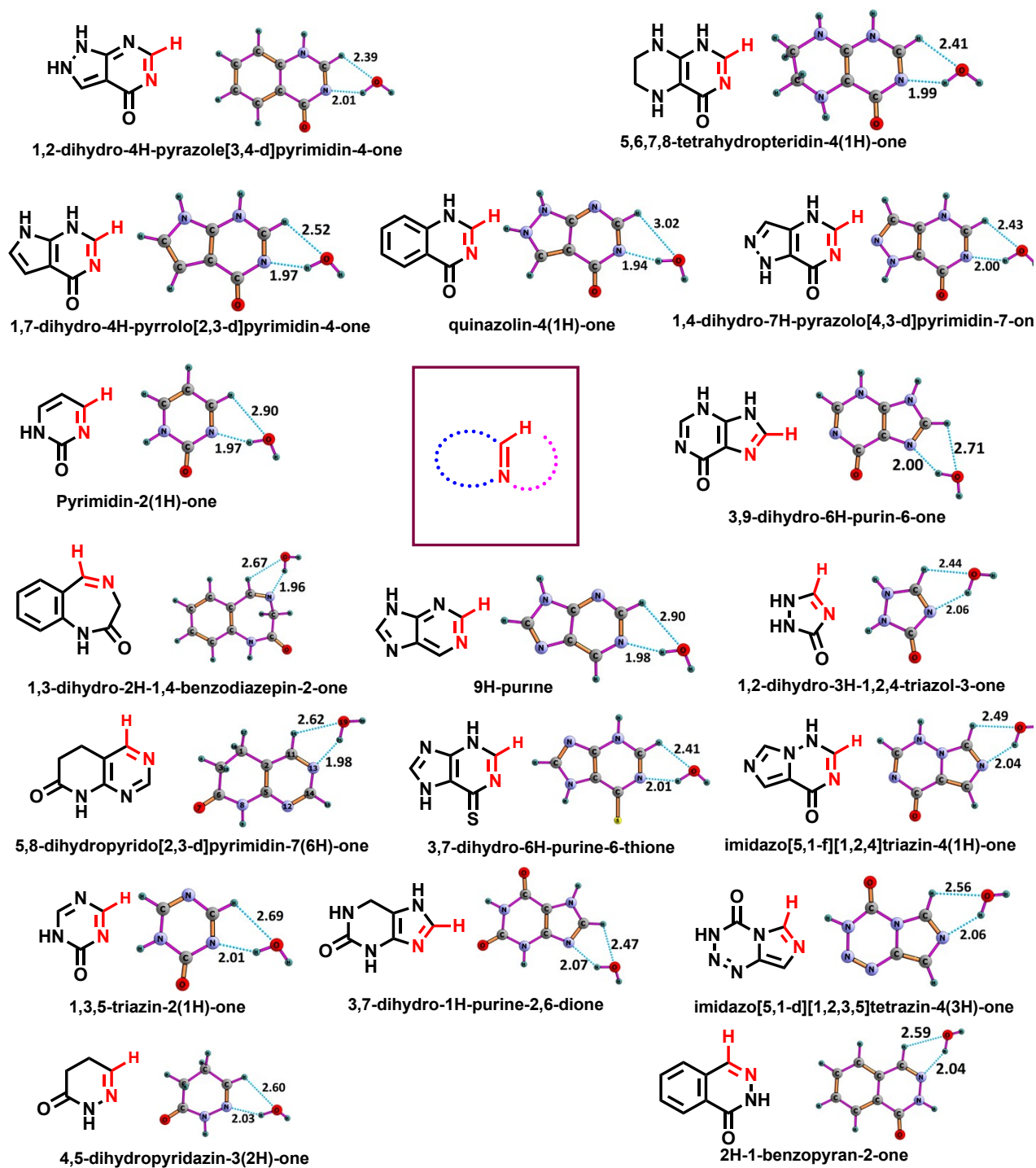


Figure S1. Dataset of ring systems in r_b category (CN⁻HN motif) and their ring...H₂O complex



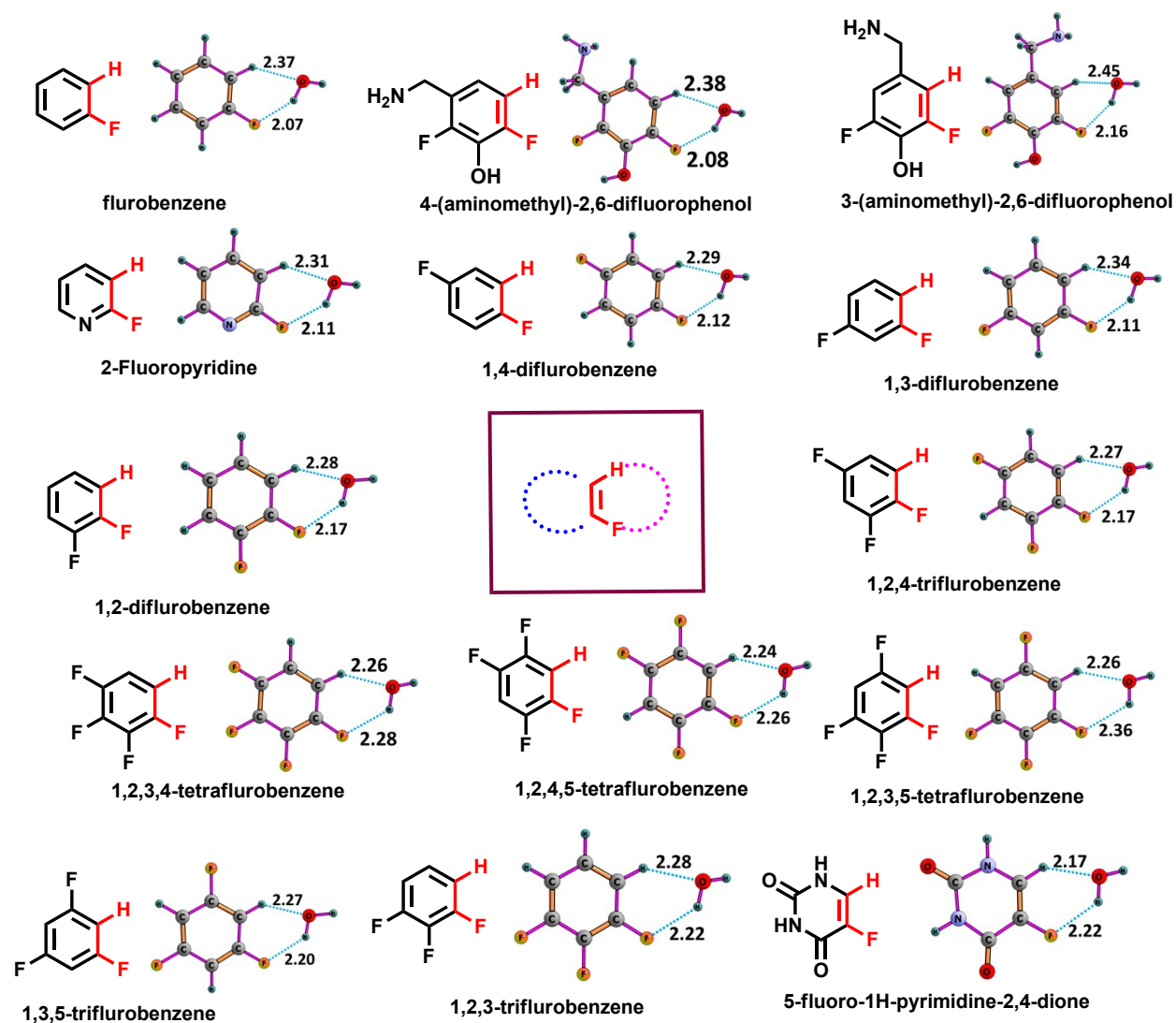


Figure S3. Dataset of ring systems in r_d category (CF⁻HC motif) and their ring...H₂O complex

