

**All-atom, Non-empirical, and Tailor-made Force Field for α -RDX from First Principles
(for Electronic Supplemental Information)**

Hua-Jie Song^a, Yan-Geng Zhang^a, Hua Li^a, Tingting Zhou^{a*} and Feng-Lei Huang^{b*}

^a Beijing Institute of Applied Physics and Computational Mathematics, Beijing, 100094

^b State Key Laboratory of Explosion Science and Technology, Beijing Institute of Technology, Beijing 100081

* Correspondence Authors: zhou_tingting@iapcm.ac.cn or huangfl@bit.edu.cn

1. The atom positions for the gas RDX conformers and transition states obtained at the B3LYP/6-31G* level of theory

(1) AAA

N	-0.433701000	1.335838000	0.820977000
C	0.954751000	1.059281000	1.179248000
N	1.372141000	-0.292611000	0.818609000
C	0.439884000	-1.357690000	1.177422000
N	-0.941108000	-1.043010000	0.821176000
C	-1.395423000	0.297485000	1.180745000
H	-1.507977000	0.321642000	2.269351000
H	-2.348890000	0.500602000	0.703388000
H	1.607257000	1.783879000	0.702246000
H	1.032369000	1.144700000	2.267912000
H	0.477300000	-1.470368000	2.265733000
H	0.739755000	-2.284013000	0.697454000
N	-0.668637000	2.058432000	-0.382198000
O	-1.808992000	2.029153000	-0.819986000
O	0.272086000	2.702152000	-0.822290000
N	-1.452298000	-1.606928000	-0.381599000
O	-2.481930000	-1.114622000	-0.818114000
O	-0.856940000	-2.578605000	-0.822393000
N	2.121079000	-0.451220000	-0.380378000
O	2.668479000	0.550586000	-0.815965000
O	2.210120000	-1.587965000	-0.819587000

(2) AAE

N	1.259750000	-0.000014000	0.104920000
C	0.774713000	1.242826000	0.730206000
N	-0.673071000	1.217155000	0.784686000
C	-1.259776000	0.000028000	1.343373000
N	-0.673101000	-1.217119000	0.784699000
C	0.774681000	-1.242831000	0.730228000
H	1.107738000	-2.093188000	0.146130000
H	1.143691000	-1.332764000	1.761970000
H	1.143725000	1.332763000	1.761947000
H	1.107794000	2.093163000	0.146095000

H	-2.332146000	0.000044000	1.177597000
H	-1.045332000	0.000029000	2.415919000
N	-1.354743000	-1.801621000	-0.330305000
O	-2.547843000	-1.561036000	-0.416659000
O	-0.699845000	-2.545961000	-1.043262000
N	-1.354727000	1.801657000	-0.330311000
O	-2.547748000	1.560746000	-0.416836000
O	-0.699961000	2.546301000	-1.043073000
N	2.618379000	-0.000036000	-0.241691000
O	3.146394000	-1.095925000	-0.392361000
O	3.146429000	1.095834000	-0.392371000

(3) EEA

N	1.172370000	-0.495827000	0.044599000
C	1.221159000	0.676299000	0.931362000
N	-0.000074000	1.440345000	0.766677000
C	-1.221200000	0.676138000	0.931385000
N	-1.172260000	-0.495972000	0.044605000
C	0.000110000	-1.364635000	0.155009000
H	0.000155000	-2.073579000	-0.666030000
H	0.000142000	-1.918384000	1.110450000
H	1.279784000	0.378772000	1.987177000
H	2.080487000	1.283256000	0.671020000
H	-2.080599000	1.283003000	0.671050000
H	-1.279799000	0.378594000	1.987196000
N	-2.385593000	-1.170719000	-0.141818000
O	-3.405475000	-0.541301000	0.114592000
O	-2.316478000	-2.317181000	-0.569230000
N	-0.000190000	2.341436000	-0.357918000
O	-1.092774000	2.707927000	-0.756080000
O	1.092240000	2.708453000	-0.756024000
N	2.385784000	-1.170427000	-0.141822000
O	2.316799000	-2.316974000	-0.569027000
O	3.405582000	-0.540964000	0.114811000

(4) EEE

N	-1.307226000	-0.320357000	-0.095225000
C	-0.402907000	-1.384822000	0.328372000
N	0.931369000	-0.971238000	-0.095045000
C	1.399771000	0.343178000	0.332108000
N	0.375850000	1.291925000	-0.093580000
C	-0.997387000	1.040386000	0.331972000
H	-1.661948000	1.734843000	-0.170143000
H	-1.106972000	1.153724000	1.424985000
H	-0.448262000	-1.540289000	1.420804000
H	-0.671056000	-2.305962000	-0.177220000

