

Supplementary Information

Host-Guest Interaction of NO and NO⁺ species with Calixerenes: Dissecting the Impact of Conformational and Confinement Effects

Hadiya Mecheri Abdulla,¹ Pookkottu K. Sajith*,¹ Subodh S. Khire,² and Karunakaran Remya³

¹*Department of Chemistry, Farook College (Autonomous), (Affiliated to the University of Calicut), Kozhikode, 673632, Kerala, India*
Email: pksajith@farookcollege.ac.in; pksajisiv@gmail.com

²RIKEN Center for Computational Science, Kobe 6500047, Japan

³*Department of Chemistry, Government. Arts and Science College Meenchanda, Kozhikode, 673018, Kerala, India*

Table of contents		Page No.
Table S1	Interaction energies calculated at two different levels of theories	S2
Fig. S1	Optimized geometries of complexes of 1 resulting from different modes of interaction of NO/NO ⁺ with 1 , where phenyl rings are not involved	S3
Fig. S2	The optimized geometries of complexes of NO/NO ⁺ @ 2 for different orientations of NO inside	S4
Fig. S3	The change in atomic charge during the complex formation of the partial cone, 1,2-alternate, and 1,3-alternate conformers of calixarene with NO and NO ⁺	S5
Fig. S4	Atomic charge distribution of 2 before and after the encapsulation of NO/NO ⁺ .	S5
Fig. S5	Molecular diagrams showing $\nabla^2\rho_b$ values (au) at the bcps of various conformers of NO/NO ⁺ @ 2 encapsulated complexes	S6
Fig. S6	Molecular diagrams showing H_b values (au) at the bcps of various conformers of NO/NO ⁺ @ 2 encapsulated complexes	S7
Fig. S7	IGMH scatterplot of complexes of NO/NO ⁺ @ 2	S8
Table S2	Percentage contribution of atomic pair δg of NO/NO ⁺ @ 2 .	S9
Table S3	Cartesian Coordinates of optimized geometries of different complexes	S10

* To whom correspondence should be addressed

Table S1 Interaction energies in kcal/mol calculated at two different levels of theories.

Complex	Mode of interaction	E_{int} (B3LYP-D3/6- 311++G(d,p)//B3LYP-D3/6- 31+G(d,p))	E_{int} (B3LYP/6- 311++G(d,p)//B3LYP/6- 31+G(d,p))
1•••NO	mode (i)	-4.3	-0.7
	mode (ii)	-3.0	-0.5
	mode (iii)	-3.2	-0.9
1•••NO⁺	mode (i)	-65.3	-60.5
	mode (iii)	-60.1	-56.9
	mode (iv)	-67.4	-63.7
	mode (v)	-56.1	-52.1

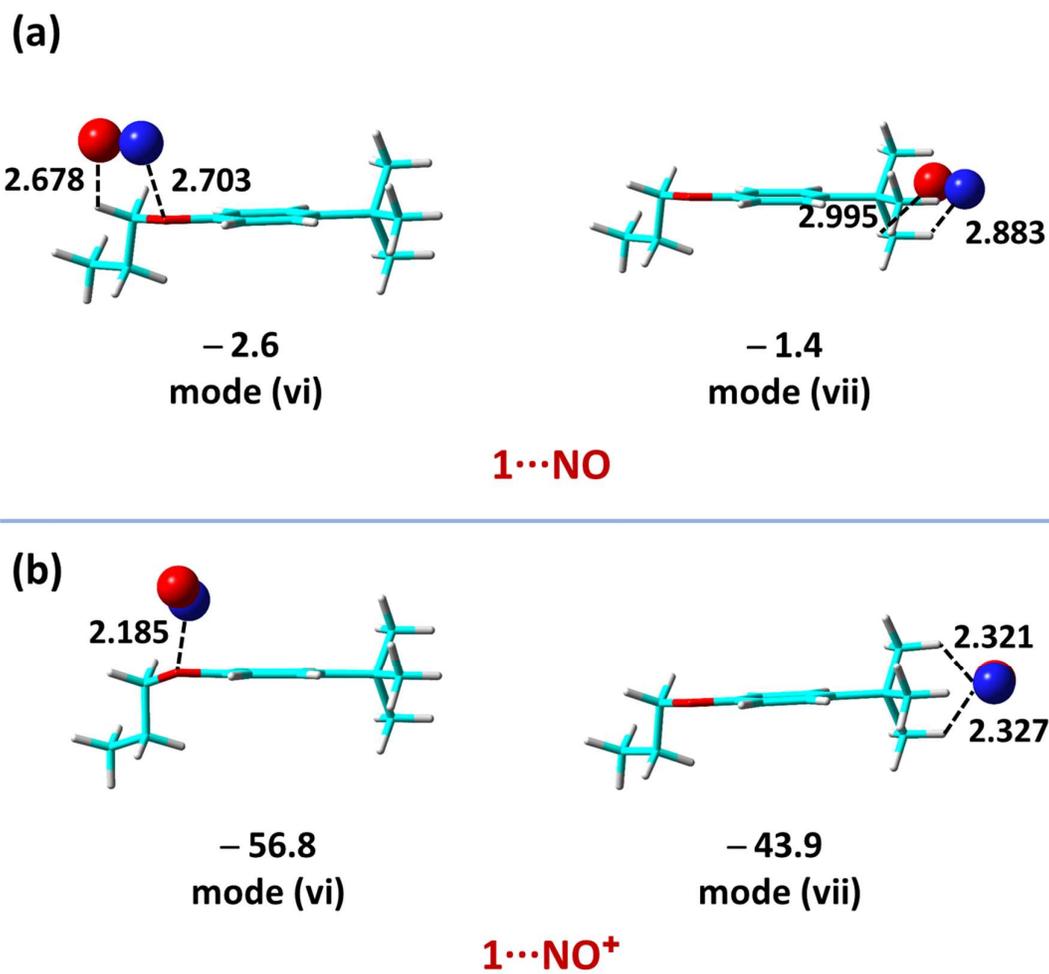


Fig. S1 Optimized geometries of complexes of **1** resulting from different modes of interaction of NO/NO⁺ with **1**, where phenyl rings are not involved. The selected bond distances are in Å. The E_{int} values are given in kcal/mol.

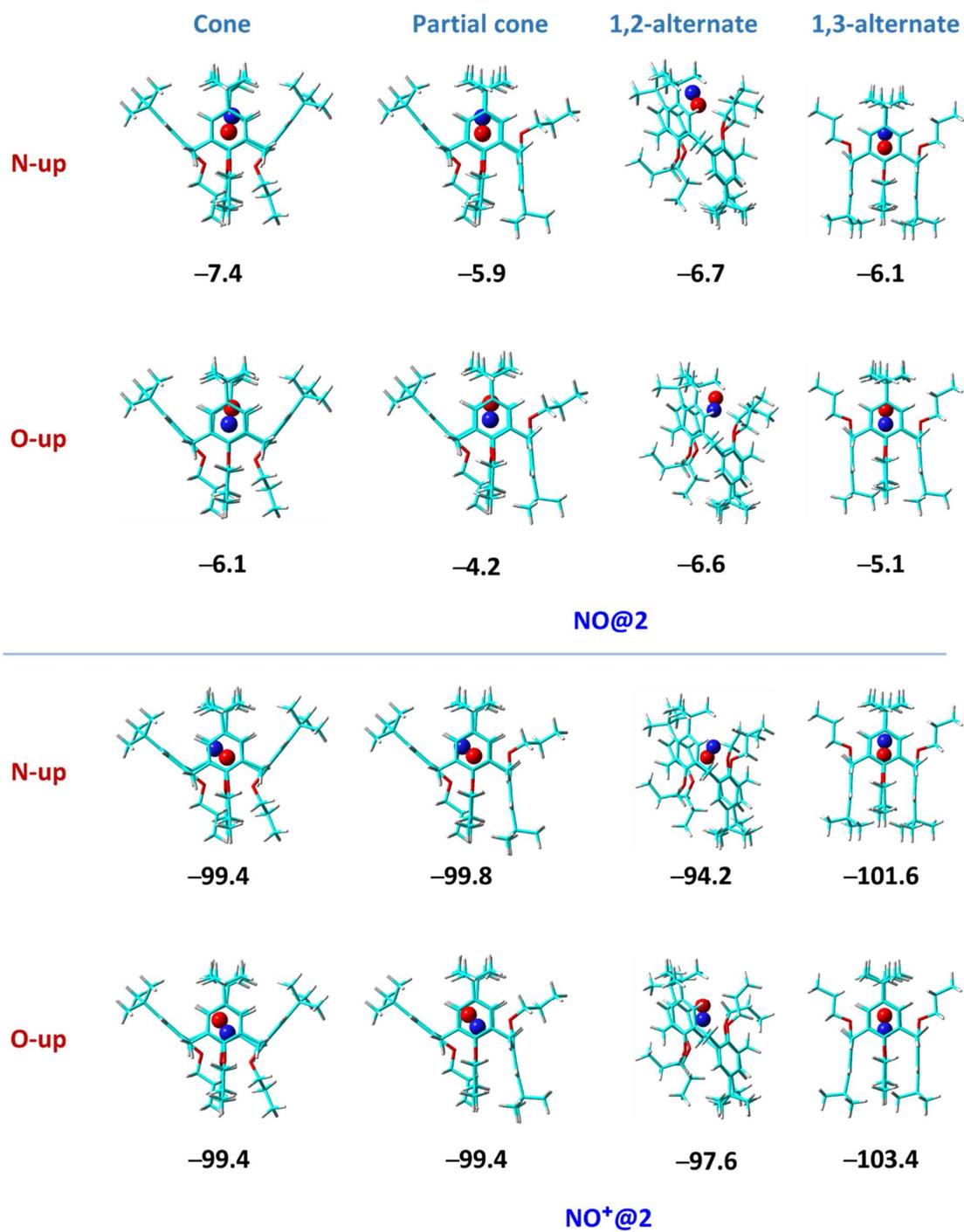


Fig. S2 The optimized geometries of complexes of NO/NO⁺@2 for different orientations of NO. The E_{int} values are given in kcal/mol.