Fi

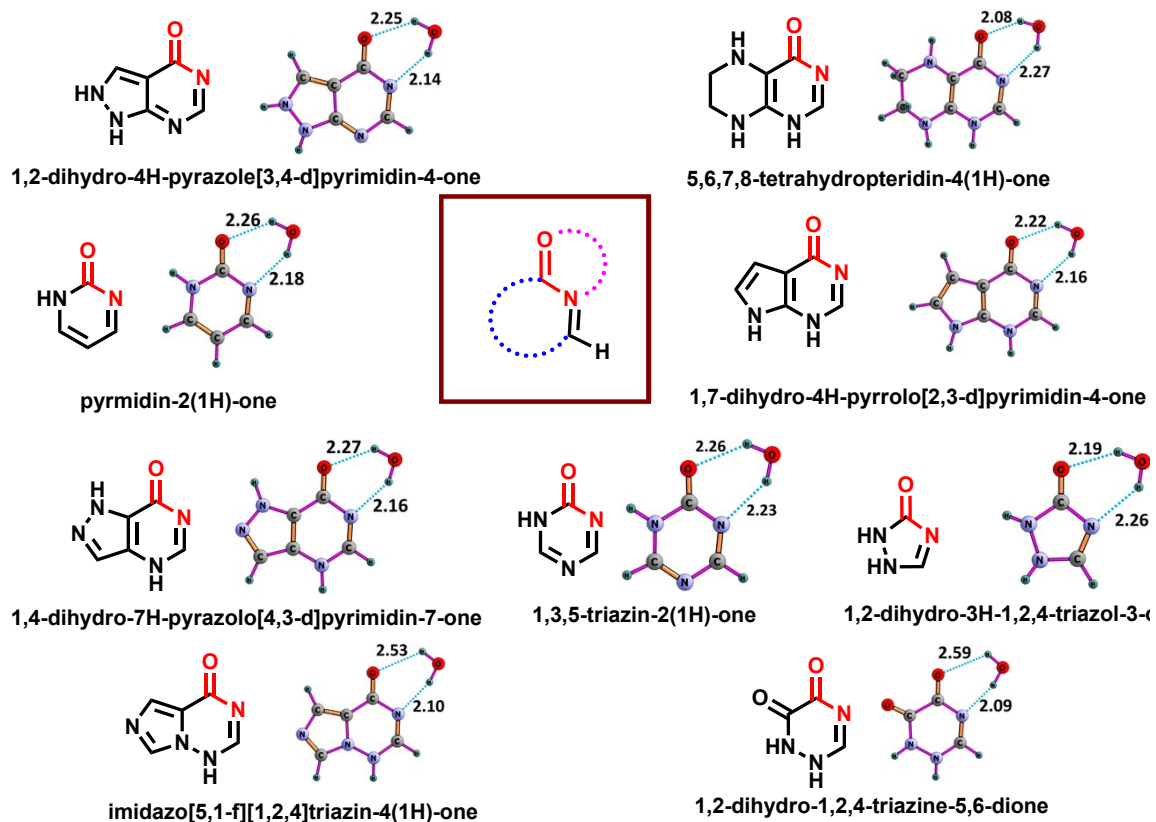


Table S1. MESP topology data and hydrogen bond energy data in kcal/mol for ring molecules in category r_b .

Label	Ring	$\Delta V_{n(CN)}$	$\Delta V_{n(NH)}$	E_{int}	ΔE_{int}
r_{b1}	3,6,7,8-tetrahydroimidazo[4,5-d][1,3]diazepine	15.3	15.8	-10.5	0.7
r_{b2}	9H-purin-6-amine	20.6	32.8	-11.4	-0.3
r_{b3}	1,2-dihydro-4H-pyrazole[3,4-d]pyrimidin-4-one	22.0	49.3	-15.0	-3.9
r_{b4}	2-amino-1H-purin-6(9H)-one	28.3	31.1	-9.4	1.7
r_{b5}	5,11-dihydro-6H-pyrido[2,3-b][1,4]benzodiazepin-6-one	28.4	7.0	-9.3	1.8
r_{b6}	1,7-Dimethyl-3H-purine-2,6-dione	30.3	26.5	-9.5	1.7
r_{b7}	1,7-Dimethyl-3H-purine-2,6-dione	33.5	22.3	-8.9	2.3
r_{b8}	5,8-dihydropyrido[2,3-d]pyrimidin-7(6H)-one	33.7	29.4	-10.5	0.6
r_{b9}	1,8-naphthyridin-4(1H)-one	34.4	40.2	-11.0	0.1
r_{b10}	9H-purine	36.3	30.9	-9.4	1.7
r_{b11}	3,7-dihydro-1H-purine-2,6-dione	37.3	37.7	-10.3	0.9
r_{b12}	1H-purin-6(9H)-one	37.7	43.1	-11.0	0.1
r_{b12}	3,7-dihydro-6H-purine-6-thione				

Table S2. MESP topology data and hydrogen bond energy data in kcal/mol for ring molecules in category r_c .

Label	Ring	$\Delta V_{n(CN)}$	$\Delta V_{n(CH)}$	E_{int}	ΔE_{int}
r_{c1}	1,2-dihydro-4H-pyrazole[3,4-d]pyrimidin-4-one	-14.9	-10.4	-7.6	-1.2
r_{c2}	5,6,7,8-tetrahydropteridin-4(1H)-one	-9.5	13.7	-8.0	-1.7
r_{c3}	1,7-dihydro-4H-pyrrolo[2,3-d]pyrimidin-4-one	-7.2	17.3	-8.2	-1.8
r_{c4}	quinazolin-4(1H)-one	-3.3	19.9	-7.8	-1.4
r_{c5}	1,4-dihydro-7H-pyrazolo[4,3-d]pyrimidin-7-one	2.2	23.3	-7.6	-1.2
r_{c6}	Pyrimidin-2(1H)-one	3.1	5.9	-7.1	-0.7
r_{c7}	3,9-dihydro-6H-purin-6-one	3.6	26.5	-7.3	-0.9
r_{c8}	1,3-dihydro-2H-1,4-benzodiazepin-2-one	3.9	1.9	-6.5	-0.2
r_{c9}	9H-purine	3.9	-3.3	-6.0	0.4
r_{c10}	1,2-dihydro-3H-1,2,4-triazol-3-one	4.3	34.5	-6.9	-0.5
r_{c11}	5,8-dihydropyrido[2,3-d]pyrimidin-7(6H)-one	5.5	8.0	-6.4	0.0
r_{c12}	3,7-dihydro-6H-purine-6-thione	7.5	24.1	-7.6	-1.2
r_{c13}	imidazo[5,1-f][1,2,4]triazin-4(1H)-one	7.7	34.9	-6.8	-0.4
r_{c14}	1,3,5-triazin-2(1H)-one	11.4	9.8	-6.1	0.3
r_{c15}	3,7-dihydro-1H-purine-2,6-dione	13.5	33.5	-5.7	0.7
r_{c16}	imidazo[5,1-d][1,2,3,5]tetrazin-4(3H)-one	15.8	32.3	-5.5	0.8
r_{c17}	4,5-dihydropyridazin-3(2H)-one	28.0	8.6	-5.2	1.2
r_{c18}	2H-1-benzopyran-2-one	33.8	10.2	-4.8	1.6

Table S3. MESP topology data and hydrogen bond energy data in kcal/mol for ring molecules in category r_d .

Label	Ring	$\Delta V_{n(CF)}$	$\Delta V_{n(CH)}$	E_{int}	ΔE_{int}
r_{d1}	Fluorobenzene	-1.6	-2.2	-3.2	-0.2
r_{d2}	4-(aminomethyl)-2,6-difluorophenol	-0.7	-6.5	-2.7	0.2
r_{d3}	3-(aminomethyl)-2,6-difluorophenol	-0.4	-3.3	-3.1	-0.1
r_{d4}	2-Fluoropyridine	0.8	6.0	-3.5	-0.6
r_{d5}	14-difluorobenzene	2.1	4.4	-3.4	-0.4
r_{d6}	13-difluorobenzene	4.7	2.3	-3.0	0.0
r_{d7}	12-difluorobenzene	6.7	4.2	-3.2	-0.2
r_{d8}	124-trifluorobenzene	10.2	10.7	-3.3	-0.4
r_{d9}	135-trifluorobenzene	10.8	14.1	-3.0	-0.1
r_{d10}	123-trifluorobenzene	12.4	8.1	-3.1	-0.2
r_{d11}	5-fluoro-1H-pyrimidine-2,4-dione	14.0	34.6	-4.9	-2.0
r_{d12}	1234-tetrafluorobenzene	15.4	14.4	-3.4	-0.4
r_{d13}	1245-tetrafluorobenzene	15.9	22.3	-3.5	-0.6
r_{d14}	1235-tetrafluorobenzene	18.5	19.9	-3.3	-0.3

Table S4. MESP topology data and hydrogen bond energy data in kcal/mol for ring molecules

Label	Ring	$\Delta V_{n(CN)}$	$\Delta V_{n(CO)}$	E_{int}	ΔE_{int}
r_{e1}	1,2-dihydro-4H-pyrazole[3,4-d]pyrimidin-4-one	-34.4	-35.8	-8.4	-3.0
r_{e2}	5,6,7,8-tetrahydropteridin-4(1H)-one	-29.1	-45.7	-8.6	-3.2
r_{e3}	1,7-dihydro-4H-pyrrolo[2,3-d]pyrimidin-4-one	-26.8	-42.5	-8.3	-2.9
r_{e4}	1,4-dihydro-7H-pyrazolo[4,3-d]pyrimidin-7-one	-17.4	-28.2	-7.3	-1.9
r_{e5}	pyrimidin-2-on	-16.7	-30.6	-7.2	-1.9
r_{e6}	1,2-dihydro-3H-1,2,4-triazol-3-one	-15.3	-26.1	-6.6	-1.2
r_{e7}	imidazo[5,1-f][1,2,4]triazin-4(1H)-one	-11.0	-21.2	-6.7	-1.3
r_{e8}	1,2-dihydro-1,2,4-triazine-5,6-dione	-9.9	-16.0	-6.5	-1.1
r_{e9}	1,3,5-triazin-2(1H)-one	-8.1	-16.9	-6.2	-0.8

in category r_e .