H	2.333225000	0.572388000	-0.170108000
H	1.553087000	0.380099000	1.425144000
N	0.767360000	2.636786000	-0.100501000
O	1.972744000	2.855221000	-0.117705000
O	-0.132441000	3.468018000	-0.118511000
N	1.900392000	-1.982538000	-0.100032000
O	3.070206000	-1.618694000	-0.115070000
O	1.487111000	-3.135751000	-0.118249000
N	-2.667634000	-0.653802000	-0.099794000
O	-3.459574000	0.280873000	-0.115513000
O	-2.937511000	-1.848752000	-0.117319000

(5) twist

N	0.325295000	-1.040669000	0.233983000
C	-0.472120000	-0.708211000	-0.966525000
N	-1.455982000	0.287989000	-0.592156000
C	-0.930683000	1.564947000	-0.087908000
N	0.353069000	1.341834000	0.590815000
C	0.488146000	0.035976000	1.220916000
H	-0.299064000	-0.030754000	1.976612000
H	1.458840000	-0.069438000	1.697078000
H	0.155788000	-0.282114000	-1.757216000
H	-0.967046000	-1.596931000	-1.344943000
H	-1.662298000	1.980223000	0.603321000
H	-0.762884000	2.261619000	-0.908213000
N	1.417632000	-1.879106000	0.007159000
O	1.433620000	-2.441402000	-1.085405000
O	2.217198000	-2.019418000	0.923119000
N	1.507658000	1.812408000	-0.096597000
O	2.566949000	1.270983000	0.185836000
O	1.344502000	2.753116000	-0.862202000
N	-2.629898000	-0.210498000	0.041624000
O	-2.875033000	-1.396318000	-0.117475000
O	-3.319714000	0.607715000	0.636209000

(6) twist_e

N	1.456039000	0.288037000	-0.592293000
C	0.472113000	-0.708261000	-0.966331000
N	-0.325294000	-1.040551000	0.234197000
C	-0.488254000	0.036132000	1.221037000
N	-0.352895000	1.342102000	0.591052000
C	0.930836000	1.564986000	-0.087886000
H	1.662495000	1.980038000	0.603307000
H	0.762884000	2.261620000	-0.908110000
H	-0.155781000	-0.282372000	-1.757105000
H	0.967151000	-1.596964000	-1.344504000

H	0.298798000	-0.030602000	1.976857000
H	-1.459045000	-0.069113000	1.696904000
N	2.629620000	-0.210803000	0.041563000
O	2.874005000	-1.396779000	-0.117437000
O	3.320171000	0.606992000	0.635909000
N	-1.507231000	1.812504000	-0.096568000
O	-1.343919000	2.752874000	-0.862580000
O	-2.566708000	1.271527000	0.186162000
N	-1.417616000	-1.879020000	0.007286000
O	-1.434167000	-2.440349000	-1.085750000
O	-2.217259000	-2.019968000	0.923079000

(7) AAA-AAE

N	-1.313915000	-0.000497000	0.537944000
C	-0.725250000	1.247480000	0.997386000
N	0.722223000	1.222108000	0.823300000
C	1.383288000	0.000465000	1.285268000
N	0.723133000	-1.221630000	0.823253000
C	-0.724341000	-1.248116000	0.997249000
H	-0.914430000	-1.378778000	2.070135000
H	-1.152269000	-2.075756000	0.440271000
H	-1.153859000	2.074866000	0.440526000
H	-0.915360000	1.377853000	2.070299000
H	1.331726000	0.000409000	2.377916000
H	2.419268000	0.000838000	0.962123000
N	-2.430760000	-0.000767000	-0.290383000
O	-2.876734000	-1.097108000	-0.609015000
O	-2.877456000	1.095451000	-0.608380000
N	1.226113000	-1.802387000	-0.381797000
O	0.472374000	-2.553585000	-0.982347000
O	2.389395000	-1.554493000	-0.655901000
N	1.224511000	1.803168000	-0.381896000
O	0.469819000	2.553380000	-0.982478000
O	2.388052000	1.556558000	-0.656084000

(8) AAE-EEA

N	1.240685000	-0.340449000	0.048859000
C	1.166047000	0.887666000	0.862033000
N	-0.176915000	1.431106000	0.788172000
C	-1.230480000	0.482927000	1.124605000
N	-1.051024000	-0.734385000	0.346872000
C	0.244171000	-1.382037000	0.342128000
H	0.265593000	-2.137222000	-0.436894000
H	0.451212000	-1.856674000	1.316155000
H	1.374687000	0.678369000	1.920113000
H	1.881846000	1.607215000	0.481808000

H	-2.205060000	0.906314000	0.906926000
H	-1.140063000	0.277914000	2.198800000
N	-2.152524000	-1.401524000	-0.179468000
O	-3.243193000	-0.867713000	-0.014469000
O	-1.931635000	-2.460721000	-0.755458000
N	-0.436784000	2.230500000	-0.380383000
O	-1.609063000	2.374957000	-0.685416000
O	0.532595000	2.747066000	-0.910120000
N	2.533430000	-0.828105000	-0.179873000
O	2.623113000	-2.005820000	-0.508903000
O	3.452593000	-0.026175000	-0.059229000