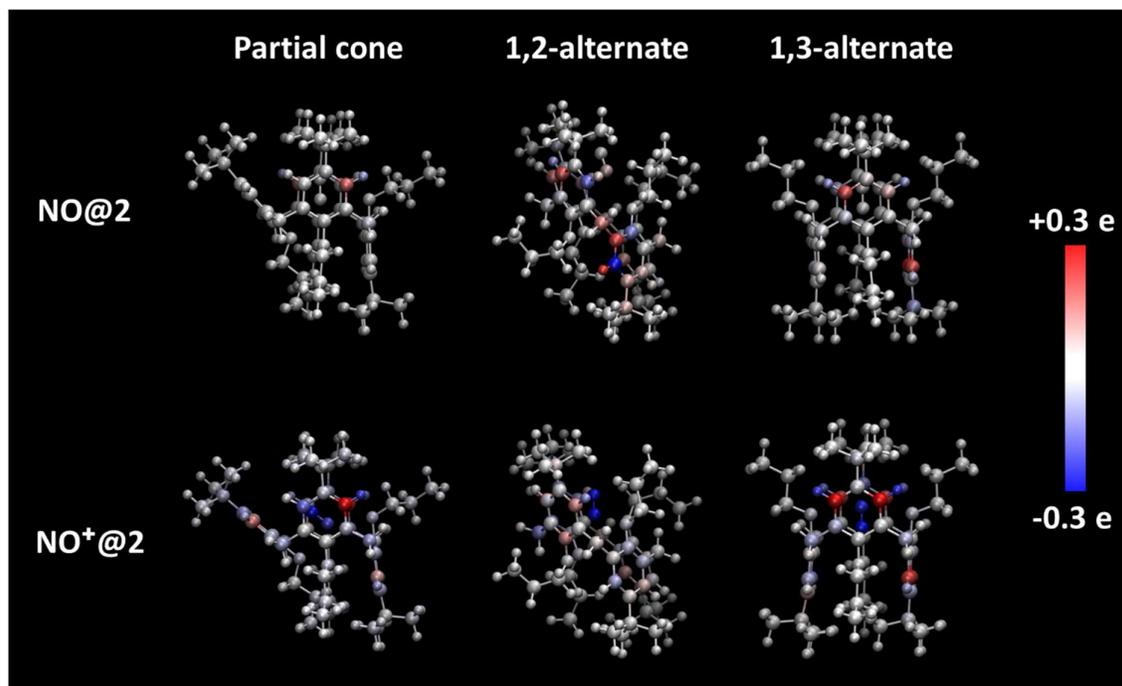


Fig. S3 The change in atomic charge during the host-guest formation of the partial cone, 1,2-alternate, and 1,3-alternate conformers of **2** with NO and NO⁺.

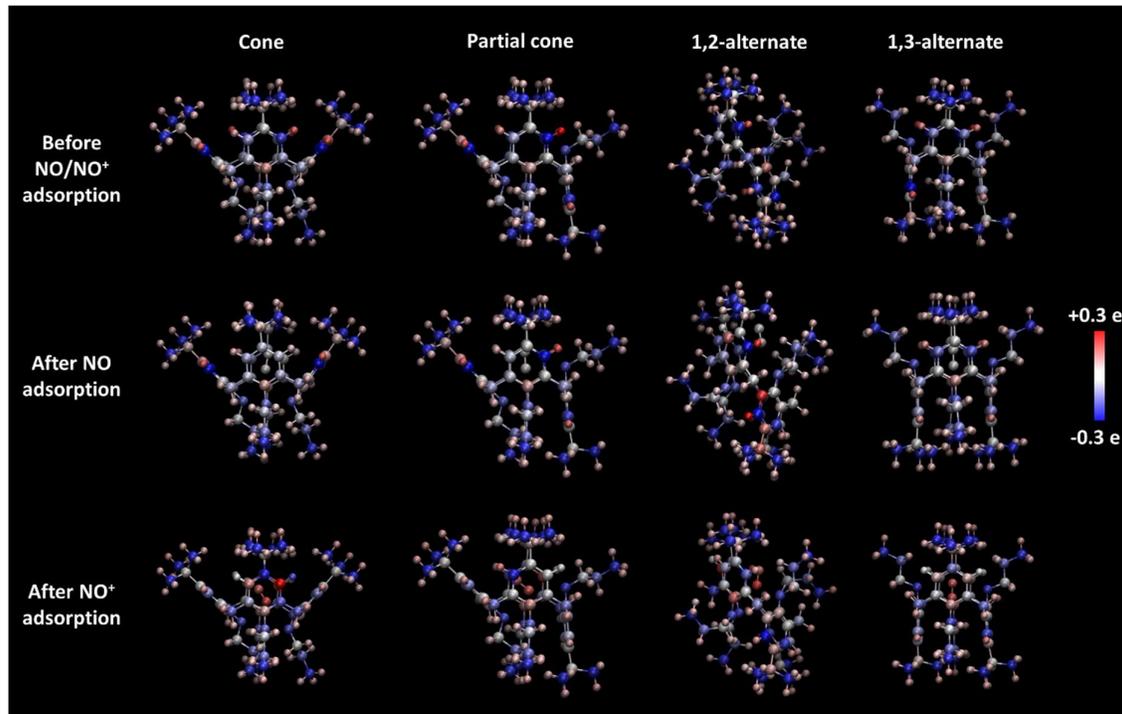


Fig. S4 Atomic charge distribution of **2** before and after the encapsulation of NO/NO⁺.

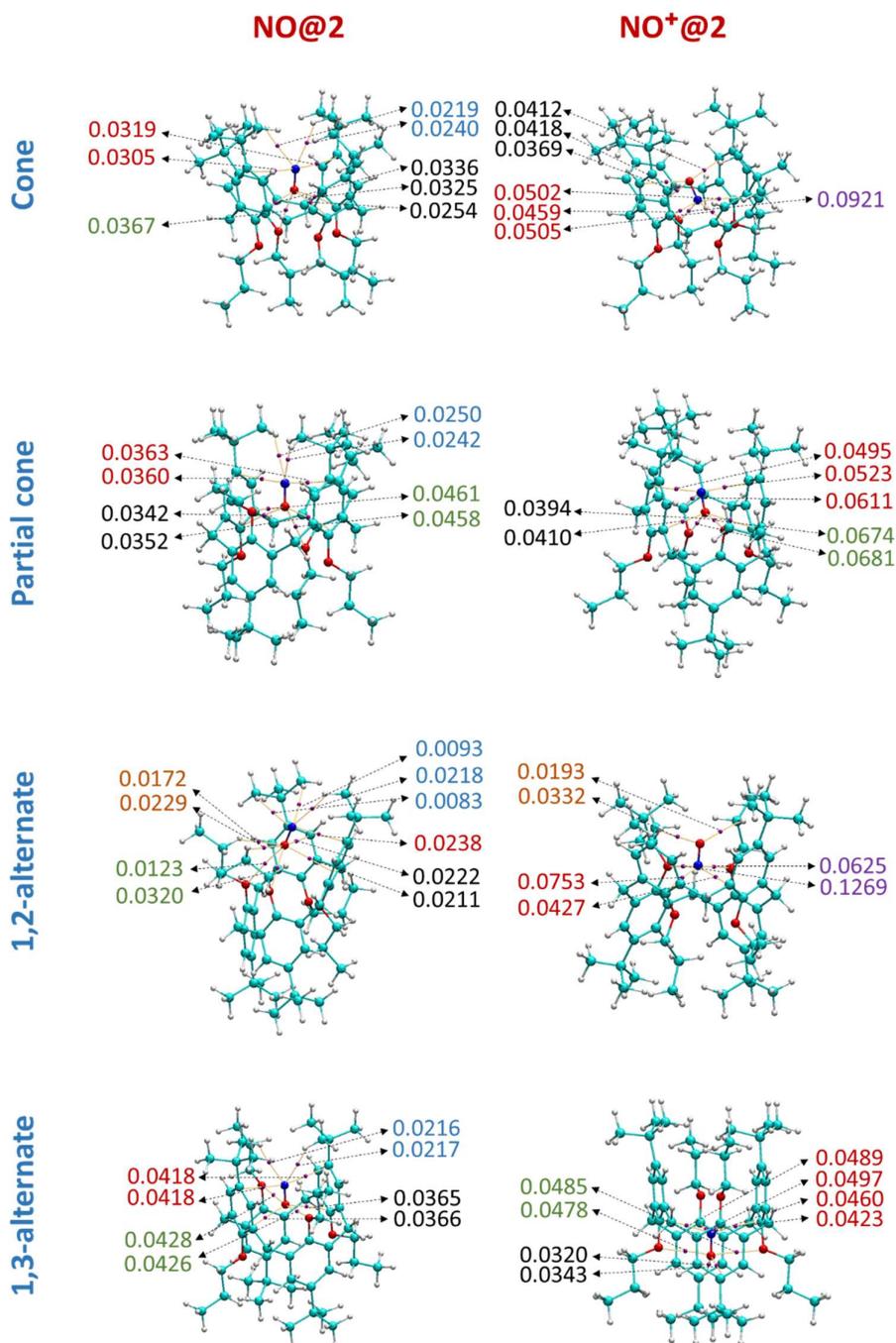


Fig. S5 Molecular diagrams showing $\nabla^2\rho_b$ values (au) of various conformers of NO/NO⁺@2 encapsulated complexes. Small purple circles represent the bcps. The $\nabla^2\rho_b$ values shown red, black, green, purple, blue, and brown color correspond to the $\text{N}_{\text{NO}}\cdots\text{C}_{\text{phenyl}}$, $\text{O}_{\text{NO}}\cdots\text{C}_{\text{phenyl}}$, $\text{O}_{\text{NO}}\cdots\text{O}_{\text{ether}}$, $\text{N}_{\text{NO}}\cdots\text{O}_{\text{ether}}$, $\text{N}_{\text{NO}}\cdots\text{H}_{\text{alkyl}}$, and $\text{O}_{\text{NO}}\cdots\text{H}_{\text{alkyl}}$ interactions, respectively.