Table S5. Cartesian coordinates of optimized geometry of rings at M06L/6-311++G(d,p) level. Atomic number followed by X, Y, Z coordinates in Å.

r_{a1}				r_{a2}			
6	-1.045850000	1.189032000	-0.000027000	6	0.790103000	-1.206263000	-0.000116000
6	0.306667000	1.221422000	0.000048000	6	-0.494836000	-0.711123000	-0.000009000
7	-1.725157000	0.000019000	-0.000008000	6	1.914401000	-0.317035000	0.000036000

1	-2.731485000	0.000036000	-0.000081000	8	3.105525000	-0.599693000	0.000054000
6	1.108533000	0.000011000	-0.000006000	6	-0.747897000	0.696800000	0.000024000
6	-1.045901000	-1.189059000	0.000030000	7	1.540070000	1.065071000	0.000086000
8	2.339070000	-0.000041000	-0.000026000	1	2.335839000	1.690145000	0.000195000
1	-1.664497000	-2.079201000	0.000021000	6	0.287660000	1.587051000	-0.000058000
6	0.306616000	-1.221404000	0.000004000	1	1.000771000	-2.268379000	-0.000335000
1	-1.664350000	2.079244000	-0.000057000	6	-1.808409000	-1.284000000	0.000093000
1	0.821795000	-2.174395000	-0.000015000	7	-2.118339000	0.833750000	-0.000616000
1	0.821685000	2.174500000	0.000099000	7	-2.744082000	-0.359972000	0.000208000
				1	0.189123000	2.665788000	-0.000182000
				1	-2.672234000	1.672793000	0.002232000
				1	-2.087380000	-2.327326000	0.000103000
		r_{a3}				r_{a4}	
6	-1.369898000	-0.967750000	-0.000268000	6	-1.356727000	0.974907000	0.000008000
6	0.032798000	-0.495734000	0.000214000	6	0.060619000	0.507696000	-0.000010000
6	-2.359346000	0.093345000	0.000526000	6	-2.334583000	-0.103681000	-0.000058000
1	-3.407206000	-0.178003000	0.001096000	1	-3.383588000	0.163716000	-0.000043000
6	0.342360000	0.877700000	-0.000145000	6	0.359478000	-0.872781000	0.000010000
6	-1.998644000	1.399892000	0.000431000	6	-1.974039000	-1.407777000	-0.000015000
1	-2.723077000	2.207108000	0.000755000	1	-2.694470000	-2.218458000	-0.000024000
7	-0.693158000	1.793407000	-0.000681000	7	-0.664472000	-1.796424000	-0.000008000
1	-0.470233000	2.775996000	0.001796000	1	-0.435031000	-2.778126000	0.000081000
8	-1.654989000	-2.164093000	-0.000700000	8	-1.663431000	2.158357000	0.000079000
6	1.087107000	-1.416956000	0.000325000	7	1.031226000	1.433295000	-0.000042000
6	1.676319000	1.308056000	-0.000422000	6	1.698245000	-1.281307000	0.000037000
6	2.402044000	-0.996034000	0.000468000	6	2.291019000	1.033063000	-0.000056000
6	2.693399000	0.374230000	-0.000017000	6	2.677938000	-0.313952000	0.000019000
1	0.821169000	-2.469194000	0.000408000	1	3.046921000	1.816361000	-0.000045000
1	3.210519000	-1.719277000	0.000912000	1	3.727805000	-0.586039000	0.000069000
1	3.725324000	0.710002000	-0.000251000	1	1.946832000	-2.339418000	0.000084000
1	1.898679000	2.371761000	-0.001031000				
		r_{a5}				r_{a6}	
6	-0.279167000	1.648005000	0.000141000	6	-1.115999000	-1.132072000	0.000000000
6	0.741584000	0.688385000	-0.000180000	7	-1.136694000	0.225918000	0.000000000
6	-1.568032000	1.193836000	0.000347000	6	0.070029000	-1.799832000	0.000000000
1	-2.405231000	1.879964000	0.000522000	1	-2.020263000	0.719264000	0.000000000
6	0.483964000	-0.666926000	-0.000053000	1	0.086299000	-2.880904000	0.000000000
6	-1.920241000	-0.216433000	-0.000030000	6	0.000000000	1.068929000	0.000000000
7	-0.811602000	-1.092401000	0.000321000	6	1.264533000	-1.034476000	0.000000000
8	2.089613000	0.904539000	-0.000300000	8	-0.143509000	2.281582000	0.000000000
6	1.742823000	-1.325970000	0.000294000	1	2.221204000	-1.549764000	0.000000000
6	2.665691000	-0.322378000	-0.000050000	6	1.239641000	0.328718000	0.000000000
1	-1.039651000	-2.077419000	-0.000477000	1	-2.080600000	-1.627232000	0.000000000
1	-0.049278000	2.708451000	0.000111000	1	2.149072000	0.916948000	0.000000000
8	-3.054310000	-0.672557000	-0.000380000				
1	1.949514000	-2.384572000	0.000373000				
1	3.743700000	-0.326586000	-0.000151000				
		r_{a7}				r_{a8}	
6	0.844256000	0.067112000	0.033594000	6	-1.375709000	0.958728000	-0.000348000
6	-0.074691000	1.195096000	0.028107000	6	0.035295000	0.514500000	-0.000088000
7	-0.002481000	-1.069063000	0.119070000	6	-2.336468000	-0.129015000	0.000160000
6	-1.330005000	0.703983000	-0.027926000	1	-3.391237000	0.113733000	0.000436000
7	-1.329728000	-0.674333000	-0.123360000	6	0.379795000	-0.849116000	-0.000067000
1	-2.282176000	1.217363000	-0.017304000	6	-1.941604000	-1.426522000	0.000129000
1	0.228210000	2.228821000	0.013618000	1	-2.646157000	-2.250627000	0.000280000
8	2.056061000	0.001167000	-0.030764000	7	-0.627088000	-1.788409000	-0.000119000
1	0.285498000	-1.890141000	-0.399340000	1	-0.344266000	-2.757630000	-0.000077000
1	-1.991916000	-1.158755000	0.476518000	8	-1.681585000	2.149002000	0.000033000
				6	1.092344000	1.426352000	0.000031000
				7	1.630394000	-1.324972000	-0.000036000
				6	2.393248000	0.960232000	0.000117000
				6	2.604310000	-0.422514000	0.000048000
				1	3.239152000	1.638027000	0.000197000
				1	3.616593000	-0.822175000	0.000073000
				1	0.848183000	2.484450000	0.000028000

<p style="text-align: center;">r_{a9}</p>				<p style="text-align: center;">r_{a10}</p>			
7	0.079878000	1.091379000	0.087254000	6	0.488371000	-1.545177000	0.000042000
6	-1.322248000	0.804640000	-0.140520000	6	-0.508512000	-0.611604000	0.000108000
6	0.902559000	-0.003189000	0.008589000	7	1.771545000	-1.112961000	0.000008000
6	-1.401344000	-0.689358000	0.193334000	1	2.524311000	-1.790350000	0.000057000
6	-0.008462000	-1.211718000	-0.140305000	6	-0.164068000	0.777621000	0.000073000
1	-1.609766000	1.001288000	-1.183726000	6	2.225098000	0.240863000	0.000054000
1	0.067993000	-1.550705000	-1.179689000	6	1.148373000	1.189933000	0.000106000
1	0.334744000	-2.034827000	0.486886000	16	-2.249879000	-0.766711000	-0.000033000
1	-2.204815000	-1.192151000	-0.346695000	6	-1.380090000	1.550187000	0.000004000
8	2.115248000	0.013919000	0.038219000	7	-2.503794000	0.896435000	-0.000137000
1	-1.599056000	-0.810614000	1.262303000	1	1.416506000	2.239396000	0.000182000
1	-1.964732000	1.415229000	0.499440000	1	0.327127000	-2.616642000	0.000063000
1	0.471470000	2.018521000	0.018363000	8	3.426798000	0.462948000	-0.000180000
				1	-1.413540000	2.636129000	0.000234000
<p style="text-align: center;">r_{a11}</p>				<p style="text-align: center;">r_{a12}</p>			
6	0.625618000	1.601024000	0.000016000	6	1.458144000	0.908241000	0.032160000
6	-0.489095000	0.783534000	0.000006000	7	0.116709000	0.396945000	-0.013437000
7	1.852961000	1.059865000	0.000015000	6	2.449907000	-0.123615000	-0.013100000
1	2.668158000	1.661634000	0.000022000	1	3.488852000	0.180463000	-0.004617000
6	-0.263858000	-0.638078000	-0.000007000	6	-0.148059000	-0.941710000	-0.021941000
6	2.179190000	-0.339256000	0.000003000	6	2.073943000	-1.430266000	-0.040672000
8	3.356342000	-0.663527000	0.000005000	1	2.823999000	-2.218516000	-0.061664000
6	1.013386000	-1.163854000	-0.000008000	7	0.785108000	-1.861352000	-0.033755000
1	1.169732000	-2.236674000	-0.000017000	8	1.637820000	2.113405000	0.101389000
1	0.558210000	2.684280000	0.000026000	6	-0.928265000	1.437446000	0.024372000
6	-1.829321000	1.255899000	0.000007000	6	-1.573123000	-1.417511000	-0.044678000
6	-1.443798000	-1.460091000	-0.000018000	6	-2.291609000	0.916913000	-0.366546000
6	-2.850500000	0.354558000	-0.000005000	6	-2.591837000	-0.373722000	0.373018000
7	-2.662520000	-1.006000000	-0.000017000	1	-0.939947000	1.852122000	1.039436000
1	-2.027495000	2.323643000	0.000016000	1	-3.032372000	1.691789000	-0.152601000
1	-3.886109000	0.679436000	-0.000004000	1	-2.538390000	-0.201037000	1.455213000
1	-1.316050000	-2.543576000	-0.000028000	1	-1.615780000	-2.322937000	0.564175000
				1	-2.329607000	0.738025000	-1.448404000
				1	-3.603566000	-0.730380000	0.164383000
				1	-1.779442000	-1.747788000	-1.071437000
				1	-0.583634000	2.247212000	-0.620927000
<p style="text-align: center;">r_{a13}</p>				<p style="text-align: center;">r_{a14}</p>			
6	1.446530000	0.117555000	-0.000539000	6	1.075873000	1.428174000	-0.000077000
7	0.280549000	0.994033000	0.000778000	6	0.022715000	0.505036000	0.000027000
6	-0.650442000	-0.015607000	0.000332000	6	2.388761000	1.000555000	-0.000066000
6	0.464702000	-1.067311000	0.000394000	1	3.199088000	1.721652000	-0.000560000
1	2.074621000	0.207674000	0.890733000	6	0.338559000	-0.857610000	0.000261000
1	2.071532000	0.207368000	-0.894120000	6	2.676940000	-0.369826000	-0.000273000
1	0.482150000	-1.698253000	-0.888653000	1	3.708256000	-0.706941000	-0.000338000
1	0.481895000	-1.697686000	0.889795000	6	1.657894000	-1.304893000	0.000046000
8	-1.853173000	-0.023313000	-0.000496000	1	1.856306000	-2.370659000	0.000515000
1	0.186604000	2.001359000	-0.000352000	1	0.813417000	2.481215000	0.000068000
				6	-1.383893000	0.950908000	0.000004000
				8	-0.633775000	-1.824855000	0.000495000
				6	-2.334337000	-0.150095000	-0.000504000
				6	-1.922471000	-1.430409000	-0.000330000
				1	-2.583956000	-2.288755000	-0.000548000
				1	-3.394753000	0.068430000	-0.000706000
				8	-1.706052000	2.132857000	0.000385000
<p style="text-align: center;">r_{a15}</p>				<p style="text-align: center;">r_{a16}</p>			
6	1.021014000	1.186728000	0.000015000	6	-1.830817000	1.248762000	0.013738000
6	-0.258862000	0.681320000	0.000004000	6	-0.525994000	0.780908000	0.117161000
6	2.155663000	0.314973000	0.000014000	6	-2.906314000	0.372220000	-0.097638000
8	3.343531000	0.588742000	0.000022000	1	-3.917185000	0.757311000	-0.174624000
6	-0.462196000	-0.750382000	-0.000009000	6	-0.307189000	-0.604044000	0.088472000
7	1.755855000	-1.055048000	0.000001000	6	-2.674696000	-0.998859000	-0.107954000
1	2.522414000	-1.722167000	0.000000000	1	-3.504342000	-1.693037000	-0.192496000
7	0.558916000	-1.600594000	-0.000010000	6	-1.378412000	-1.489662000	-0.020411000
1	1.204539000	2.255894000	0.000024000	1	-1.190623000	-2.559566000	-0.039899000
6	-1.436906000	1.493749000	0.000005000	1	-2.003944000	2.321747000	0.029847000