(9) AAE-EEA_e

N	1.050587000	-0.735267000	0.348103000
C	1.230488000	0.482247000	1.125343000
N	0.177616000	1.431009000	0.788350000
C	-1.165694000	0.888371000	0.861935000
N	-1.240867000	-0.339960000	0.049207000
C	-0.244988000	-1.382106000	0.342653000
H	-0.266483000	-2.137063000	-0.436589000
H	-0.452696000	-1.856934000	1.316431000
H	1.139640000	0.277631000	2.199569000
H	2.205406000	0.904932000	0.907804000
H	-1.880930000	1.608220000	0.481215000
H	-1.374800000	0.679635000	1.920034000
N	-2.533837000	-0.826817000	-0.180028000
O	-3.452555000	-0.024315000	-0.059877000
O	-2.624184000	-2.004527000	-0.508882000
N	0.438251000	2.229832000	-0.380498000
O	-0.530697000	2.746768000	-0.910635000
O	1.610673000	2.373462000	-0.685327000
N	2.151631000	-1.402094000	-0.179618000
O	1.930227000	-2.460983000	-0.755968000
O	3.242456000	-0.868457000	-0.015143000

(10) EEA-EEE

N	1.170925000	-0.654120000	-0.096178000
C	1.247672000	0.707721000	0.437388000
N	-0.001249000	1.348526000	0.076150000
C	-1.248935000	0.705388000	0.437530000
N	-1.169703000	-0.656271000	-0.096073000
C	0.001347000	-1.451916000	0.267028000
H	0.002175000	-2.370488000	-0.309454000
H	0.001622000	-1.697937000	1.343770000
H	1.391891000	0.697766000	1.531635000
H	2.071682000	1.234849000	-0.031414000

H	-2.073975000	1.231004000	-0.031160000
H	-1.392993000	0.695134000	1.531796000
N	-2.381347000	-1.359844000	-0.106234000
O	-3.403204000	-0.685820000	-0.048870000
O	-2.307206000	-2.578979000	-0.202703000
N	-0.002556000	2.725962000	-0.135779000
O	-1.099364000	3.264896000	-0.225504000
O	1.093223000	3.266856000	-0.226337000
N	2.383875000	-1.355477000	-0.106135000
O	2.312008000	-2.574758000	-0.202495000
O	3.404479000	-0.679562000	-0.048729000

(11) EEA-twist

N	-1.048227000	-1.007264000	-0.600423000
C	-0.000236000	-1.846243000	0.000972000
N	1.048389000	-1.007273000	0.601009000
C	0.609293000	0.282296000	1.106617000
N	0.000238000	1.023410000	0.000139000
C	-0.608449000	0.281969000	-1.106303000
H	0.113540000	0.088457000	-1.907720000
H	-1.447503000	0.844131000	-1.505324000
H	-0.467894000	-2.471864000	0.759408000
H	0.466863000	-2.473552000	-0.756402000
H	1.448719000	0.844360000	1.504997000
H	-0.112354000	0.089319000	1.908471000
N	0.000181000	2.393720000	0.000029000
O	0.449690000	2.940502000	1.005528000
O	-0.449353000	2.940389000	-1.005513000
N	2.302762000	-0.994709000	-0.080711000
O	3.037488000	-0.046068000	0.147657000
O	2.554788000	-1.965417000	-0.782006000
N	-2.303139000	-0.994161000	0.080257000
O	-3.037485000	-0.045433000	-0.148976000
O	-2.555934000	-1.964604000	0.781652000

(12) EEA-twist_e

N	1.048227000	1.007264000	0.600423000
C	0.000236000	1.846243000	-0.000972000
N	-1.048389000	1.007273000	-0.601009000
C	-0.609293000	-0.282296000	-1.106617000
N	-0.000238000	-1.023410000	-0.000139000
C	0.608449000	-0.281969000	1.106303000
H	-0.113540000	-0.088457000	1.907720000
H	1.447503000	-0.844131000	1.505324000
H	0.467894000	2.471864000	-0.759408000
H	-0.466863000	2.473552000	0.756402000

H	-1.448719000	-0.844360000	-1.504997000
H	0.112354000	-0.089319000	-1.908471000
N	-0.000181000	-2.393720000	-0.000029000
O	-0.449690000	-2.940502000	-1.005528000
O	0.449353000	-2.940389000	1.005513000
N	-2.302762000	0.994709000	0.080711000
O	-3.037488000	0.046068000	-0.147657000
O	-2.554788000	1.965417000	0.782006000
N	2.303139000	0.994161000	-0.080257000
O	3.037485000	0.045433000	0.148976000
O	2.555934000	1.964604000	-0.781652000