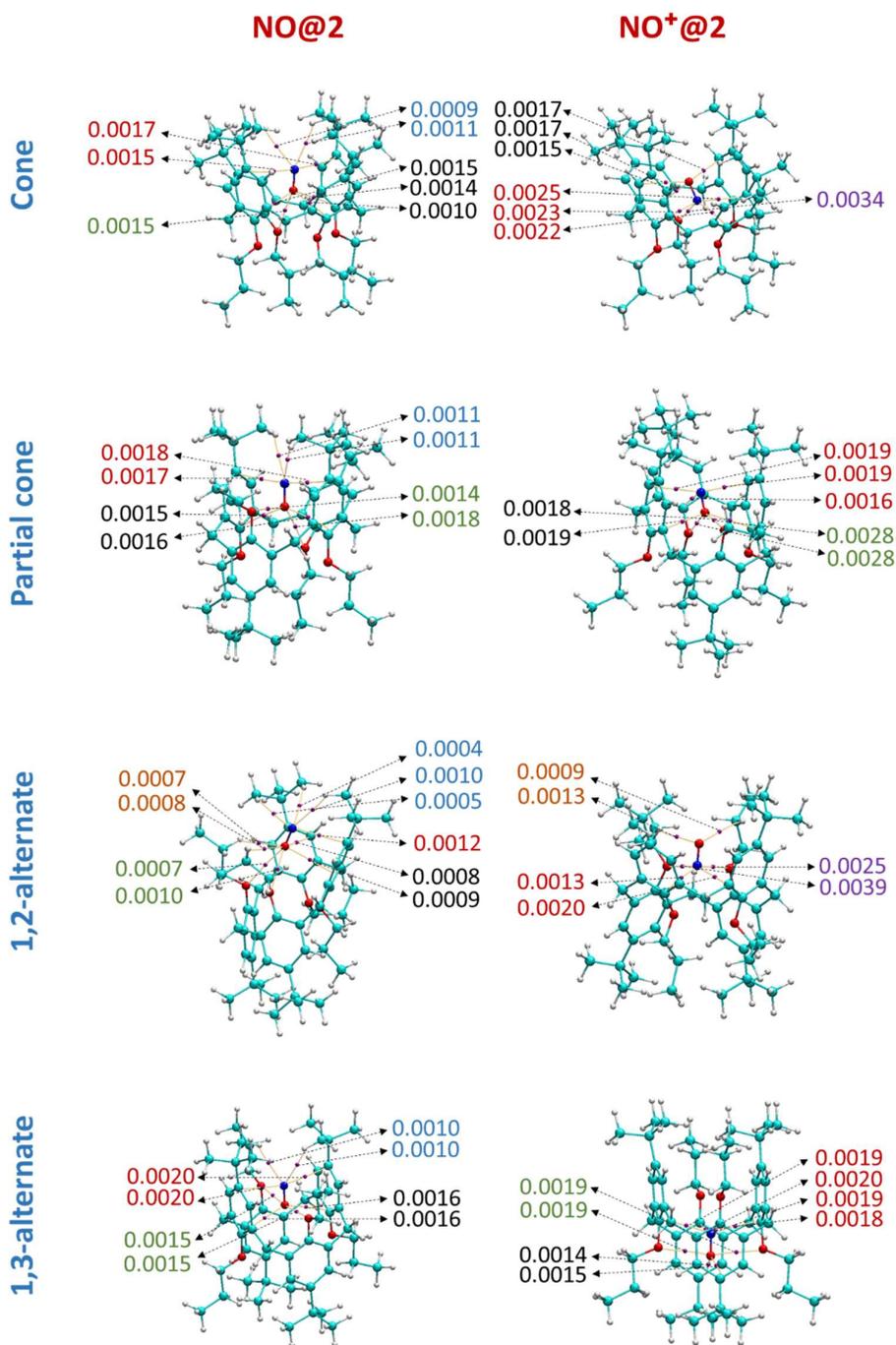


Fig. S6 Molecular diagrams showing H_b values (au) of various conformers of NO/NO⁺@2 encapsulated complexes. Small purple circles represent the bcps. The H_b values shown red, black, green, purple, blue, and brown color correspond to the N_{NO}...C_{phenyl}, O_{NO}...C_{phenyl}, O_{NO}...O_{ether}, N_{NO}...O_{ether}, N_{NO}...HC_{alkyl}, and O_{NO}...HC_{alkyl} interactions, respectively.

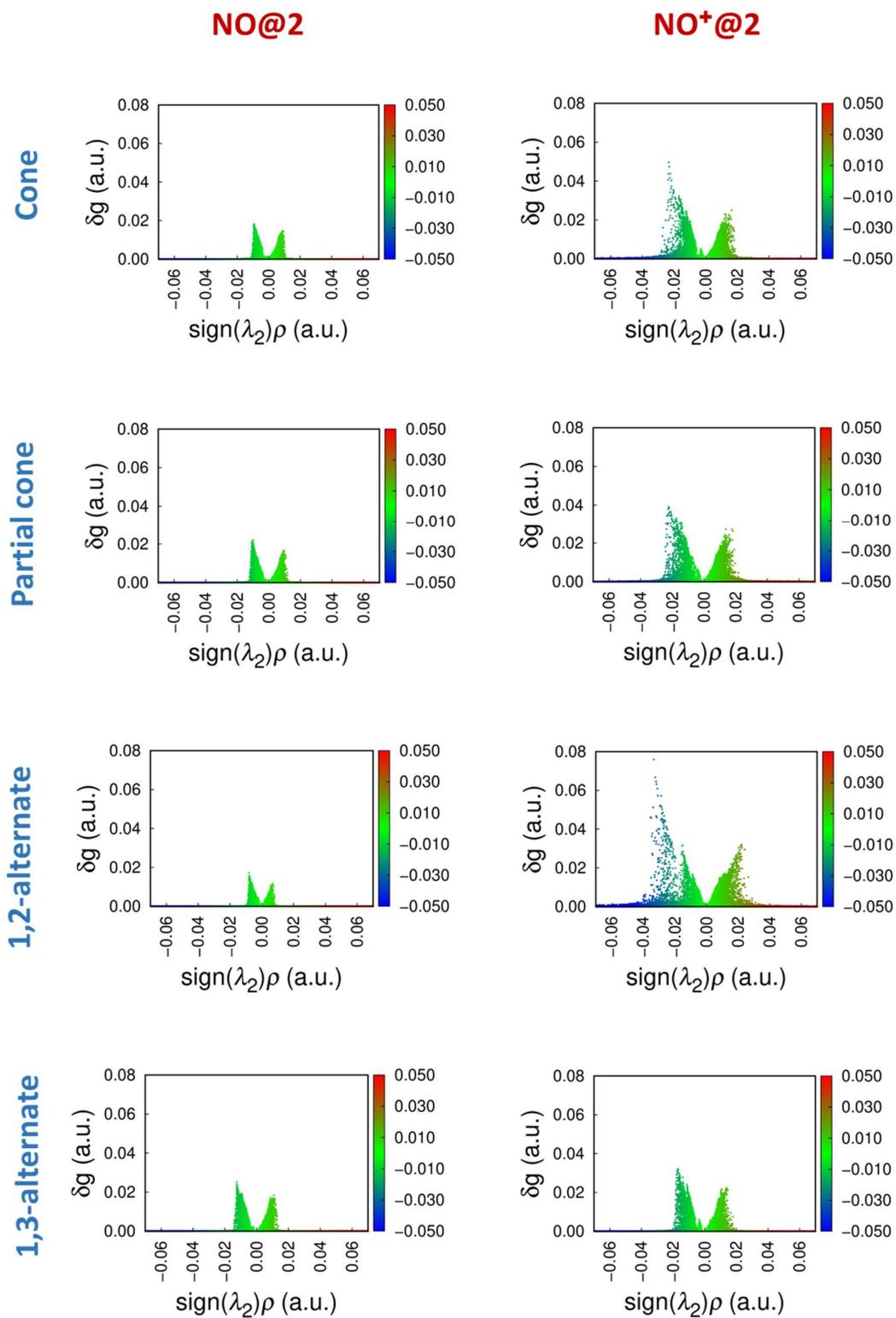


Fig. S7 IGMH scatterplot of complexes of NO/NO⁺@2.