7	-1.698449000	-1.335414000	-0.000020000	6	0.666588000	1.670941000	0.302926000
6	-2.653083000	0.890721000	-0.000006000	7	1.006672000	-1.080546000	0.192640000
6	-2.728754000	-0.539844000	-0.000019000	6	1.891857000	1.100543000	-0.400298000
1	-1.333262000	2.574694000	0.000014000	6	2.150415000	-0.345789000	-0.048635000
1	-3.568896000	1.471846000	-0.000006000	1	1.154604000	-2.072667000	0.322715000
1	-3.708553000	-1.016398000	-0.000028000	8	3.252286000	-0.856352000	-0.004143000
				1	2.799416000	1.664725000	-0.182841000
				1	1.751004000	1.138129000	-1.488659000
				1	0.453098000	2.683232000	-0.050963000
				1	0.880357000	1.764645000	1.377422000
		r_{a17}				r_{a18}	
6	-1.201404000	-1.149051000	-0.000014000	6	-1.019852000	-1.195041000	0.000015000
6	0.279348000	-1.265735000	0.000102000	6	0.268983000	-0.697328000	0.000004000
6	-1.812534000	0.046346000	-0.000089000	6	-2.163213000	-0.343489000	0.000015000
1	0.613930000	-1.861018000	-0.860173000	8	-3.347384000	-0.629035000	0.000022000
1	-2.895156000	0.115480000	-0.000206000	6	0.511947000	0.718002000	-0.000009000
6	1.079869000	0.028797000	0.000016000	7	-1.808887000	1.063457000	0.000001000
6	-1.037168000	1.268243000	0.000016000	1	-2.615056000	1.678717000	0.000001000
8	2.300733000	0.006642000	-0.000129000	6	-0.580447000	1.573717000	-0.000010000
1	-1.575265000	2.213413000	0.000006000	1	-0.453299000	2.651467000	-0.000019000
6	0.314712000	1.273028000	0.000096000	1	-1.204810000	-2.262935000	0.000024000
1	-1.783963000	-2.066550000	-0.000045000	6	1.460747000	-1.476921000	0.000005000
1	0.883835000	2.196625000	0.000147000	7	1.753379000	1.296012000	-0.000020000
1	0.613825000	-1.860858000	0.860540000	6	2.654062000	-0.824704000	-0.000007000
				7	2.806057000	0.549684000	-0.000020000
				1	1.408781000	-2.561319000	0.000014000
				1	3.596248000	-1.363141000	-0.000007000
		r_{a19}				r_{a20}	
6	1.307929000	-1.423277000	0.000000000	6	-1.294528000	-0.344409000	-0.000069000
6	0.151991000	-0.658663000	-0.000359000	7	-0.033022000	-0.980768000	-0.000104000
6	2.528712000	-0.748303000	0.000312000	6	1.222930000	-0.407935000	0.000024000
1	3.450100000	-1.321474000	0.000598000	7	1.171608000	0.984771000	-0.000464000
6	0.186449000	0.742326000	-0.000418000	6	0.005420000	1.702580000	0.000044000
6	2.582434000	0.641612000	0.000233000	6	-1.201582000	1.103249000	0.000312000
1	3.543925000	1.143684000	0.000482000	1	-0.046703000	-1.992802000	-0.000133000
6	1.405171000	1.394973000	-0.000145000	1	2.068264000	1.446627000	-0.000386000
1	1.267489000	-2.507515000	0.000211000	1	0.124186000	2.780032000	0.000223000
7	-1.178007000	-1.079117000	-0.000712000	1	-2.116527000	1.676411000	0.000762000
6	-1.222086000	1.245450000	-0.000032000	8	2.263001000	-1.026245000	0.000315000
6	-2.073453000	-0.021239000	-0.000066000	8	-2.312095000	-1.006155000	-0.000108000
1	1.449281000	2.480137000	-0.000140000				
1	-1.475780000	1.850369000	0.875755000				
1	-1.485754000	-2.039592000	0.001151000				
8	-3.278691000	-0.117595000	0.000547000				
1	-1.476557000	1.851709000	-0.874592000				
		r_{a21}				r_{a22}	
6	-1.315142000	0.777373000	-0.000127000	6	1.259868000	-0.445804000	0.023784000
6	-0.051855000	1.199007000	0.000073000	6	1.249089000	1.050669000	0.206293000
6	0.841178000	0.026663000	0.000058000	6	-0.000001000	1.709460000	-0.357199000
8	0.041613000	-1.096439000	-0.000311000	6	-1.249089000	1.050669000	0.206294000
6	-1.324993000	-0.708068000	0.000198000	6	-1.259868000	-0.445804000	0.023787000
1	-2.216984000	1.376479000	-0.000644000	7	0.000000000	-1.040076000	-0.061852000
1	0.323968000	2.211507000	-0.000017000	1	2.169126000	1.439158000	-0.233135000
8	2.037622000	-0.040792000	0.000050000	1	1.323726000	1.236984000	1.286051000
1	-1.817444000	-1.129510000	0.885082000	1	-0.000001000	2.778831000	-0.133098000
1	-1.818543000	-1.130473000	-0.883544000	1	-0.000001000	1.624052000	-1.449914000
				1	-2.169127000	1.439157000	-0.233133000
				1	-1.323726000	1.236985000	1.286053000
				1	0.000000000	-2.048562000	-0.172751000
				8	2.262224000	-1.121326000	-0.033428000
				8	-2.262223000	-1.121326000	-0.033430000
		r_{a23}				r_{a24}	
7	0.695491000	1.120785000	-0.142257000	6	0.704532000	1.239527000	0.021778000
7	-0.695598000	1.120852000	0.142259000	7	-0.730317000	1.121398000	-0.064561000
6	1.197860000	-0.176826000	-0.039788000	6	1.166882000	-0.211637000	0.002491000
6	-1.197879000	-0.176898000	0.039872000	6	-1.166433000	-0.176678000	-0.009071000