(13) boat

N	-0.694888000	1.492963000	0.000000000
C	-0.776737000	0.729671000	1.228729000
N	0.274339000	-0.315614000	1.210787000
C	1.079831000	-0.442995000	0.000000000
N	0.274339000	-0.315614000	-1.210787000
C	-0.776737000	0.729671000	-1.228729000
H	-1.761665000	0.258285000	-1.276375000
H	-0.654991000	1.394688000	-2.080160000
H	-0.654991000	1.394688000	2.080160000
H	-1.761665000	0.258285000	1.276375000
H	1.566496000	-1.415179000	0.000000000
H	1.837529000	0.344854000	0.000000000
N	0.196265000	2.610917000	0.000000000
O	0.513068000	3.053799000	1.093196000
O	0.513068000	3.053799000	-1.093196000
N	-0.017579000	-1.468102000	-1.943090000
O	-0.939161000	-1.356809000	-2.749323000
O	0.686523000	-2.452542000	-1.761551000
N	-0.017579000	-1.468102000	1.943090000
O	-0.939161000	-1.356809000	2.749323000
O	0.686523000	-2.452542000	1.761551000

2. The Born–Mayer repulsion parameters

(Note: We found that \bar{S} -function expansion for RDX dimer converges at $l = 1$.)

atom pair	$l_a k_a$	$l_b k_b$	l	ρ	α
C-C	00	00	0	5.274554	1.769427
	00	10	1	-0.077880	
	10	00	1	-0.077880	
C-H	00	00	0	4.405158	1.878563
	00	10	1	-0.018652	
	10	00	1	0.014848	

	00	00	0	5.108723	
C-N	00	10	1	-0.089986	2.100451
	10	00	1	-0.122216	
	00	00	0	5.549693	
C-O	00	10	1	-0.144367	2.189134
	10	00	1	0.008035	
	00	00	0	3.880241	
H-H	00	10	1	0.056932	1.786859
	10	00	1	0.056932	
	00	00	0	4.182617	
H-N	00	10	1	-0.302414	2.026678
	10	00	1	0.025731	
	00	00	0	4.759655	
H-O	00	10	1	-0.020237	2.115238
	10	00	1	0.123452	
	00	00	0	4.397317	
N-N	00	10	1	-0.475086	1.984348
	10	00	1	-0.475086	
	00	00	0	5.236072	
N-O	00	10	1	-0.156987	2.668108
	10	00	1	-0.126141	
	00	00	0	5.768799	
O-O	00	10	1	0.007358	2.087284
	10	00	1	0.007358	

3. Energy ranks of low energy structures for 216 Space groups

(Note: The table gives the low energy structures for 216 space groups, since other 14 space groups failed to be built in the search.)

Rank No.	Space group	Density (g/cm ³)	Total energy (kJ/mol)	<i>a</i> (Å)	<i>b</i> (Å)	<i>c</i> (Å)	<i>α</i> (deg)	<i>β</i> (deg)	<i>γ</i> (deg)
1	PBCA	1.915	-38.510	13.029	11.264	10.498	90.0	90.0	90.0
2	P21/C	1.901	-35.288	7.257	14.510	8.235	90.0	116.5	90.0
3	P21	1.842	-35.223	7.333	6.119	9.120	90.0	78.1	90.0
4	PNA21	1.865	-35.161	9.992	12.199	6.488	90.0	90.0	90.0
5	P212121	1.871	-34.969	13.663	7.549	7.645	90.0	90.0	90.0
6	P41212	1.853	-34.830	7.645	7.645	27.238	90.0	90.0	90.0
7	PCA21	1.807	-34.729	12.226	7.643	8.737	90.0	90.0	90.0
8	P43212	1.843	-34.562	7.638	7.638	27.444	90.0	90.0	90.0
9	IBA2	1.840	-34.546	25.018	10.562	6.069	90.0	90.0	90.0
10	P-1	1.870	-34.079	6.942	6.157	10.438	111.7	74.9	104.4
11	C2/C	1.876	-34.035	12.744	7.242	19.612	90.0	119.7	90.0
12	CC	1.895	-33.993	7.146	20.020	5.896	90.0	67.4	90.0
13	FDD2	1.797	-33.700	44.392	9.625	7.685	90.0	90.0	90.0
14	PCCN	1.815	-33.605	25.107	11.008	5.882	90.0	90.0	90.0