Table S2 Percentage contribution of atomic pair δg of NO/NO⁺@2.

	NO			NO ⁺		
	Atom1	Atom2	δG^{pair} (%)	Atom1	Atom2	δG^{pair} (%)
Cone	C ₆₅	N ₁₄₁	3.13	O ₅	N ₂	5.04
	C ₁₂₇	N ₁₄₁	3.07	C ₁₃₂	N ₂	3.56
	C ₆₃	N ₁₄₁	3.02	C ₁₂₅	N ₂	3.53
	C ₁₂₃	O ₁₄₂	2.84	C ₃₂	N ₂	3.39
	C ₁₂₈	N ₁₄₁	2.82	C ₆₃	N ₂	3.38
	C ₆₁	O ₁₄₂	2.77	C ₆₄	N ₂	3.24
	C ₁₂₄	O ₁₄₂	2.59	O ₃	N ₂	2.79
	C ₁₃₀	O ₁₄₂	2.57	C ₁₂₇	O ₁	2.78
	C ₆₈	O ₁₄₂	2.56	C ₆₈	O ₁	2.70
	C ₉₂	O ₁₄₂	2.51	C ₉₄	O ₁	2.45
	C ₃	O ₁₄₂	2.5	C ₆₇	O ₁	2.27
	C ₆₂	O ₁₄₂	2.5	C ₁₂₆	O ₁	2.26
Partial cone	C ₃₄	N ₁₄₁	3.28	C ₆₁	N ₁₄₁	4.68
	C ₉₆	N ₁₄₁	3.25	C ₉₄	N ₁₄₁	4.05
	O ₄	O ₁₄₂	3.01	C ₃₅	N ₁₄₁	3.85
	C ₉₄	N ₁₄₁	2.83	O ₂	O ₁₄₂	3.28
	O ₂	O ₁₄₂	2.79	O ₄	O ₁₄₂	3.21
	C ₆₁	O ₁₄₂	2.77	C ₉₃	N ₁₄₁	2.88
	C ₃₅	N ₁₄₁	2.64	C ₃₇	N ₁₄₁	2.73
	C ₉₂	O ₁₄₂	2.62	C ₆₈	N ₁₄₁	2.68
	C ₉₃	O ₁₄₂	2.61	O ₂	N ₁₄₁	2.57
	C ₃₀	O ₁₄₂	2.59	C ₃₁	O ₁₄₂	2.53
	C ₃₂	N ₁₄₁	2.51	C ₆₂	N ₁₄₁	2.51
	C ₃₇	O ₁₄₂	2.49	C ₃₀	O ₁₄₂	2.42
1,2-alternate	C ₁₄	N ₁₄₁	3.84	O ₇₂	N ₁₄₂	7.25
	C ₁₂	N ₁₄₁	3.6	C ₁₀	N ₁₄₂	6.46
	O ₇₂	O ₁₄₂	3.51	C ₁₁	N ₁₄₂	4.38
	C ₃₆	O ₁₄₂	3.34	O ₇₁	N ₁₄₂	3.99
	H ₂₁	N ₁₄₁	3.22	C ₃₈	N ₁₄₂	3.55
	C ₁₁	O ₁₄₂	2.9	C ₁₇	N ₁₄₂	3.27
	H ₁₃₆	O ₁₄₂	2.78	C ₃₁	N ₁₄₂	3.07
	C ₁₀	O ₁₄₂	2.78	O ₁	N ₁₄₂	2.97
	C ₁₅	N ₁₄₁	2.65	O ₇₂	O ₁₄₁	2.42
	C ₁₃₁	O ₁₄₂	2.55	C ₃₆	O ₁₄₁	2.17
	C ₃₆	N ₁₄₁	2.26	H ₁₃₃	O ₁₄₁	2.06
C ₁₁	N ₁₄₁	2.21	C ₁₁	O ₁₄₁	1.98	

1,3- alternate	C ₁₂₆	N ₁₄₁	3.41	C ₁₂₂	N ₁₄₀	3.88
	C ₆₅	N ₁₄₁	3.41	C ₉₁	N ₁₄₀	3.86
	C ₁₂₇	N ₁₄₁	2.81	C ₆₁	N ₁₄₀	3.60
	C ₆₆	N ₁₄₁	2.8	C ₃₀	N ₁₄₀	3.33
	C ₆₃	N ₁₄₁	2.67	C ₁₂₃	N ₁₄₀	2.85
	C ₁₂₄	N ₁₄₁	2.67	C ₁₂₉	N ₁₄₀	2.74
	O ₃	O ₁₄₀	2.5	C ₆₈	N ₁₄₀	2.73
	C ₆₁	O ₁₄₀	2.49	O ₃	O ₁₄₁	2.59
	O ₁	O ₁₄₀	2.49	C ₆₂	N ₁₄₀	2.57
	C ₁₂₂	O ₁₄₀	2.49	O ₁	O ₁₄₁	2.55
	C ₉₁	O ₁₄₀	2.47	O ₃	N ₁₄₀	2.43
	C ₃₀	O ₁₄₀	2.46	O ₁	N ₁₄₀	2.42

Table S3. Cartesian coordinates of optimized geometries of different complexes.

Coordinates of NO@2 complexes							
NO@ Cone			NO@Partial cone				
8	2.505190000	-1.097088000	0.223058000	8	1.452764000	-1.960616000	2.104391000
8	0.769979000	-1.989003000	2.738482000	8	0.232227000	-1.947885000	-0.869157000
8	-0.862602000	-2.407709000	-0.078960000	8	1.526398000	0.258864000	-2.797130000
8	0.929329000	-2.073706000	-2.583765000	8	0.807546000	2.572158000	1.155781000
6	2.487422000	0.341574000	2.724701000	6	-1.112935000	-3.097742000	1.373904000
1	2.803206000	-0.697243000	2.812247000	1	-1.701191000	-3.833986000	1.933740000
1	2.944636000	0.897443000	3.551211000	1	-0.128335000	-3.528058000	1.189428000
6	-2.109747000	-1.850188000	2.411239000	6	-1.055484000	-0.981045000	-3.230208000
1	-2.851280000	-1.962830000	3.210880000	1	-1.630424000	-1.029496000	-4.162258000
1	-1.487935000	-2.745901000	2.403110000	1	-0.075651000	-1.419531000	-3.421181000
6	-1.940389000	-1.770592000	-2.642888000	6	1.891911000	2.782110000	-1.504149000
1	-1.381113000	-2.706447000	-2.648320000	1	1.779154000	3.822506000	-1.187405000
1	-2.632411000	-1.792069000	-3.492574000	1	2.578327000	2.786998000	-2.357991000
6	2.766526000	0.159912000	-2.343351000	6	1.795187000	0.668520000	3.155498000
1	3.005629000	-0.899459000	-2.269635000	1	2.451560000	0.007914000	3.732088000
1	3.382124000	0.596093000	-3.138880000	1	1.674323000	1.575255000	3.756350000
6	3.882645000	4.472320000	0.151548000	6	-3.293309000	0.861650000	3.674770000
6	5.136224000	4.737853000	1.017349000	6	-3.843499000	0.142900000	4.929882000
1	6.005323000	4.206545000	0.614398000	1	-3.111221000	0.165610000	5.744474000
1	4.992743000	4.409376000	2.051151000	1	-4.072020000	-0.905864000	4.712856000
1	5.367195000	5.809520000	1.036661000	1	-4.763345000	0.627248000	5.279562000
6	2.674612000	5.239594000	0.743590000	6	-3.033324000	2.340290000	4.024586000
1	2.870310000	6.318538000	0.748102000	1	-2.351448000	2.447607000	4.874786000
1	2.465475000	4.932937000	1.772909000	1	-3.975948000	2.825812000	4.298904000
1	1.771769000	5.054779000	0.151651000	1	-2.610970000	2.880715000	3.170345000
6	4.150378000	5.023571000	-1.262012000	6	-4.366266000	0.823758000	2.560092000
1	4.998047000	4.520266000	-1.739669000	1	-3.998228000	1.297179000	1.646290000
1	4.387257000	6.091201000	-1.202289000	1	-5.265720000	1.355908000	2.890660000
1	3.274769000	4.917036000	-1.911545000	1	-4.665325000	-0.197061000	2.306904000
6	2.869827000	0.230301000	0.201325000	6	0.305483000	-1.261321000	2.440294000
6	3.072552000	0.867279000	-1.031007000	6	0.429503000	0.018017000	3.003720000
6	3.433617000	2.223355000	-1.032428000	6	-0.731833000	0.692793000	3.390149000
1	3.601148000	2.694904000	-1.994226000	1	-0.617636000	1.686628000	3.805866000
6	3.558997000	2.968678000	0.143138000	6	-2.010392000	0.140967000	3.222771000
6	3.305087000	2.302404000	1.352326000	6	-2.087724000	-1.121553000	2.617889000
1	3.355894000	2.852732000	2.288008000	1	-3.058589000	-1.561522000	2.415271000
6	2.945915000	0.954448000	1.407480000	6	-0.956483000	-1.822116000	2.193346000
6	3.512145000	-2.023065000	0.656831000	6	1.859917000	-2.910495000	3.099483000
1	2.984125000	-2.791166000	1.227498000	1	1.028349000	-3.594979000	3.325708000
1	4.222423000	-1.525776000	1.331545000	1	2.115194000	-2.384536000	4.032940000
6	4.261047000	-2.645274000	-0.518202000	6	3.059221000	-3.677972000	2.566122000
1	4.821550000	-1.862614000	-1.044084000	1	3.848539000	-2.961870000	2.316172000
1	3.522120000	-3.039786000	-1.223013000	1	2.772631000	-4.168005000	1.627987000
6	5.208225000	-3.759061000	-0.059374000	6	3.575829000	-4.711394000	3.572260000