6	-0.000058000	-1.096407000	-0.000188000	7	0.007823000	-0.954219000	-0.013764000
1	1.218833000	1.831128000	0.357664000	1	1.047494000	1.717676000	0.946381000
1	-1.219231000	1.830414000	-0.358513000	1	-1.377613000	1.873270000	0.102415000
1	-0.048644000	-1.748814000	-0.874396000	1	-0.019455000	-1.962220000	-0.020621000
1	0.049326000	-1.749185000	0.873590000	8	2.301506000	-0.618721000	0.004369000
8	-2.371410000	-0.447184000	-0.026190000	8	-2.297466000	-0.592279000	0.026855000
8	2.371526000	-0.447093000	0.026473000	1	1.144831000	1.781741000	-0.820878000
r_{a25}				r_{a26}			
6	1.352599000	1.416847000	0.000171000	6	1.465726000	1.395126000	0.000233000
6	0.161109000	0.698569000	0.000213000	6	0.255512000	0.702758000	0.000544000
6	2.542719000	0.700904000	-0.000185000	6	2.665337000	0.697363000	-0.000157000
1	3.490846000	1.229528000	-0.000449000	1	3.606198000	1.238341000	-0.000264000
6	0.161098000	-0.698570000	0.000192000	6	0.255447000	-0.702602000	0.000139000
6	2.542706000	-0.700910000	-0.000204000	6	2.665327000	-0.697476000	-0.000395000
1	3.490817000	-1.229563000	-0.000451000	1	3.606254000	-1.238326000	-0.000654000
6	1.352582000	-1.416847000	0.000134000	6	1.465672000	-1.395131000	-0.000241000
1	1.338555000	2.501910000	0.000309000	1	1.438570000	-2.479953000	-0.000499000
6	-1.230550000	1.211077000	-0.000090000	1	1.438891000	2.479968000	0.000351000
6	-1.230597000	-1.211064000	0.000031000	6	-1.020878000	1.459811000	0.000736000
6	-2.150680000	-0.000004000	-0.000495000	6	-1.021019000	-1.459800000	0.000389000
1	1.338569000	-2.501911000	0.000217000	6	-2.268949000	0.670419000	-0.000274000
8	-1.565384000	-2.374235000	0.000208000	6	-2.269070000	-0.670626000	-0.000729000
1	-2.809785000	0.000085000	0.872314000	1	-3.189204000	-1.247597000	-0.001273000
1	-2.808682000	-0.000019000	-0.874143000	1	-3.188934000	1.247616000	-0.000669000
8	-1.565396000	2.374229000	0.000181000	8	-1.054489000	2.680928000	-0.000252000
				8	-1.054313000	-2.680816000	0.000443000
r_{a27}							
6	1.295036000	0.708950000	-0.001402000				
6	0.000070000	1.476774000	0.062535000				
6	-1.294945000	0.709151000	-0.001402000				
7	-1.166846000	-0.673321000	0.010676000				
6	-0.000111000	-1.427371000	0.006581000				
7	1.166796000	-0.673428000	0.010651000				
1	0.000153000	2.229192000	-0.729784000				
1	0.000141000	2.055002000	0.992281000				
1	-2.024448000	-1.210707000	-0.017854000				
1	2.024274000	-1.211048000	-0.017889000				
8	2.379125000	1.239214000	-0.046455000				
8	-0.000113000	-2.633630000	-0.003816000				
8	-2.379021000	1.239388000	-0.046468000				
r_{b1}				r_{b2}			
6	0.537768000	0.666320000	0.003907000	6	0.990121000	1.374265000	-0.000218000
6	0.587593000	-0.712145000	0.130384000	6	-0.246009000	0.738747000	0.000035000
7	-0.426170000	1.641830000	0.029975000	7	2.112301000	0.652803000	0.000041000
6	-0.569476000	-1.632950000	0.264295000	6	-0.202411000	-0.668280000	-0.000014000
6	-1.677772000	1.361613000	0.109374000	6	2.000139000	-0.683177000	0.000287000
6	-1.808072000	-1.097107000	-0.442443000	1	2.935822000	-1.237088000	0.000141000
1	-0.300671000	-2.600219000	-0.173096000	7	0.886634000	-1.422494000	-0.000261000
1	-1.589539000	-0.968489000	-1.510663000	7	-1.551057000	1.193196000	0.000027000
7	-2.319952000	0.151608000	0.120273000	7	-1.517837000	-1.058095000	0.000234000
6	2.621723000	-0.077206000	-0.068866000	6	-2.263351000	0.099260000	0.000016000
7	1.861887000	1.047210000	-0.115648000	1	-1.857216000	-2.007877000	-0.000980000
7	1.884268000	-1.156401000	0.074789000	1	-3.344588000	0.063833000	0.000054000
1	2.165039000	2.003875000	-0.215069000	1	1.084762000	2.458373000	-0.000130000
1	3.699013000	-0.054027000	-0.147106000				
1	-3.325396000	0.225957000	0.132784000				
1	-0.812406000	-1.828869000	1.315554000				
1	-2.622755000	-1.821251000	-0.369322000				
1	-2.364099000	2.202150000	0.221289000				
r_{b3}				r_{b4}			
7	-0.180053000	-1.865639000	-0.005361000	6	0.198729000	1.472895000	0.002519000
6	0.574894000	-0.797971000	-0.048670000	6	-0.853385000	0.499287000	0.006926000
6	-1.508093000	-1.512036000	0.025197000	7	1.467094000	0.790935000	0.000143000
1	-2.177880000	-2.372495000	0.060824000	6	-0.519134000	-0.851681000	-0.000696000
6	0.136639000	0.555217000	-0.031968000	6	1.669594000	-0.560043000	-0.001376000
7	-2.086185000	-0.339958000	0.019996000	7	2.970653000	-0.993825000	-0.075020000

6	-1.308331000	0.817876000	-0.008829000	7	0.699216000	-1.439718000	0.007802000
7	1.953396000	-0.785655000	-0.099696000	7	-2.218422000	0.674891000	0.007155000
6	1.261861000	1.330408000	0.027290000	7	-1.719145000	-1.506440000	-0.003310000
7	2.359275000	0.529860000	0.111235000	6	-2.700564000	-0.536641000	0.000744000
1	2.502536000	-1.503569000	0.357588000	1	-1.840112000	-2.507687000	-0.010349000
8	-1.776701000	1.944063000	-0.011566000	1	-3.748975000	-0.798124000	-0.000630000
1	3.244774000	0.787433000	-0.307170000	8	0.178536000	2.684374000	-0.004412000
1	1.377325000	2.404904000	0.019956000	1	2.261367000	1.414787000	-0.064309000
				1	3.668441000	-0.427844000	0.384379000
				1	3.063784000	-1.979924000	0.120118000
		Γ_{b5}				Γ_{b6}	
6	3.517755000	-1.263691000	0.302588000	7	-0.798222000	-1.693769000	0.000104000
7	2.305937000	-1.640414000	-0.112984000	6	0.494284000	-1.246304000	0.000058000
6	3.842488000	0.053385000	0.584320000	6	-1.874268000	-0.821280000	0.000012000
1	4.832376000	0.321754000	0.934038000	6	0.759056000	0.104222000	0.000073000
6	1.373928000	-0.709330000	-0.291646000	7	-1.547472000	0.544160000	0.000131000
6	2.864380000	1.022307000	0.391135000	6	-2.692203000	1.446883000	-0.000022000
1	3.077626000	2.072059000	0.572838000	6	-0.247005000	1.117961000	0.000037000
6	1.605509000	0.657987000	-0.072012000	7	1.620068000	-1.993924000	-0.000022000
1	4.251205000	-2.058291000	0.4111792000	7	2.138863000	0.193104000	-0.000020000
7	0.155654000	-1.186386000	-0.779998000	6	2.587234000	-1.084194000	-0.000068000
7	0.674997000	1.650676000	-0.404734000	6	2.928716000	1.408497000	-0.000009000
6	-1.106895000	-0.826464000	-0.299134000	1	3.645001000	-1.308329000	-0.000141000
6	-0.696762000	1.722873000	-0.225644000	1	-1.013720000	-2.679527000	-0.000090000
1	0.240117000	-2.183544000	-0.940359000	1	2.705451000	2.008030000	-0.883039000
1	1.060169000	2.582001000	-0.504062000	1	2.706824000	2.007180000	0.883971000
8	-1.224663000	2.821400000	-0.288143000	1	3.983290000	1.135215000	-0.000910000
6	-2.051050000	-1.855930000	-0.173096000	8	-3.023946000	-1.210053000	-0.000124000
6	-1.496426000	0.492273000	0.004509000	8	-0.067224000	2.325741000	-0.000058000
6	-3.336551000	-1.604856000	0.269886000	1	-3.308410000	1.273310000	-0.883034000
6	-2.803341000	0.716771000	0.459399000	1	-3.308532000	1.273449000	0.882932000
1	-4.039442000	-2.427038000	0.359745000	1	-2.308094000	2.463453000	-0.000059000
1	-3.076873000	1.744325000	0.670348000				
6	-3.718503000	-0.308400000	0.607198000				
1	-4.720521000	-0.102103000	0.965721000				
1	-1.750653000	-2.869053000	-0.425920000				
		Γ_{b7}				Γ_{b8}	
6	-0.633007000	1.688686000	-0.296365000	6	-1.375676000	0.958608000	-0.000006000
6	0.546626000	0.789027000	-0.107144000	6	0.035577000	0.514461000	0.000013000
6	-1.872829000	1.101785000	0.369830000	6	-2.336827000	-0.128892000	0.000010000
1	-2.779766000	1.651846000	0.117479000	1	-3.391421000	0.114301000	0.000001000
6	0.337774000	-0.597570000	-0.078630000	6	0.379829000	-0.849268000	0.000011000
6	-2.110430000	-0.354371000	0.037805000	6	-1.941716000	-1.426395000	0.000005000
8	-3.201725000	-0.876515000	-0.006203000	1	-2.646156000	-2.250598000	0.000006000
7	-0.951694000	-1.093976000	-0.164991000	7	-0.627038000	-1.788244000	0.000005000
1	-1.053402000	-2.099507000	-0.235989000	1	-0.345013000	-2.757715000	-0.000034000
1	-0.821746000	1.808237000	-1.372198000	8	-1.681324000	2.148970000	-0.000082000
6	1.867431000	1.181151000	0.007163000	6	1.092249000	1.426432000	0.000023000
7	1.326030000	-1.485366000	0.009577000	7	1.630416000	-1.325089000	0.000003000
7	2.889860000	0.320657000	0.110257000	6	2.393277000	0.960156000	0.000024000
6	2.552015000	-0.965295000	0.091189000	6	2.604223000	-0.422481000	0.000020000
1	3.367766000	-1.682627000	0.155187000	1	0.848311000	2.484519000	0.000022000
1	2.123259000	2.240716000	0.009815000	1	3.239209000	1.637881000	0.000021000
1	-0.425115000	2.691574000	0.086433000	1	3.616401000	-0.822537000	-0.000017000
1	-1.772050000	1.152196000	1.461912000				
		Γ_{b9}				Γ_{b10}	
6	0.990121000	1.374265000	-0.000218000	6	0.275388000	1.439617000	0.000446000
6	-0.246009000	0.738747000	0.000035000	6	-0.768546000	0.461045000	-0.000134000
7	2.112301000	0.652803000	0.000041000	7	1.528333000	0.790784000	-0.000003000
6	-0.202411000	-0.668280000	-0.000014000	1	2.337271000	1.398329000	0.000042000
6	2.000139000	-0.683177000	0.000287000	6	-0.544856000	-0.897226000	-0.000057000
1	2.935822000	-1.237088000	0.000141000	6	1.840567000	-0.571390000	-0.000021000
7	0.886634000	-1.422494000	-0.000261000	8	2.978821000	-0.983832000	-0.000036000
7	-1.551057000	1.193196000	0.000027000	7	0.729581000	-1.401833000	-0.000053000
7	-1.517837000	-1.058095000	0.000234000	8	0.172285000	2.652242000	-0.000023000
6	-2.263351000	0.099260000	0.000016000	7	-2.140480000	0.582245000	-0.000320000
1	-1.857216000	-2.007877000	-0.000980000	7	-1.698373000	-1.608236000	0.000025000