15	P42BC	1.796	-33.536	16.717	16.717	5.878	90.0	90.0	90.0
16	P-421C	1.791	-33.399	16.883	16.883	5.780	90.0	90.0	90.0
17	P1	1.773	-33.389	6.408	5.686	7.824	114.8	120.7	93.6
18	PBCN	1.835	-33.335	25.472	10.244	6.163	90.0	90.0	90.0
19	ABA2	1.816	-33.321	9.608	26.359	6.415	90.0	90.0	90.0
20	P21212	1.828	-33.226	8.527	13.050	7.253	90.0	90.0	90.0
21	I-4	1.776	-33.031	16.270	16.270	6.278	90.0	90.0	90.0
22	C2	1.877	-32.971	12.871	7.686	8.055	90.0	99.4	90.0
23	P42/N	1.805	-32.891	15.833	15.833	6.521	90.0	90.0	90.0
24	R3C	1.822	-32.615	25.706	25.706	6.366	90.0	90.0	120.0
25	I41CD	1.762	-32.566	24.107	24.107	5.763	90.0	90.0	90.0
26	PC	1.733	-32.464	6.297	11.982	5.785	90.0	77.2	90.0
27	PCCA	1.868	-32.405	24.603	7.878	8.152	90.0	90.0	90.0
28	PCC2	1.874	-32.393	12.296	7.888	8.118	90.0	90.0	90.0
29	C2221	1.822	-32.302	8.312	13.057	14.923	90.0	90.0	90.0
30	PNN2	1.679	-32.179	10.550	12.939	6.435	90.0	90.0	90.0
31	P2/C	1.861	-32.121	12.337	7.875	8.160	90.0	90.0	90.0
32	P61	1.690	-32.077	15.596	15.596	6.217	90.0	90.0	120.0
33	R3	1.860	-31.858	16.338	16.338	7.721	90.0	90.0	120.0
34	P42	1.698	-31.808	9.084	9.084	10.527	90.0	90.0	90.0
35	I-43D	1.759	-31.700	21.593	21.593	21.593	90.0	90.0	90.0
36	R-3	1.449	-31.576	29.066	29.066	6.260	90.0	90.0	120.0
37	P65	1.685	-31.518	15.569	15.569	6.259	90.0	90.0	120.0
38	I4	1.710	-31.480	15.935	15.935	6.797	90.0	90.0	90.0
39	FDDD	1.852	-31.470	19.813	24.476	13.140	90.0	90.0	90.0
40	CCC2	1.767	-31.389	11.590	25.521	5.647	90.0	90.0	90.0
41	P-4	1.705	-31.305	9.021	9.021	10.631	90.0	90.0	90.0
42	P4122	1.752	-31.272	9.214	9.214	19.840	90.0	90.0	90.0
43	IBCA	1.724	-31.062	22.727	5.843	25.772	90.0	90.0	90.0
44	P42212	1.792	-31.056	13.186	13.186	9.471	90.0	90.0	90.0
45	P41	1.601	-30.999	12.353	12.353	6.039	90.0	90.0	90.0
46	I41/A	1.627	-30.945	24.065	24.065	6.262	90.0	90.0	90.0
47	P31C	1.793	-30.871	14.805	14.805	6.502	90.0	90.0	120.0
48	CMC21	1.662	-30.770	28.694	9.655	6.407	90.0	90.0	90.0
49	PBA2	1.752	-30.759	11.518	11.263	6.491	90.0	90.0	90.0
50	PNNA	1.760	-30.675	5.679	25.401	11.620	90.0	90.0	90.0
51	I222	1.635	-30.617	10.678	14.719	11.484	90.0	90.0	90.0
52	PNC2	1.714	-30.585	6.409	22.485	5.975	90.0	90.0	90.0
53	P4/NCC	1.658	-30.551	17.460	17.460	11.678	90.0	90.0	90.0
54	P3121	1.731	-30.528	7.375	7.375	27.138	90.0	90.0	120.0
55	P64	1.603	-30.514	14.960	14.960	7.125	90.0	90.0	120.0
56	P43	1.614	-30.465	12.116	12.116	6.226	90.0	90.0	90.0
57	P-3C1	1.646	-30.446	17.149	17.149	10.557	90.0	90.0	120.0
58	P4/N	1.657	-30.435	16.742	16.742	6.354	90.0	90.0	90.0