1	5.744609000	-4.198966000	-0.906335000	1	4.438055000	-5.252724000	3.170406000
1	4.655188000	-4.564195000	0.439533000	1	2.803683000	-5.449902000	3.818111000
1	5.956569000	-3.381685000	0.647916000	1	3.889421000	-4.233867000	4.508103000
6	-1.756503000	3.165287000	3.018594000	6	-5.432939000	-2.746949000	-1.259723000
6	-2.750647000	3.340812000	1.845085000	6	-6.070133000	-1.938072000	-0.103202000
1	-3.246070000	4.316274000	1.915703000	1	-5.813445000	-0.876524000	-0.184970000
1	-3.529739000	2.573349000	1.847371000	1	-5.724665000	-2.289237000	0.874023000
1	-2.231741000	3.282236000	0.884386000	1	-7.162313000	-2.032532000	-0.125687000
6	-2.532943000	3.227136000	4.355525000	6	-5.794620000	-4.242472000	-1.101279000
1	-3.051805000	4.188254000	4.453966000	1	-6.882537000	-4.377134000	-1.125280000
1	-1.852270000	3.115108000	5.206692000	1	-5.428677000	-4.650185000	-0.154058000
1	-3.281675000	2.430696000	4.417337000	1	-5.357316000	-4.834916000	-1.912228000
6	-0.759550000	4.339407000	2.974082000	6	-6.039934000	-2.243983000	-2.583409000
1	-1.304969000	5.287805000	3.026114000	1	-5.858245000	-1.174097000	-2.732114000
1	-0.177940000	4.337252000	2.046336000	1	-7.124509000	-2.396158000	-2.572399000
1	-0.062151000	4.315066000	3.818576000	1	-5.637001000	-2.786043000	-3.445800000
6	0.172096000	-0.738284000	2.761851000	6	-1.115426000	-2.201931000	-1.004782000
6	0.968943000	0.411672000	2.841310000	6	-1.815708000	-2.796174000	0.059210000
6	0.340574000	1.660342000	2.925961000	6	-3.194229000	-2.978850000	-0.070503000
1	0.975180000	2.537385000	2.959106000	1	-3.727114000	-3.431762000	0.761456000
6	-1.051773000	1.801449000	2.916643000	6	-3.905336000	-2.571680000	-1.210366000
6	-1.810341000	0.628513000	2.790957000	6	-3.173074000	-1.970957000	-2.240519000
1	-2.891143000	0.695471000	2.720760000	1	-3.676224000	-1.622760000	-3.135893000
6	-1.229996000	-0.635907000	2.690657000	6	-1.788061000	-1.770081000	-2.155821000
6	0.903641000	-2.577894000	4.039918000	6	1.106787000	-2.981842000	-1.332085000
1	-0.081107000	-2.624869000	4.529766000	1	0.924940000	-3.174297000	-2.401574000
1	1.554268000	-1.946733000	4.665537000	1	0.896583000	-3.919287000	-0.792567000
6	1.492025000	-3.972141000	3.883489000	6	2.539047000	-2.531255000	-1.098337000
1	0.824956000	-4.567216000	3.248811000	1	2.661577000	-2.320085000	-0.032763000
1	2.446672000	-3.893280000	3.349586000	1	2.687953000	-1.582287000	-1.620010000
6	1.695732000	-4.663269000	5.235955000	6	3.535582000	-3.592294000	-1.575027000
1	2.116600000	-5.665156000	5.105641000	1	4.569145000	-3.274851000	-1.410343000
1	0.747363000	-4.768143000	5.775896000	1	3.421937000	-3.795619000	-2.647315000
1	2.381226000	-4.094054000	5.874668000	1	3.395294000	-4.541786000	-1.043133000
6	-6.162747000	-0.232791000	-0.185972000	6	-3.131589000	3.463367000	-1.806855000
6	-7.152301000	-1.185960000	0.524858000	6	-3.102542000	4.630949000	-2.821874000
1	-7.205935000	-2.147774000	0.003433000	1	-3.135601000	4.253675000	-3.849885000
1	-8.157586000	-0.748550000	0.543557000	1	-2.190333000	5.226719000	-2.712371000
1	-6.854184000	-1.382232000	1.559242000	1	-3.962720000	5.294428000	-2.670661000
6	-6.694480000	0.037891000	-1.606408000	6	-4.455453000	2.692704000	-1.978232000
1	-6.767993000	-0.883653000	-2.193946000	1	-4.583892000	2.322744000	-3.001043000
1	-6.057928000	0.744258000	-2.150127000	1	-5.299258000	3.356688000	-1.761903000
1	-7.697031000	0.474904000	-1.547198000	1	-4.5111718000	1.840243000	-1.292697000
6	-6.114485000	1.116371000	0.572136000	6	-3.104075000	4.039693000	-0.370553000
1	-5.410124000	1.805081000	0.093572000	1	-3.097047000	3.237411000	0.371730000
1	-5.798224000	0.985534000	1.611624000	1	-3.988506000	4.664919000	-0.201646000
1	-7.104881000	1.586789000	0.581046000	1	-2.222331000	4.662978000	-0.194739000
6	-2.156472000	-1.943014000	-0.122782000	6	0.387989000	1.000723000	-2.526756000
6	-2.831300000	-1.688752000	1.082492000	6	-0.877807000	0.471678000	-2.805198000
6	-4.124180000	-1.163800000	1.021499000	6	-2.002585000	1.275344000	-2.578887000
1	-4.639622000	-0.969998000	1.958530000	1	-2.974647000	0.839305000	-2.775598000
6	-4.756007000	-0.856215000	-0.194406000	6	-1.904428000	2.567801000	-2.051960000
6	-4.037908000	-1.101905000	-1.371045000	6	-0.617898000	3.036108000	-1.736094000
1	-4.472958000	-0.864443000	-2.335704000	1	-0.498581000	4.012385000	-1.278817000
6	-2.742445000	-1.637506000	-1.357553000	6	0.529128000	2.273380000	-1.944521000
6	-0.711239000	-3.830779000	-0.126857000	6	1.986680000	0.384600000	-4.149754000
1	-1.076902000	-4.216734000	-1.091539000	1	2.271594000	1.429394000	-4.350678000
1	-1.317373000	-4.299631000	0.664874000	1	1.174221000	0.126362000	-4.845937000
6	0.764784000	-4.130651000	0.059890000	6	3.174483000	-0.545598000	-4.339944000
1	1.062904000	-3.708477000	1.021447000	1	3.944066000	-0.283763000	-3.606587000
1	1.309620000	-3.578228000	-0.708358000	1	2.857925000	-1.569719000	-4.109204000
6	1.077602000	-5.626719000	-0.004254000	6	3.743944000	-0.469872000	-5.760163000
1	2.149398000	-5.807286000	0.133285000	1	4.597015000	-1.145582000	-5.877135000
1	0.793044000	-6.057693000	-0.971969000	1	4.087342000	0.543883000	-5.997944000
1	0.545599000	-6.185587000	0.775820000	1	2.991927000	-0.750055000	-6.507171000
6	-1.153524000	3.236487000	-3.268067000	6	5.748777000	-0.140189000	0.066059000
6	-0.628868000	4.179460000	-2.158165000	6	5.924947000	-1.470480000	0.829439000
1	-0.992086000	5.199450000	-2.330027000	1	5.902367000	-1.330456000	1.914323000
1	0.464191000	4.216352000	-2.132021000	1	6.894634000	-1.916956000	0.583171000
1	-0.971300000	3.850451000	-1.173562000	1	5.141422000	-2.184055000	0.561222000
6	-2.692933000	3.301404000	-3.254129000	6	5.989529000	-0.423760000	-1.431984000
1	-3.019417000	4.337556000	-3.393764000	1	6.015035000	0.494039000	-2.027144000
1	-3.099899000	2.946950000	-2.300910000	1	5.210222000	-1.073475000	-1.839516000
1	-3.133502000	2.705834000	-4.060979000	1	6.955977000	-0.921647000	-1.566975000
6	-0.651832000	3.741580000	-4.642100000	6	6.820397000	0.862100000	0.560313000