1	-3.344588000	0.063833000	0.000054000	6	-2.639839000	-0.676549000	0.000315000
1	1.084762000	2.458373000	-0.000130000	1	-3.701593000	-0.874379000	0.000483000
				1	-2.652420000	1.451746000	-0.000807000
				1	0.898185000	-2.396685000	-0.000096000
		r_{b11}				r_{b12}	
7	0.142164000	-1.880209000	0.000088000	6	1.143899000	0.113737000	0.000112000
6	-0.628958000	-0.765098000	-0.000146000	6	-0.182778000	-0.400217000	0.000005000
6	1.409703000	-1.587400000	-0.000350000	7	1.201360000	1.508753000	0.000039000
1	2.141978000	-2.390715000	0.000610000	6	-1.320013000	0.383898000	0.000039000
6	-0.242981000	0.572666000	0.000140000	6	0.120314000	2.219439000	0.000036000
7	1.912279000	-0.324098000	0.000023000	1	0.200306000	3.304370000	0.000049000
1	2.916165000	-0.192834000	-0.000069000	7	-1.164611000	1.743682000	0.000056000
6	1.158504000	0.899229000	0.000447000	7	-0.673182000	-1.681132000	-0.000032000
7	-1.996160000	-0.734896000	0.000283000	7	-2.465046000	-0.337335000	0.000080000
7	-1.335439000	1.403220000	0.000386000	6	-2.028244000	-1.588087000	-0.000040000
6	-2.359717000	0.590883000	-0.000537000	1	-2.665346000	-2.459810000	-0.000070000
1	-2.600864000	-1.542487000	-0.000424000	16	2.489315000	-0.856806000	-0.000120000
8	1.732677000	1.965647000	-0.000317000	1	-0.088485000	-2.506926000	-0.000061000
1	-3.397905000	0.891050000	-0.000371000	1	-1.964230000	2.360863000	0.000097000
		r_{c1}				r_{c2}	
7	-0.180053000	-1.865639000	-0.005361000	7	1.530878000	1.364099000	-0.070804000
6	0.574894000	-0.797971000	-0.048670000	6	0.233824000	0.871377000	0.010775000
6	-1.508093000	-1.512036000	0.025197000	6	2.582419000	0.386917000	0.233685000
1	-2.177880000	-2.372495000	0.060824000	6	-0.061057000	-0.458315000	0.088143000
6	0.136639000	0.555217000	-0.031968000	6	2.223429000	-0.964492000	-0.364834000
7	-2.086185000	-0.339958000	0.019996000	7	0.958018000	-1.398444000	0.192885000
6	-1.308331000	0.817876000	-0.008829000	1	0.622639000	-2.315245000	-0.085017000
7	1.953396000	-0.785655000	-0.099696000	7	-0.815372000	1.763062000	-0.051672000
6	1.261861000	1.330408000	0.027290000	6	-1.435748000	-0.921019000	0.038844000
7	2.359275000	0.529860000	0.111235000	6	-2.101270000	1.296969000	-0.058284000
1	2.502536000	-1.503569000	0.357588000	7	-2.440722000	0.056863000	-0.004022000
8	-1.776701000	1.944063000	-0.011566000	1	-0.632955000	2.742978000	-0.211477000
1	3.244774000	0.787433000	-0.307170000	1	-2.861477000	2.075163000	-0.108568000
1	1.377325000	2.404904000	0.019956000	8	-1.688766000	-2.122057000	0.035626000
		r_{c3}		1	1.665074000	2.242357000	0.415967000
				1	2.192170000	-0.874719000	-1.462667000
				1	3.520926000	0.751907000	-0.191793000
				1	3.003711000	-1.686554000	-0.112754000
				1	2.720855000	0.272881000	1.316613000
		r_{c4}				r_{c5}	
6	1.213663000	0.897133000	0.000392000	6	1.070900000	1.419396000	0.000006000
6	-0.203503000	0.573900000	0.000134000	6	0.027971000	0.488817000	0.000004000
7	2.085404000	-0.230927000	0.000087000	6	2.388989000	1.000629000	0.000014000
6	-0.612394000	-0.747476000	-0.000188000	1	3.194815000	1.726704000	0.000010000
6	1.619859000	-1.425077000	-0.000211000	6	0.345127000	-0.877587000	-0.000002000
7	0.286669000	-1.778802000	-0.000313000	6	2.686662000	-0.366598000	0.000007000
6	-1.390179000	1.362884000	0.000033000	1	3.720400000	-0.696235000	0.000007000
7	-1.968928000	-0.801867000	-0.000176000	6	1.674297000	-1.309181000	0.000001000
6	-2.452257000	0.505026000	-0.000084000	1	1.900866000	-2.371475000	0.000001000
1	-2.539091000	-1.631214000	-0.000289000	1	0.803607000	2.470500000	-0.000047000
1	-1.433870000	2.440511000	0.000143000	6	-1.386620000	0.927247000	-0.000002000
8	1.663537000	2.027337000	0.000447000	7	-0.715979000	-1.768206000	-0.000008000
1	0.009841000	-2.748415000	-0.000605000	7	-2.371443000	-0.078937000	-0.000006000
1	2.297139000	-2.279488000	-0.000352000	6	-2.000124000	-1.310860000	-0.000007000
1	-3.515464000	0.682741000	-0.000115000	8	-1.694906000	2.103734000	0.000005000
		r_{c5}		1	-2.754281000	-2.099091000	-0.000016000
				1	-0.537418000	-2.761445000	-0.000013000
						r_{c6}	
7	0.357677000	-1.804628000	0.000064000	6	1.064273000	1.171435000	0.000000000
6	-0.626549000	-0.841482000	-0.000038000	7	1.134793000	-0.175107000	0.000000000
6	1.657967000	-1.381427000	0.000095000	6	-0.160952000	1.767202000	0.000000000
1	2.387731000	-2.190950000	0.000080000	1	2.029918000	-0.646678000	0.000000000
6	-0.228641000	0.485772000	-0.000121000	1	-0.270192000	2.842047000	0.000000000
7	2.071854000	-0.158971000	-0.000025000	6	0.000000000	-1.040197000	0.000000000
6	1.158073000	0.912697000	-0.000215000	6	-1.278386000	0.894591000	0.000000000
1	0.139122000	-2.789118000	0.000075000	8	0.179352000	-2.237120000	0.000000000