59	I-42D	1.673	-30.289	12.175	12.175	23.790	90.0	90.0	90.0
60	P62	1.573	-29.909	15.050	15.050	7.171	90.0	90.0	120.0
61	P-3	1.771	-29.892	10.660	10.660	12.699	90.0	90.0	120.0
62	P63	1.592	-29.833	15.867	15.867	6.377	90.0	90.0	120.0
63	R-3C	1.623	-29.802	31.318	31.318	9.633	90.0	90.0	120.0
64	P2	1.740	-29.795	5.962	6.381	11.685	90.0	107.4	90.0
65	P3221	1.709	-29.766	7.459	7.459	26.876	90.0	90.0	120.0
66	P2221	1.730	-29.736	6.391	5.907	22.599	90.0	90.0	90.0
67	PNMA	1.610	-29.675	10.275	27.529	6.479	90.0	90.0	90.0
68	P31	1.657	-29.650	11.290	11.290	6.049	90.0	90.0	120.0
69	P32	1.731	-29.648	10.782	10.782	6.350	90.0	90.0	120.0
70	PMN21	1.543	-29.478	27.330	6.442	5.430	90.0	90.0	90.0
71	P21/M	1.706	-29.353	6.046	22.447	6.431	90.0	82.3	90.0
72	ABM2	1.663	-29.293	11.024	27.434	5.868	90.0	90.0	90.0
73	P6122	1.694	-29.279	7.339	7.339	56.029	90.0	90.0	120.0
74	CCCA	1.703	-28.991	21.657	26.586	6.019	90.0	90.0	90.0
75	CMCA	1.648	-28.984	27.363	5.875	22.279	90.0	90.0	90.0
76	P-4C2	1.654	-28.952	12.596	12.596	11.246	90.0	90.0	90.0
77	CM	1.565	-28.894	5.704	26.717	6.327	90.0	77.9	90.0
78	P3112	1.715	-28.827	6.985	6.985	30.533	90.0	90.0	120.0
79	P6	1.581	-28.764	15.865	15.865	6.420	90.0	90.0	120.0
80	I41	1.663	-28.711	18.326	18.326	5.282	90.0	90.0	90.0
81	PA-3	1.627	-28.588	17.587	17.587	17.587	90.0	90.0	90.0
82	P4322	1.651	-28.568	6.300	6.300	45.030	90.0	90.0	90.0
83	P-4B2	1.735	-28.474	11.742	11.742	12.338	90.0	90.0	90.0
84	PBAN	1.693	-28.428	5.838	22.491	13.270	90.0	90.0	90.0
85	P213	1.714	-28.421	13.719	13.719	13.719	90.0	90.0	90.0
86	P4CC	1.598	-28.367	14.802	14.802	8.427	90.0	90.0	90.0
87	PBCM	1.576	-28.328	6.448	10.382	27.971	90.0	90.0	90.0
88	I-4C2	1.764	-28.287	11.690	11.690	24.485	90.0	90.0	90.0
89	PNNN	1.661	-28.251	24.639	12.905	5.587	90.0	90.0	90.0
90	IMA2	1.610	-28.148	28.130	11.394	5.719	90.0	90.0	90.0
91	P4NC	1.631	-28.117	17.578	17.578	5.855	90.0	90.0	90.0
92	C2/M	1.634	-28.092	5.860	27.482	12.448	90.0	115.7	90.0
93	P6CC	1.287	-27.982	25.823	25.823	5.954	90.0	90.0	120.0
94	P-4N2	1.682	-27.965	17.457	17.457	5.756	90.0	90.0	90.0
95	P-42C	1.472	-27.931	12.697	12.697	12.438	90.0	90.0	90.0
96	AMA2	1.594	-27.859	25.173	13.117	5.608	90.0	90.0	90.0
97	P4	1.657	-27.712	11.780	11.780	6.416	90.0	90.0	90.0
98	PNNM	1.562	-27.473	6.446	10.158	28.847	90.0	90.0	90.0
99	PMA2	1.656	-27.443	22.920	6.073	6.401	90.0	90.0	90.0
100	I41/ACD	1.677	-27.357	11.401	11.401	54.156	90.0	90.0	90.0
101	C222	1.623	-27.204	5.898	26.781	11.508	90.0	90.0	90.0
102	IBAM	1.603	-27.065	22.858	5.760	27.966	90.0	90.0	90.0