1	-1.008286000	4.761560000	-4.829901000	1	6.740582000	1.812725000	0.022130000
1	-1.014270000	3.096364000	-5.449914000	1	7.829185000	0.460336000	0.402939000
1	0.442022000	3.752069000	-4.686531000	1	6.695218000	1.069186000	1.628534000
6	0.418353000	-0.791162000	-2.698677000	6	1.961300000	1.858956000	0.882742000
6	-0.969407000	-0.608209000	-2.804894000	6	2.538492000	1.965032000	-0.393813000
6	-1.468032000	0.687338000	-2.981585000	6	3.732483000	1.281032000	-0.645374000
1	-2.544312000	0.804807000	-3.032286000	1	4.165362000	1.386495000	-1.633506000
6	-0.630503000	1.806428000	-3.046070000	6	4.362322000	0.481344000	0.314926000
6	0.745908000	1.582963000	-2.890546000	6	3.699212000	0.324412000	1.538200000
1	1.422536000	2.430234000	-2.879824000	1	4.103258000	-0.342185000	2.291802000
6	1.288127000	0.312421000	-2.689529000	6	2.498387000	0.975724000	1.837904000
6	1.246168000	-2.677463000	-3.845176000	6	0.928082000	3.689102000	2.044103000
1	2.071535000	-2.127415000	-4.324126000	1	1.618754000	3.457604000	2.865868000
1	0.374562000	-2.615199000	-4.514914000	1	-0.072284000	3.824794000	2.470573000
6	1.629505000	-4.129499000	-3.601781000	6	1.384263000	4.965691000	1.340639000
1	0.798012000	-4.627874000	-3.089737000	1	0.683625000	5.189322000	0.527718000
1	2.482756000	-4.161511000	-2.914842000	1	2.365048000	4.787279000	0.883589000
6	1.971030000	-4.859955000	-4.904543000	6	1.462884000	6.148855000	2.311944000
1	2.243638000	-5.902106000	-4.710593000	1	1.782705000	7.061495000	1.799175000
1	2.815334000	-4.384792000	-5.417715000	1	2.178443000	5.952661000	3.119267000
1	1.119725000	-4.861103000	-5.595362000	1	0.488154000	6.349680000	2.772519000
7	-0.443747000	1.519933000	-0.029867000	7	-1.692564000	1.012987000	0.435586000
8	-0.206244000	0.386344000	-0.011788000	8	-0.713419000	0.444314000	0.195715000
NO@1,2-alternate				NO@1,3-alternate			
8	0.268482000	1.114702000	-1.318762000	8	1.267923000	0.169345000	-2.820866000
8	0.287281000	-1.937878000	-1.955166000	8	-1.374278000	2.823632000	0.169494000
6	-1.873997000	-0.208198000	-2.658229000	8	1.268617000	-0.170356000	2.820986000
1	-0.901284000	-0.273503000	-3.142007000	8	-1.375212000	-2.823782000	-0.168589000
1	-2.637939000	-0.289447000	-3.440531000	6	-0.055153000	-2.383084000	-2.672084000
6	0.041548000	3.815029000	-0.105564000	1	0.665555000	-2.427452000	-3.495155000
1	-0.386954000	4.506583000	0.629469000	1	-0.782866000	-3.182542000	-2.849276000
1	0.412121000	4.459972000	-0.912790000	6	-0.052093000	2.703699000	-2.391910000
6	-4.899445000	3.614879000	-1.268860000	1	0.672130000	2.842768000	-3.201129000
6	-0.946071000	1.761042000	-1.333680000	1	-0.777897000	3.519441000	-2.478393000
6	-2.036150000	1.137704000	-1.972972000	6	-0.053594000	2.382734000	2.672444000
6	-3.284064000	1.759054000	-1.936673000	1	-0.781066000	3.182376000	2.849754000
1	-4.110774000	1.272034000	-2.445701000	1	0.667294000	2.426881000	3.495369000
6	-3.502037000	2.969797000	-1.260307000	6	-0.052315000	-2.704060000	2.392273000
6	-2.392309000	3.560342000	-0.645579000	1	-0.778317000	-3.519637000	2.478796000
1	-2.505064000	4.503698000	-0.122008000	1	0.672056000	-2.843353000	3.201313000
6	-1.107883000	2.994350000	-0.683827000	6	-4.463343000	0.203519000	-2.734471000
6	-5.959781000	2.607030000	-0.765242000	6	-4.851672000	0.696111000	-4.149755000
1	-5.993475000	1.704429000	-1.382462000	1	-4.467479000	0.015213000	-4.917070000
1	-6.955589000	3.064432000	-0.793008000	1	-4.437610000	1.690619000	-4.346274000
1	-5.748508000	2.299894000	0.262702000	1	-5.942415000	0.752565000	-4.253518000
6	-5.244346000	4.033581000	-2.718805000	6	-5.054867000	1.173719000	-1.687403000
1	-4.510975000	4.752003000	-3.100965000	1	-6.149444000	1.118676000	-1.692623000
1	-6.235747000	4.500647000	-2.756696000	1	-4.782251000	2.211398000	-1.897499000
1	-5.251743000	3.171276000	-3.392958000	1	-4.700343000	0.930587000	-0.682617000
6	-4.972256000	4.865627000	-0.372144000	6	-5.097494000	-1.183155000	-2.510113000
1	-4.722021000	4.629002000	0.667791000	1	-4.788952000	-1.902679000	-3.275619000
1	-5.989776000	5.270404000	-0.387268000	1	-6.188799000	-1.102956000	-2.559237000
1	-4.299434000	5.657277000	-0.718706000	1	-4.833166000	-1.590123000	-1.529884000
6	-4.842583000	-3.002571000	0.401837000	6	-0.113445000	0.168273000	-2.706310000
6	-0.929844000	-2.180263000	-1.349920000	6	-0.800260000	-1.053455000	-2.694594000
6	-1.056328000	-3.152905000	-0.337972000	6	-2.199739000	-1.027684000	-2.668541000
6	-2.322063000	-3.383299000	0.205110000	1	-2.713577000	-1.980488000	-2.665356000
1	-2.409259000	-4.144949000	0.976076000	6	-2.927699000	0.166471000	-2.636331000
6	-3.461040000	-2.659494000	-0.184467000	6	-2.195066000	1.359527000	-2.552883000
6	-3.268905000	-1.638401000	-1.115987000	1	-2.715137000	2.307602000	-2.463633000
1	-4.096171000	-1.002666000	-1.408054000	6	-0.798944000	1.387036000	-2.568652000
6	-2.021052000	-1.373587000	-1.693353000	6	1.736182000	0.248693000	-4.172355000
6	-5.948791000	-2.070189000	-0.129778000	1	1.405364000	1.193922000	-4.630498000
1	-5.751295000	-1.023630000	0.126003000	1	1.304104000	-0.569366000	-4.769207000
1	-6.909899000	-2.347897000	0.316328000	6	3.253770000	0.160500000	-4.153823000
1	-6.054651000	-2.146083000	-1.217377000	1	3.639283000	0.948397000	-3.498406000
6	-5.204693000	-4.456885000	0.016175000	1	3.542754000	-0.790873000	-3.694432000
1	-5.228253000	-4.574262000	-1.072647000	6	3.858374000	0.282173000	-5.555984000
1	-6.191414000	-4.724943000	0.412674000	1	4.950082000	0.211278000	-5.519966000
1	-4.476653000	-5.170907000	0.413980000	1	3.602061000	1.242487000	-6.019039000
6	-4.821410000	-2.878238000	1.942775000	1	3.495059000	-0.512994000	-6.217888000
1	-4.067161000	-3.527250000	2.396949000	6	4.358640000	2.897118000	0.136330000
1	-5.796037000	-3.158647000	2.359238000	6	4.947687000	2.006064000	-0.981969000
1	-4.607246000	-1.848638000	2.246356000	1	4.662984000	2.358169000	-1.977398000
6	1.154065000	1.412022000	-2.404697000	1	4.606957000	0.972436000	-0.878998000