6	-1.207341000	0.872146000	-0.002712000	7	1.219690000	0.382525000	0.000000000
6	2.024369000	-0.722175000	-0.010245000	7	-1.125717000	0.150630000	0.000000000
6	1.391050000	1.327569000	0.014275000	1	-2.039708000	0.587810000	0.000000000
7	2.480699000	0.516752000	0.011481000	6	0.000000000	1.032233000	0.000000000
8	-1.651419000	1.998893000	-0.015501000	8	-0.177431000	2.224386000	0.000000000
1	1.474812000	2.403570000	0.023662000				
1	2.611103000	-1.628984000	-0.022905000				
1	0.109552000	-2.656583000	0.253050000				
1	-2.198279000	-2.314325000	0.060653000				
		r_{c15}				r_{c16}	
6	0.275388000	1.439617000	0.000446000	6	1.116497000	0.859364000	0.000306000
6	-0.768546000	0.461045000	-0.000134000	7	-0.237846000	0.504490000	0.000055000
7	1.528333000	0.790784000	-0.000003000	7	1.881003000	-0.291509000	0.000180000
1	2.337271000	1.398329000	0.000042000	6	-0.647356000	-0.837315000	-0.000304000
6	-0.544856000	-0.897226000	-0.000057000	7	1.482014000	-1.625162000	-0.000122000
6	1.840567000	-0.571390000	-0.000021000	7	0.240466000	-1.867608000	-0.000570000
8	2.978821000	-0.983832000	-0.000036000	6	-1.371213000	1.261080000	-0.000173000
7	0.729581000	-1.401833000	-0.000053000	6	-2.024580000	-0.785620000	0.000028000
8	0.172285000	2.652242000	-0.000023000	7	-2.451194000	0.507000000	0.000033000
7	-2.140480000	0.582245000	-0.000320000	1	-2.710109000	-1.619441000	0.000094000
7	-1.698373000	-1.608236000	0.000025000	1	-1.335977000	2.340162000	-0.000145000
6	-2.639839000	-0.676549000	0.000315000	8	1.539968000	1.985463000	0.000443000
1	-3.701593000	-0.874379000	0.000483000	1	2.885152000	-0.179960000	0.000339000
1	-2.652420000	1.451746000	-0.000807000				
1	0.898185000	-2.396685000	-0.000096000				
		r_{c17}				r_{c18}	
6	-1.072550000	0.031263000	0.002609000	6	1.341601000	0.906899000	0.000006000
7	-0.343162000	-1.139155000	-0.111527000	6	-0.057788000	0.480056000	0.000107000
6	-0.224909000	1.247734000	0.275939000	7	2.237003000	-0.161637000	0.000012000
1	-0.742285000	2.124891000	-0.114031000	1	3.220628000	0.076331000	-0.000105000
7	1.002852000	-1.308248000	0.136583000	6	-0.361405000	-0.897101000	0.000055000
6	1.183691000	1.097546000	-0.280129000	7	1.980626000	-1.486006000	-0.000033000
1	1.844196000	1.889645000	0.080681000	6	0.729220000	-1.828973000	-0.000003000
6	1.723861000	-0.252456000	0.060349000	1	0.541134000	-2.898830000	-0.000133000
1	2.785346000	-0.403747000	0.238307000	8	1.744264000	2.058228000	-0.000054000
8	-2.283782000	0.027727000	-0.077214000	6	-1.083757000	1.428332000	0.000055000
1	-0.870383000	-2.001528000	-0.106154000	6	-1.706945000	-1.300412000	0.000019000
1	-0.193605000	1.363299000	1.366856000	6	-2.402695000	1.013561000	-0.000035000
1	1.168604000	1.192921000	-1.375943000	6	-2.712674000	-0.353285000	-0.000055000
		r_{d1}		1	-3.203390000	1.745886000	-0.000152000
6	0.000000000	0.000000000	0.926028000	1	-3.750824000	-0.669125000	-0.000140000
6	0.000000000	-1.213653000	0.259712000	1	-1.944838000	-2.359981000	0.000102000
6	0.000000000	1.213653000	0.259712000	1	-0.813569000	2.478934000	0.000116000
1	0.000000000	-2.136920000	0.827133000				
1	0.000000000	2.136920000	0.827133000				
6	0.000000000	-1.203779000	-1.131052000				
6	0.000000000	1.203779000	-1.131052000				
1	0.000000000	-2.145710000	-1.669960000				
1	0.000000000	2.145710000	-1.669960000				
6	0.000000000	0.000000000	-1.828730000				
1	0.000000000	0.000000000	-2.913189000				
9	0.000000000	0.000000000	2.274570000				
		r_{d3}				r_{d2}	
6	0.618935000	-1.793318000	-0.058702000	6	-0.789471000	0.946847000	0.130010000
6	1.605378000	-0.828305000	-0.000377000	6	0.565233000	1.209109000	0.057208000
6	-0.719283000	-1.413920000	-0.101370000	6	-1.248342000	-0.370479000	0.130119000
				6	1.514471000	0.191611000	-0.015474000
				6	-0.323406000	-1.412078000	0.052797000
				1	-0.635258000	-2.450895000	0.040912000
				6	1.020901000	-1.108148000	-0.009783000
				9	1.951712000	-2.093980000	-0.085827000
				1	-1.494633000	1.767824000	0.183562000
				8	2.833665000	0.480074000	-0.094926000
				1	3.314720000	-0.354314000	-0.142483000
				9	1.004318000	2.477074000	0.052220000
				6	-2.720609000	-0.668999000	0.248396000
				7	-3.533054000	0.399070000	-0.320600000
				1	-4.514930000	0.227396000	-0.136037000
				1	-3.428175000	0.415199000	-1.330770000
				1	-2.910970000	-1.667010000	-0.179829000
				1	-2.985638000	-0.747310000	1.311082000
						r_{d4}	
				6	0.000000000	0.889749000	0.000000000
				7	1.189140000	0.340878000	0.000000000
				6	-1.213882000	0.214763000	0.000000000

6	1.291362000	0.529317000	0.016319000	1	-2.149067000	0.760932000	0.000000000
6	-1.088347000	-0.068959000	-0.084300000	6	1.226006000	-0.996569000	0.000000000
6	-0.058256000	0.857520000	-0.026309000	6	-1.152819000	-1.170039000	0.000000000
9	-0.337940000	2.191971000	-0.010950000	1	2.218890000	-1.441413000	0.000000000
1	0.911447000	-2.836462000	-0.070688000	1	-2.067427000	-1.753880000	0.000000000
8	2.270847000	1.459619000	0.074982000	6	0.091528000	-1.795337000	0.000000000
1	1.852718000	2.328688000	0.072092000	1	0.180212000	-2.875164000	0.000000000
9	2.899587000	-1.180714000	0.044277000	9	-0.023510000	2.229775000	0.000000000
6	-2.519533000	0.393323000	-0.133729000				
7	-3.445644000	-0.694818000	0.152015000				
1	-4.397707000	-0.377360000	0.008869000				
1	-3.378740000	-0.954823000	1.132027000				
1	-2.629056000	1.268228000	0.526328000				
1	-2.739872000	0.763662000	-1.143214000				
1	-1.502409000	-2.160426000	-0.158516000				
r_{d5}				r_{d6}			
6	0.000000000	0.000000000	1.363766000	6	1.080483000	1.210886000	0.000000000
6	0.000000000	1.212555000	0.694991000	6	-0.304365000	1.180521000	0.000000000
6	0.000000000	-1.212555000	0.694991000	6	1.763603000	0.000000000	0.000000000
1	0.000000000	2.137735000	1.258738000	9	-0.980893000	2.342685000	0.000000000
1	0.000000000	-2.137735000	1.258738000	1	2.848130000	0.000000000	0.000000000
6	0.000000000	1.212598000	-0.695031000	6	-1.028749000	0.000000000	0.000000000
6	0.000000000	-1.212598000	-0.695031000	6	1.080483000	-1.210886000	0.000000000
1	0.000000000	2.137695000	-1.258871000	1	-2.110692000	0.000000000	0.000000000
1	0.000000000	-2.137695000	-1.258871000	1	1.598056000	-2.162035000	0.000000000
6	0.000000000	0.000000000	-1.363681000	6	-0.304365000	-1.180521000	0.000000000
9	0.000000000	0.000000000	-2.711555000	9	-0.980894000	-2.342685000	0.000000000
9	0.000000000	0.000000000	2.711581000	1	1.598055000	2.162035000	0.000000000
r_{d7}				r_{d8}			
6	1.052712000	-1.684335000	0.000000000	6	1.189739000	1.008665000	0.000000000
6	-0.327940000	-1.508840000	0.000000000	6	0.011130000	1.733870000	0.000000000
6	1.899265000	-0.581411000	0.000000000	6	1.212156000	-0.377032000	0.000000000
1	-1.012444000	-2.348983000	0.000000000	1	0.041402000	2.815950000	0.000000000
1	2.974644000	-0.717897000	0.000000000	1	2.144198000	-0.926908000	0.000000000
6	-0.846309000	-0.226490000	0.000000000	6	-1.195582000	1.042274000	0.000000000
6	1.372739000	0.706766000	0.000000000	6	0.000000000	-1.043230000	0.000000000
9	-2.171224000	-0.029479000	0.000000000	1	-2.143296000	1.567417000	0.000000000
1	2.007202000	1.585259000	0.000000000	9	-0.025950000	-2.379039000	0.000000000
6	0.000000000	0.875951000	0.000000000	6	-1.199357000	-0.340368000	0.000000000
9	-0.532664000	2.104986000	0.000000000	9	-2.354175000	-1.019104000	0.000000000
1	1.462783000	-2.687785000	0.000000000	9	2.363368000	1.664640000	0.000000000
r_{d9}				r_{d10}			
6	-0.000064000	-1.408082000	0.000000000	6	1.209208000	-1.369794000	0.000000000
6	1.179257000	-0.681401000	0.000000000	6	-0.000020000	-2.055187000	0.000000000
6	-1.179471000	-0.681449000	0.000000000	6	1.195941000	0.014068000	0.000000000
9	2.341860000	-1.350810000	0.000000000	1	-0.000078000	-3.138824000	0.000000000
9	-2.341696000	-1.350558000	0.000000000	9	2.340318000	0.706255000	0.000000000
6	1.218271000	0.703221000	0.000000000	6	-1.209234000	-1.369739000	0.000000000
6	-1.218261000	0.703231000	0.000000000	6	0.000000000	0.720896000	0.000000000
1	2.154740000	1.243780000	0.000000000	1	-2.161848000	-1.885179000	0.000000000
1	-2.154692000	1.243862000	0.000000000	9	0.000035000	2.052245000	0.000000000
6	0.000000000	1.361883000	0.000000000	6	-1.195984000	0.014143000	0.000000000
9	0.000011000	2.703281000	0.000000000	9	-2.340284000	0.706259000	0.000000000
1	-0.000015000	-2.489278000	0.000000000	1	2.161843000	-1.885156000	0.000000000
r_{d11}				r_{d12}			
9	-2.442534000	-0.803836000	-0.000166000	6	0.000000000	1.378605000	-0.525288000
8	-1.517969000	1.829044000	0.000103000	6	0.000000000	0.694542000	0.684814000
8	2.816319000	0.326762000	-0.000076000	6	0.000000000	0.695203000	-1.726531000
7	0.634288000	1.045467000	0.000278000	9	0.000000000	1.355394000	1.838346000
1	1.120218000	-1.208598000	-0.000018000	1	0.000000000	1.258018000	-2.651379000
6	-0.763681000	0.882379000	0.000104000	6	0.000000000	-0.694542000	0.684814000
6	1.631934000	0.082363000	0.000054000	6	0.000000000	-0.695203000	-1.726531000
6	-1.139725000	-0.522514000	-0.000045000	9	0.000000000	-1.355394000	1.838346000
6	-0.221353000	-1.504819000	-0.000146000	1	0.000000000	-1.258018000	-2.651379000