103	P622	1.552	-26.854	16.695	16.695	11.814	90.0	90.0	120.0
104	P321	1.680	-26.595	15.379	15.379	6.430	90.0	90.0	120.0
105	P4/NNC	1.272	-26.584	27.913	27.913	5.955	90.0	90.0	90.0
106	P3C1	1.505	-26.567	17.398	17.398	5.609	90.0	90.0	120.0
107	P-31C	1.189	-26.514	26.989	26.989	5.902	90.0	90.0	120.0
108	FMM2	1.586	-26.509	22.941	27.261	5.952	90.0	90.0	90.0
109	P422	1.448	-26.402	13.131	13.131	11.816	90.0	90.0	90.0
110	P6522	1.566	-26.287	9.746	9.746	34.352	90.0	90.0	120.0
111	I212121	1.628	-26.209	11.910	5.585	27.250	90.0	90.0	90.0
112	FD-3	1.563	-26.058	28.296	28.296	28.296	90.0	90.0	90.0
113	P42/MBC	1.604	-26.009	11.386	11.386	28.387	90.0	90.0	90.0
114	F222	1.633	-25.976	26.409	24.842	5.510	90.0	90.0	90.0
115	P6222	1.473	-25.952	16.945	16.945	12.085	90.0	90.0	120.0
116	P312	1.178	-25.816	13.596	13.596	11.738	90.0	90.0	120.0
117	I23	1.249	-25.729	19.208	19.208	19.208	90.0	90.0	90.0
118	P4212	1.555	-25.675	18.401	18.401	5.605	90.0	90.0	90.0
119	PMNA	1.584	-25.652	24.955	12.821	5.822	90.0	90.0	90.0
120	CCCM	1.593	-25.604	22.442	6.058	27.252	90.0	90.0	90.0
121	P-43N	1.484	-25.415	18.137	18.137	18.137	90.0	90.0	90.0
122	IA-3	1.654	-25.400	22.038	22.038	22.038	90.0	90.0	90.0
123	PMC21	1.498	-25.084	15.333	10.962	5.861	90.0	90.0	90.0
124	P6422	1.442	-25.080	17.217	17.217	11.960	90.0	90.0	120.0
125	I4122	1.345	-25.054	27.259	27.259	5.905	90.0	90.0	90.0
126	P222	1.584	-25.051	5.528	13.083	12.876	90.0	90.0	90.0
127	P42/NBC	1.298	-24.930	28.004	28.004	5.800	90.0	90.0	90.0
128	PN-3	1.264	-24.916	19.133	19.133	19.133	90.0	90.0	90.0
129	PBAM	1.488	-24.881	5.932	21.838	15.309	90.0	90.0	90.0
130	P42CM	1.161	-24.822	20.762	20.762	5.893	90.0	90.0	90.0
131	PN-3N	1.305	-24.652	23.847	23.847	23.847	90.0	90.0	90.0
132	CMCM	1.513	-24.640	23.878	5.856	27.887	90.0	90.0	90.0
133	P3	1.605	-24.502	11.153	11.153	6.401	90.0	90.0	120.0
134	I4CM	1.269	-24.464	28.133	28.133	5.874	90.0	90.0	90.0
135	R32	1.430	-24.396	19.981	19.981	13.432	90.0	90.0	120.0
136	I422	1.227	-24.362	27.928	27.928	6.168	90.0	90.0	90.0
137	P42/NCM	1.269	-24.277	28.129	28.129	5.879	90.0	90.0	90.0
138	FD-3C	1.133	-24.169	39.690	39.690	39.690	90.0	90.0	90.0
139	P4132	1.494	-24.025	18.094	18.094	18.094	90.0	90.0	90.0
140	P42/NMC	1.125	-23.914	29.886	29.886	5.873	90.0	90.0	90.0
141	F432	1.289	-23.888	30.175	30.175	30.175	90.0	90.0	90.0
142	P63CM	1.143	-23.883	27.577	27.577	5.881	90.0	90.0	120.0
143	PCCM	1.510	-23.795	11.665	12.660	13.231	90.0	90.0	90.0
144	P4222	1.525	-23.770	12.467	12.467	12.449	90.0	90.0	90.0
145	P4332	1.485	-23.747	18.132	18.132	18.132	90.0	90.0	90.0
146	IA-3D	1.480	-23.715	28.815	28.815	28.815	90.0	90.0	90.0