1	1.379426000	2.489258000	-2.417467000	1	6.042458000	2.021246000	-0.935143000
1	0.666029000	1.162283000	-3.359440000	6	4.756333000	4.368917000	-0.128134000
6	2.425834000	0.599407000	-2.221140000	1	4.346913000	4.719654000	-1.081461000
1	2.139072000	-0.435502000	-2.017566000	1	5.847707000	4.473169000	-0.164921000
1	2.950742000	0.963137000	-1.333053000	1	4.374500000	5.023681000	0.662868000
6	3.321325000	0.690041000	-3.460916000	6	4.985225000	2.445002000	1.470342000
1	4.271832000	0.171240000	-3.303622000	1	4.688409000	3.089101000	2.304534000
1	3.555316000	1.731072000	-3.713557000	1	6.077276000	2.489105000	1.398861000
1	2.835809000	0.237737000	-4.334413000	1	4.701824000	1.415359000	1.709635000
6	0.846931000	-2.936881000	-2.822467000	6	0.010188000	2.760445000	0.156885000
1	0.455883000	-3.930137000	-2.569359000	6	0.696223000	2.797933000	-1.068996000
1	1.921245000	-2.930222000	-2.612363000	6	2.090656000	2.845205000	-1.039750000
6	0.593295000	-2.632571000	-4.298895000	1	2.613303000	2.871162000	-1.989778000
1	1.316958000	-3.214272000	-4.887079000	6	2.822175000	2.804880000	0.158606000
1	0.828647000	-1.575199000	-4.473437000	6	2.095179000	2.679363000	1.350517000
6	-0.827530000	-2.958355000	-4.773636000	1	2.612251000	2.566414000	2.295118000
1	-0.955686000	-2.712869000	-5.833318000	6	0.697952000	2.635688000	1.372669000
1	-1.579703000	-2.406558000	-4.206023000	6	-1.863667000	4.171977000	0.237620000
1	-1.041757000	-4.026407000	-4.648470000	1	-1.565375000	4.722453000	-0.668147000
8	0.000668000	-1.632238000	1.969225000	1	-1.409682000	4.689376000	1.096560000
8	-0.049181000	1.700328000	1.989473000	6	-3.377060000	4.137565000	0.369729000
6	2.208443000	0.076097000	2.624609000	1	-3.785341000	3.543461000	-0.453504000
1	1.252417000	0.044601000	3.142370000	1	-3.639484000	3.610140000	1.292492000
1	3.007847000	0.068462000	3.375235000	6	-3.986297000	5.543330000	0.370660000
6	0.145890000	-3.914903000	0.198488000	1	-3.762175000	6.075710000	-0.561266000
1	0.480821000	-4.663343000	-0.528990000	1	-3.597562000	6.146543000	1.199710000
1	-0.188857000	-4.490626000	1.068985000	6	-4.462678000	-0.202311000	2.735208000
6	5.136535000	-2.914711000	-0.243365000	6	-5.054282000	-1.171737000	1.687455000
6	1.232166000	-1.965018000	1.441729000	1	-4.781877000	-2.209589000	1.896903000
6	2.344248000	-1.164383000	1.747829000	1	-4.699473000	-0.928009000	0.682931000
6	3.581578000	-1.515950000	1.201290000	1	-6.148852000	-1.116459000	1.692502000
1	4.439983000	-0.899079000	1.444345000	6	-4.851558000	-0.695411000	4.150149000
6	3.749534000	-2.616185000	0.351501000	1	-4.437966000	-1.690165000	4.346377000
6	2.611364000	-3.375510000	0.057290000	1	-5.942349000	-0.751486000	4.253576000
1	2.683331000	-4.230960000	-0.605028000	1	-4.467324000	-0.015001000	4.917882000
6	1.349800000	-3.065828000	0.578704000	6	-5.096240000	1.184689000	2.511311000
6	5.577639000	-1.713969000	-1.114422000	1	-6.187563000	1.104996000	2.560801000
1	5.630438000	-0.788734000	-0.532604000	1	-4.832071000	1.591697000	1.531041000
1	6.567011000	-1.896864000	-1.550474000	1	-4.787057000	1.903933000	3.276834000
1	4.865691000	-1.551083000	-1.929413000	6	-0.112771000	-0.168697000	2.706672000
6	6.161760000	-3.128061000	0.894981000	6	-0.799085000	1.053311000	2.695081000
1	5.868375000	-3.972514000	1.527935000	6	-2.198589000	1.028044000	2.669334000
1	7.154851000	-3.337781000	0.480189000	1	-2.712105000	1.981011000	2.666121000
1	6.247798000	-2.244452000	1.534439000	6	-2.927007000	-0.165830000	2.637283000
6	5.137368000	-4.174119000	-1.130708000	6	-2.194869000	-1.359187000	2.553799000
1	4.462518000	-4.067468000	-1.987153000	1	-2.715315000	-2.307067000	2.464606000
1	6.144502000	-4.347343000	-1.524756000	6	-0.798765000	-1.387211000	2.569259000
1	4.841620000	-5.066330000	-0.568265000	6	1.736883000	-0.249134000	4.172504000
6	5.070408000	3.408567000	0.028171000	1	1.405373000	-1.193783000	4.631376000
6	1.154146000	2.077378000	1.440546000	1	1.305476000	0.569683000	4.768793000
6	1.250713000	3.114951000	0.489540000	6	3.254520000	-0.162048000	4.153913000
6	2.520496000	3.505288000	0.057343000	1	3.639562000	-0.951461000	3.500053000
1	2.579119000	4.313711000	-0.667077000	1	3.544160000	0.788241000	3.692704000
6	3.701540000	2.894103000	0.505060000	6	3.858940000	-0.281451000	5.556342000
6	3.552205000	1.804177000	1.363184000	1	3.601509000	-1.240484000	6.021435000
1	4.426100000	1.268882000	1.713036000	1	3.496539000	0.515536000	6.216550000
6	2.300048000	1.357071000	1.810126000	1	4.950733000	-0.211924000	5.520194000
6	6.239726000	2.615819000	0.643372000	6	4.357751000	-2.897513000	-0.137303000
1	6.205388000	1.558271000	0.359436000	6	4.983846000	-2.445052000	-1.471451000
1	7.190818000	3.022616000	0.283435000	1	6.075930000	-2.488964000	-1.400320000
1	6.242715000	2.679848000	1.736832000	1	4.700163000	-1.415437000	-1.710529000
6	5.229897000	4.893767000	0.431125000	1	4.686895000	-3.089085000	-2.305642000
1	5.163270000	5.009550000	1.518350000	6	4.755680000	-4.369317000	0.126758000
1	6.203386000	5.277492000	0.103190000	1	4.346727000	-4.720242000	1.080220000
1	4.454062000	5.519913000	-0.020098000	1	5.847078000	-4.473490000	0.163031000
6	5.168251000	3.281519000	-1.510231000	1	4.373533000	-5.023986000	-0.664171000
1	4.371311000	3.835854000	-2.015412000	6	4.947101000	-2.006642000	0.980961000
1	6.127813000	3.675021000	-1.866133000	1	4.663017000	-2.359178000	1.976408000
1	5.092825000	2.234349000	-1.817124000	1	4.605968000	-0.973091000	0.878507000
6	-0.361809000	-2.345011000	3.156419000	1	6.041853000	-2.021476000	0.933556000
1	-0.466700000	-3.418680000	2.938704000	6	0.009271000	-2.760814000	-0.156517000
1	0.430506000	-2.238004000	3.913733000	6	0.695660000	-2.798362000	1.069165000
6	-1.678830000	-1.773114000	3.651770000	6	2.090110000	-2.845655000	1.039535000
1	-1.516644000	-0.732806000	3.946400000	1	2.613036000	-2.871632000	1.989409000
1	-2.370259000	-1.758787000	2.805371000	6	2.821268000	-2.805350000	-0.159011000

6	-2.265665000	-2.574600000	4.816173000	6	2.093891000	-2.679897000	-1.350721000
1	-3.210594000	-2.138286000	5.155588000	1	2.610676000	-2.566974000	-2.295475000
1	-2.467214000	-3.612148000	4.523678000	6	0.696658000	-2.636201000	-1.372478000
1	-1.582269000	-2.597358000	5.673517000	6	-1.864682000	-4.172013000	-0.238190000
6	-0.829901000	2.721432000	2.637461000	1	-1.411610000	-4.688113000	-1.098381000
1	-0.180192000	3.569994000	2.892359000	1	-1.565455000	-4.723806000	0.666466000
1	-1.608443000	3.067770000	1.949176000	6	-3.378177000	-4.137409000	-0.368710000
6	-1.480093000	2.158530000	3.894277000	1	-3.641553000	-3.607411000	-1.289717000
1	-2.174234000	2.923298000	4.268863000	1	-3.785792000	-3.545716000	0.456590000
1	-2.091030000	1.297030000	3.608532000	6	-3.987174000	-5.543293000	-0.373000000
6	-0.487269000	1.771149000	4.993124000	1	-5.075971000	-5.498108000	-0.475508000
1	-1.006976000	1.393962000	5.880408000	1	-3.761765000	-6.078395000	0.557059000
1	0.195853000	0.991847000	4.646768000	1	-3.599387000	-6.143972000	-1.204327000
1	0.118934000	2.632528000	5.298210000	8	1.097868000	0.000301000	0.001009000
7	-3.599794000	0.950834000	1.147456000	7	2.257144000	-0.000139000	-0.002102000
8	-2.555947000	0.451347000	1.138852000	1	-5.074950000	5.498231000	0.474707000