1	0.962113000	2.003413000	0.000257000	6	0.000000000	-1.378605000	-0.525288000
1	1.807025000	-1.946905000	-0.000294000	9	0.000000000	-2.715385000	-0.499078000
1	-0.497719000	-2.550967000	-0.000304000	9	0.000000000	2.715385000	-0.499078000
r_{d13}				r_{d14}			
6	0.000000000	1.379124000	0.000000000	6	1.216583000	-1.002477000	0.000000000
6	1.207706000	0.703506000	0.000000000	6	1.194344000	0.381770000	0.000000000
6	-1.200434000	0.680471000	0.000000000	6	0.000000000	-1.663261000	0.000000000
1	2.142306000	1.249238000	0.000000000	9	2.339132000	1.067001000	0.000000000
9	-2.353741000	1.356306000	0.000000000	9	0.000000000	-3.004791000	0.000000000
6	1.200183000	-0.680594000	0.000000000	6	0.000000000	1.090921000	0.000000000
6	-1.207815000	-0.703509000	0.000000000	6	-1.216583000	-1.002477000	0.000000000
9	2.353793000	-1.356123000	0.000000000	9	0.000000000	2.422393000	0.000000000
1	-2.142324000	-1.249312000	0.000000000	1	-2.154580000	-1.540948000	0.000000000
6	0.000150000	-1.379404000	0.000000000	6	-1.194344000	0.381770000	0.000000000
9	0.018531000	-2.715355000	0.000000000	9	-2.339132000	1.067000000	0.000000000
9	-0.018441000	2.715452000	0.000000000	1	2.154581000	-1.540948000	0.000000000
r_{e1}				r_{e2}			
7	-0.180053000	-1.865639000	-0.005361000	7	1.530878000	1.364099000	-0.070804000
6	0.574894000	-0.797971000	-0.048670000	6	0.233824000	0.871377000	0.010775000
6	-1.508093000	-1.512036000	0.025197000	6	2.582419000	0.386917000	0.233685000
1	-2.177880000	-2.372495000	0.060824000	6	-0.061057000	-0.458315000	0.088143000
6	0.136639000	0.555217000	-0.031968000	6	2.223429000	-0.964492000	-0.364834000
7	-2.086185000	-0.339958000	0.019996000	7	0.958018000	-1.398444000	0.192885000
6	-1.308331000	0.817876000	-0.008829000	1	0.622639000	-2.315245000	-0.085017000
7	1.953396000	-0.785655000	-0.099696000	7	-0.815372000	1.763062000	-0.051672000
6	1.261861000	1.330408000	0.027290000	6	-1.435748000	-0.921019000	0.038844000
7	2.359275000	0.529860000	0.111235000	6	-2.101270000	1.296969000	-0.058284000
1	2.502536000	-1.503569000	0.357588000	7	-2.440722000	0.056863000	-0.004022000
8	-1.776701000	1.944063000	-0.011566000	1	-0.632955000	2.742978000	-0.211477000
1	3.244774000	0.787433000	-0.307170000	1	-2.861477000	2.075163000	-0.108568000
1	1.377325000	2.404904000	0.019956000	8	-1.688766000	-2.122057000	0.035626000
r_{e3}				r_{e4}			
6	1.213663000	0.897133000	0.000392000	7	-0.357677000	-1.804555000	0.000018000
6	-0.203503000	0.573900000	0.000134000	6	0.626597000	-0.841490000	0.000135000
7	2.085404000	-0.230927000	0.000087000	6	-1.658002000	-1.381423000	0.000039000
6	-0.612394000	-0.747476000	-0.000188000	1	-2.387649000	-2.190993000	-0.000254000
6	1.619859000	-1.425077000	-0.000211000	6	0.228666000	0.485739000	0.000106000
7	0.286669000	-1.778802000	-0.000313000	7	-2.071925000	-0.158925000	-0.000128000
6	-1.390179000	1.362884000	0.000033000	6	-1.158095000	0.912661000	0.000072000
7	-1.968928000	-0.801867000	-0.000176000	1	-0.139196000	-2.789017000	0.000324000
6	-2.452257000	0.505026000	-0.000084000	6	2.031356000	-0.826347000	-0.000075000
1	-2.539091000	-1.631214000	-0.000289000	7	1.379027000	1.201591000	0.000043000
1	-1.433870000	2.440511000	0.000143000	7	2.474819000	0.431871000	-0.000076000
8	1.663537000	2.027337000	0.000447000	8	-1.508459000	2.079127000	-0.000055000
1	0.009841000	-2.748415000	-0.000605000	1	1.465614000	2.206698000	0.000176000
1	2.297139000	-2.279488000	-0.000352000	1	2.736070000	-1.644427000	-0.000463000
1	-3.515464000	0.682741000	-0.000115000	r_{e5}			
r_{e5}				r_{e6}			
6	-1.064273346	-1.171435443	0.000000000	7	-1.332748000	0.621852000	-0.117815000
7	-1.134793093	0.175106868	0.000000000	7	-0.029986000	1.073859000	0.124130000
6	0.160951906	-1.767202240	0.000000000	6	0.814368000	-0.070916000	0.029671000
1	-2.029918106	0.646677882	0.000000000	7	-0.023846000	-1.204183000	0.019808000
1	0.270192082	-2.842047489	0.000000000	6	-1.227025000	-0.742400000	-0.022021000
6	0.000000000	1.040196839	0.000000000	1	-2.054034000	1.091727000	0.420467000
6	1.278385869	-0.894591602	0.000000000	1	0.242206000	1.875034000	-0.432825000
8	-0.179351928	2.237120104	0.000000000	8	2.015285000	-0.022817000	-0.026214000
1	2.279696118	-1.330768596	0.000000000	1	-2.128448000	-1.345027000	-0.006695000
7	1.230332871	0.410783894	0.000000000	r_{e6}			
1	-2.004322332	-1.713862232	0.000000000	r_{e6}			

r_{e7}				r_{e8}			
7	-0.229795000	-1.764066000	-0.078879000	6	-0.698979000	-0.794688000	0.019617000
7	0.667148000	-0.724750000	0.001492000	7	0.515417000	-1.478120000	-0.071659000
6	-1.557064000	-1.433263000	0.019905000	6	-0.673640000	0.739373000	0.000553000
6	0.224199000	0.590608000	0.004422000	8	-1.645754000	1.444954000	-0.100593000
7	-2.066211000	-0.257098000	0.016719000	6	1.614019000	-0.803969000	-0.049986000
6	-1.207341000	0.872146000	-0.002712000	7	0.593662000	1.303310000	0.139867000
6	2.024369000	-0.722175000	-0.010245000	1	2.574358000	-1.320261000	-0.066093000
6	1.391050000	1.327569000	0.014275000	1	0.679184000	2.271068000	-0.151727000
7	2.480699000	0.516752000	0.011481000	7	1.743882000	0.543069000	-0.044196000
8	-1.651419000	1.998893000	-0.015501000	1	2.581250000	0.948465000	0.357864000
1	1.474812000	2.403570000	0.023662000	8	-1.760986000	-1.360125000	0.084439000
1	2.611103000	-1.628984000	-0.022905000				
1	0.109552000	-2.656583000	0.253050000				
1	-2.198279000	-2.314325000	0.060653000				
r_{e9}							
6	0.992772000	1.186454000	0.000000000				
7	-0.161481000	1.786277000	0.000000000				
7	1.125749000	-0.150629000	0.000000000				
1	2.039733000	-0.587814000	0.000000000				
6	-1.223187000	0.918221000	0.000000000				
6	0.000000000	-1.032227000	0.000000000				
1	-2.199543000	1.403239000	0.000000000				
8	0.177439000	-2.224366000	0.000000000				
7	-1.219671000	-0.382538000	0.000000000				
1	1.910603000	1.773033000	0.000000000				