147	F-43C	1.280	-23.697	30.242	30.242	30.242	90.0	90.0	90.0
148	R3M	1.221	-23.635	31.385	31.385	6.376	90.0	90.0	120.0
149	P42NM	1.267	-23.501	18.731	18.731	6.636	90.0	90.0	90.0
150	P2/M	1.464	-23.289	11.293	15.379	5.805	90.0	91.8	90.0
151	P42/M	1.372	-23.267	8.996	8.996	26.565	90.0	90.0	90.0
152	PM	1.366	-23.177	6.414	15.696	5.370	90.0	92.9	90.0
153	P-421M	1.384	-22.852	18.214	18.214	6.426	90.0	90.0	90.0
154	P6322	1.287	-22.800	13.001	13.001	23.499	90.0	90.0	120.0
155	P3212	1.370	-22.709	17.416	17.416	6.150	90.0	90.0	120.0
156	P6/MCC	1.334	-22.683	16.639	16.639	27.677	90.0	90.0	120.0
157	I4/M	1.380	-22.646	12.675	12.675	26.622	90.0	90.0	90.0
158	I213	1.561	-22.550	17.833	17.833	17.833	90.0	90.0	90.0
159	AMM2	1.425	-22.276	15.339	22.808	5.919	90.0	90.0	90.0
160	P63/M	1.003	-22.046	13.643	13.643	27.366	90.0	90.0	120.0
161	IMMA	1.364	-21.979	26.527	27.652	5.897	90.0	90.0	90.0
162	P-31M	1.111	-21.782	27.983	27.983	5.873	90.0	90.0	120.0
163	I41/AMD	1.220	-21.566	40.537	40.537	5.886	90.0	90.0	90.0
164	I41MD	1.381	-21.554	30.823	30.823	4.499	90.0	90.0	90.0
165	P-6C2	0.973	-21.451	13.624	13.624	28.310	90.0	90.0	120.0
166	P42/NNM	1.084	-21.437	30.956	30.956	5.679	90.0	90.0	90.0
167	P4232	1.152	-21.336	19.734	19.734	19.734	90.0	90.0	90.0
168	P63MC	0.998	-20.948	29.332	29.332	5.950	90.0	90.0	120.0
169	I-42M	1.233	-20.917	27.122	27.122	6.505	90.0	90.0	90.0
170	P42MC	1.164	-20.916	20.780	20.780	5.869	90.0	90.0	90.0
171	I4MM	0.998	-20.841	31.729	31.729	5.874	90.0	90.0	90.0
172	CMMA	1.397	-20.839	30.499	23.847	5.809	90.0	90.0	90.0
173	P432	0.900	-20.566	21.427	21.427	21.427	90.0	90.0	90.0
174	F23	0.881	-20.483	27.186	27.186	27.186	90.0	90.0	90.0
175	P4BM	1.290	-20.411	18.937	18.937	6.378	90.0	90.0	90.0
176	IMM2	1.369	-20.098	15.340	23.719	5.924	90.0	90.0	90.0
177	I-4M2	0.975	-19.898	30.721	30.721	6.415	90.0	90.0	90.0
178	I432	1.151	-19.854	24.869	24.869	24.869	90.0	90.0	90.0
179	P4/MNC	1.223	-19.637	13.405	13.405	26.841	90.0	90.0	90.0
180	P4/NBM	1.112	-19.588	34.326	34.326	4.504	90.0	90.0	90.0
181	P-4M2	1.130	-19.586	21.126	21.126	5.851	90.0	90.0	90.0
182	R-3M	0.996	-19.571	58.032	58.032	4.571	90.0	90.0	120.0
183	P-42M	0.979	-19.545	22.784	22.784	5.804	90.0	90.0	90.0
184	PMMN	1.343	-19.481	17.098	28.750	4.469	90.0	90.0	90.0
185	I4132	1.209	-19.400	24.468	24.468	24.468	90.0	90.0	90.0
186	P-62C	1.313	-19.355	11.971	11.971	27.153	90.0	90.0	120.0
187	P4/MCC	0.880	-19.331	15.533	15.533	27.808	90.0	90.0	90.0
188	P31M	1.210	-19.057	18.155	18.155	6.410	90.0	90.0	120.0
189	P6/M	1.117	-18.956	16.810	16.810	16.196	90.0	90.0	120.0
190	PMMA	1.295	-18.236	29.925	16.888	4.509	90.0	90.0	90.0

191	CMM2	1.309	-18.042	17.156	29.567	4.444	90.0	90.0	90.0
192	P4/M	1.191	-17.901	12.355	12.355	16.236	90.0	90.0	90.0
193	F4132	0.598	-17.733	38.972	38.972	38.972	90.0	90.0	90.0
194	P-3M1	0.777	-17.659	38.027	38.027	4.549	90.0	90.0	120.0
195	P4/NMM	1.026	-17.649	35.807	35.807	4.486	90.0	90.0	90.0
196	P-6	0.847	-17.340	13.621	13.621	16.266	90.0	90.0	120.0
197	P23	0.848	-17.059	17.349	17.349	17.349	90.0	90.0	90.0
198	FM-3	0.766	-16.478	35.884	35.884	35.884	90.0	90.0	90.0
199	PMM2	1.213	-16.257	16.893	16.104	4.469	90.0	90.0	90.0
200	P4MM	0.957	-15.440	26.261	26.261	4.469	90.0	90.0	90.0
201	P3M1	0.900	-15.380	25.167	25.167	4.484	90.0	90.0	120.0
202	P6MM	0.859	-15.306	36.465	36.465	4.474	90.0	90.0	120.0
203	I4/MCM	0.843	-13.756	22.082	22.082	28.722	90.0	90.0	90.0
204	FMMM	1.044	-12.549	28.950	14.135	27.626	90.0	90.0	90.0
205	I-43M	0.704	-12.404	29.293	29.293	29.293	90.0	90.0	90.0
206	P42/MNM	1.047	-12.226	19.536	19.536	14.764	90.0	90.0	90.0
207	P42/MCM	0.599	-11.030	18.808	18.808	27.845	90.0	90.0	90.0
208	P4/MBM	0.956	-10.149	18.389	18.389	18.248	90.0	90.0	90.0
209	IMMM	1.100	-8.894	13.674	29.072	13.498	90.0	90.0	90.0
210	P-43M	0.017	-7.543	80.491	80.491	80.491	90.0	90.0	90.0
211	P42/MMC	0.249	-7.481	29.473	29.473	27.262	90.0	90.0	90.0
212	CMMM	0.361	-6.868	48.917	14.521	22.987	90.0	90.0	90.0
213	P-6M2	0.001	-0.677	232.366	232.366	129.228	90.0	90.0	120.0
214	P-62M	0.002	-0.677	188.189	188.189	61.081	90.0	90.0	120.0
215	P6/MMM	0.001	-0.677	289.753	289.753	91.224	90.0	90.0	120.0
216	PMMM	0.002	-0.677	176.544	58.241	132.212	90.0	90.0	90.0