Coordinates of NO ⁺ @2 complexes							
NO ⁺ @Cone				NO ⁺ @Partial cone			
8	-0.658338000	-0.746884000	0.045460000	8	1.359033000	-1.620196000	2.446398000
7	0.180647000	-0.012985000	-0.001973000	8	0.042109000	-1.930099000	-0.510455000
8	2.427558000	1.497386000	-0.294906000	1	1.433670000	-0.317297000	-2.875085000
8	0.390300000	2.075408000	-2.759215000	8	0.962572000	2.673508000	0.648624000
8	-1.184880000	2.020887000	0.153376000	6	-1.274502000	-2.719710000	1.894184000
8	0.552145000	2.111907000	2.672747000	1	-1.883609000	-3.298571000	2.596124000
6	2.429086000	0.025032000	-2.753220000	1	-0.318079000	-3.231080000	1.780492000
1	2.581867000	1.098310000	-2.857986000	6	-1.244001000	-1.418557000	-3.014200000
1	2.893265000	-0.466904000	-3.614503000	1	-1.860790000	-1.551001000	-3.909012000
6	-2.442318000	1.545738000	-2.334907000	1	-0.307054000	-1.953602000	-3.173315000
1	-3.186008000	1.555113000	-3.138722000	6	2.027581000	2.335852000	-1.993018000
1	-1.954270000	2.521409000	-2.324674000	1	2.010126000	3.424820000	-1.901074000
6	-2.229560000	1.329001000	2.725255000	1	2.663677000	2.099520000	-2.850924000
1	-1.842718000	2.345721000	2.806683000	6	1.863545000	1.132559000	2.960354000
1	-2.896503000	1.164037000	3.577494000	1	2.459014000	0.525142000	3.648310000
6	2.750710000	0.244151000	2.265559000	1	1.806064000	2.131338000	3.402329000
1	2.799143000	1.329311000	2.197080000	6	-3.211164000	1.764640000	3.235950000
1	3.399991000	-0.079390000	3.086801000	6	-3.849566000	1.283769000	4.562443000
6	4.622847000	-3.800157000	-0.242729000	1	-3.148711000	1.393127000	5.396416000
6	5.897678000	-3.806095000	-1.119408000	1	-4.144003000	0.230839000	4.504367000
1	6.649981000	-3.119120000	-0.718110000	1	-4.744878000	1.873382000	4.787759000
1	5.685566000	-3.508212000	-2.150626000	6	-2.863249000	3.259649000	3.369315000
1	6.332612000	-4.810930000	-1.146499000	1	-2.207798000	3.451243000	4.224815000
6	3.582261000	-4.782014000	-0.836571000	1	-3.778488000	3.838424000	3.525575000
1	3.986604000	-5.799832000	-0.848428000	1	-2.375442000	3.644779000	2.467439000
1	3.313484000	-4.520713000	-1.864597000	6	-4.241121000	1.602389000	2.092868000
1	2.664245000	-4.786561000	-0.238716000	1	-3.807265000	1.880617000	1.128616000
6	5.001221000	-4.296436000	1.165572000	1	-5.105452000	2.249599000	2.272912000
1	5.743180000	-3.646233000	1.640979000	1	-4.614046000	0.577552000	2.009232000
1	5.436834000	-5.297811000	1.096547000	6	0.261147000	-0.808697000	2.607840000
1	4.127481000	-4.365886000	1.823280000	6	0.458907000	0.562097000	2.881124000
6	2.915513000	0.212888000	-0.266722000	6	-0.661187000	1.385875000	3.071384000
6	3.209619000	-0.395822000	0.965102000	1	-0.481166000	2.429591000	3.295982000
6	3.788418000	-1.672867000	0.958544000	6	-1.967993000	0.904978000	2.962587000
1	4.047268000	-2.112331000	1.914932000	6	-2.118127000	-0.449883000	2.601621000
6	4.020478000	-2.386346000	-0.223142000	1	-3.113542000	-0.854695000	2.454246000
6	3.617705000	-1.781652000	-1.427597000	6	-1.029859000	-1.316652000	2.430414000
1	3.729585000	-2.324164000	-2.361770000	6	1.714821000	-2.403204000	3.607096000
6	3.052366000	-0.508542000	-1.472592000	1	0.851219000	-3.005329000	3.923872000
6	3.368747000	2.513015000	-0.714064000	1	1.973590000	-1.729085000	4.436430000
1	2.772922000	3.266874000	-1.234384000	6	2.891718000	-3.288195000	3.232872000
1	4.081214000	2.085302000	-1.430964000	1	3.710276000	-2.650721000	2.882318000
6	4.109453000	3.126475000	0.468197000	1	2.600319000	-3.918983000	2.384204000
1	4.687691000	2.344328000	0.975141000	6	3.354490000	-4.154590000	4.408934000
1	3.369198000	3.498058000	1.186144000	1	4.201532000	-4.782837000	4.118966000
6	5.034959000	4.264550000	0.023919000	1	2.553825000	-4.816245000	4.758357000
1	5.559081000	4.701594000	0.878781000	1	3.673136000	-3.538357000	5.257233000
1	4.469890000	5.066440000	-0.465454000	6	-5.594058000	-2.902623000	-0.764816000
1	5.792673000	3.909557000	-0.683786000	6	-6.262558000	-1.925907000	0.235460000
6	-1.373977000	-3.383018000	-2.683397000	1	-6.047558000	-0.885198000	-0.031048000
6	-2.341229000	-3.609763000	-1.495978000	1	-5.917500000	-2.092088000	1.260668000
1	-2.679237000	-4.650996000	-1.482549000	1	-7.348874000	-2.063162000	0.224983000

1	-3.231390000	-2.977119000	-1.555990000	6	-5.899363000	-4.361427000	-0.346712000
1	-1.847295000	-3.403359000	-0.542239000	1	-6.980436000	-4.534830000	-0.358758000
6	-2.133368000	-3.625526000	-4.010538000	1	-5.539915000	-4.584627000	0.662112000
1	-2.519179000	-4.650175000	-4.043326000	1	-5.432476000	-5.071497000	-1.037037000
1	-1.472617000	-3.481035000	-4.871528000	6	-6.204565000	-2.660046000	-2.157959000
1	-2.982091000	-2.942475000	-4.117331000	1	-6.063698000	-1.626461000	-2.492390000
6	-0.226333000	-4.405161000	-2.574782000	1	-7.281883000	-2.846966000	-2.121600000
1	-0.637746000	-5.418786000	-2.552816000	1	-5.780023000	-3.331692000	-2.911565000
1	0.360524000	-4.264234000	-1.660790000	6	-1.301360000	-2.179589000	-0.589685000
1	0.453150000	-4.348733000	-3.431430000	6	-1.996414000	-2.626768000	0.562437000
6	-0.026262000	0.768723000	-2.712210000	6	-3.363207000	-2.864503000	0.459019000
6	0.933637000	-0.269983000	-2.750937000	1	-3.891332000	-3.199813000	1.346308000
6	0.491296000	-1.601130000	-2.742264000	6	-4.076588000	-2.668959000	-0.739475000
1	1.243401000	-2.379774000	-2.761204000	6	-3.356880000	-2.228054000	-1.859803000
6	-0.862173000	-1.935488000	-2.672736000	1	-3.867270000	-2.062787000	-2.801309000
6	-1.782952000	-0.869649000	-2.589384000	6	-1.982122000	-1.981032000	-1.813303000
1	-2.839752000	-1.089106000	-2.480331000	6	0.907823000	-3.056939000	-0.805929000
6	-1.397688000	0.468319000	-2.599045000	1	0.710589000	-3.392775000	-1.832661000
6	0.373259000	2.673491000	-4.075199000	1	0.654252000	-3.883270000	-0.128131000
1	-0.639638000	2.602199000	-4.496092000	6	2.354213000	-2.635603000	-0.638041000
1	1.053602000	2.115324000	-4.734436000	1	2.499225000	-2.277741000	0.384402000
6	0.808606000	4.122997000	-3.936736000	1	2.551801000	-1.791580000	-1.303033000
1	0.124198000	4.631448000	-3.247135000	6	3.284114000	-3.814170000	-0.949820000
1	1.801375000	4.147279000	-3.471086000	1	4.333497000	-3.529956000	-0.844218000
6	0.836724000	4.842883000	-5.289378000	1	3.144825000	-4.174941000	-1.975918000
1	1.151336000	5.883452000	-5.169557000	1	3.103583000	-4.658883000	-0.274282000
1	-0.152964000	4.846956000	-5.759728000	6	-2.950685000	3.297810000	-2.035251000
1	1.535316000	4.361847000	-5.983093000	6	-2.949215000	4.273972000	-3.236996000
6	-6.406447000	-0.317214000	0.249433000	1	-3.102738000	3.736586000	-4.178574000
6	-7.425851000	0.632931000	-0.423659000	1	-2.000256000	4.814851000	-3.307939000
1	-7.500686000	1.577021000	0.125900000	1	-3.752847000	5.010561000	-3.128382000
1	-8.417706000	0.168833000	-0.441491000	6	-4.323029000	2.599242000	-1.969555000
1	-7.149914000	0.865095000	-1.456604000	1	-4.566363000	2.089257000	-2.907310000
6	-6.915358000	-0.646378000	1.665544000	1	-5.106065000	3.342754000	-1.793250000
1	-7.014478000	0.253317000	2.282030000	1	-4.370304000	1.866799000	-1.156539000
1	-6.256602000	-1.352463000	2.182899000	6	-2.746875000	4.102380000	-0.729296000
1	-7.904355000	-1.109969000	1.600114000	1	-2.652759000	3.436831000	0.133252000
6	-6.323261000	-1.638926000	-0.553951000	1	-3.601635000	4.764217000	-0.557011000
1	-5.596977000	-2.324590000	-0.103426000	1	-1.851134000	4.728714000	-0.766519000
1	-6.027172000	-1.466541000	-1.593418000	6	0.365854000	0.526175000	-2.673624000
1	-7.299164000	-2.135858000	-0.565996000	6	-0.942851000	0.055444000	-2.791998000
6	-2.460937000	1.508395000	0.201167000	6	-2.006267000	0.943264000	-2.542540000
6	-3.140190000	1.278449000	-1.010163000	1	-3.013774000	0.550951000	-2.614252000
6	-4.412380000	0.711079000	-0.952585000	6	-1.799507000	2.298410000	-2.222281000
1	-4.937247000	0.536524000	-1.887216000	6	-0.473201000	2.715842000	-2.077134000
6	-5.019128000	0.345316000	0.263120000	1	-0.259497000	3.735745000	-1.781760000
6	-4.299971000	0.580110000	1.443643000	6	0.613661000	1.855638000	-2.261498000
1	-4.726909000	0.308727000	2.402263000	6	1.882152000	-0.424439000	-4.243150000
6	-3.023651000	1.156864000	1.438248000	1	2.179590000	0.567884000	-4.611545000
6	-1.085041000	3.469418000	0.253720000	1	1.054245000	-0.779806000	-4.873664000
1	-1.414184000	3.772622000	1.254853000	6	3.052033000	-1.393891000	-4.275996000
1	-1.770639000	3.911129000	-0.481542000	1	3.831879000	-1.022830000	-3.601747000
6	0.346307000	3.886581000	-0.006265000	1	2.720340000	-2.357301000	-3.870276000
1	0.626107000	3.520470000	-0.994554000	6	3.609887000	-1.573393000	-5.691706000
1	0.983754000	3.379320000	0.718454000	1	4.449699000	-2.274109000	-5.692693000
6	0.516545000	5.405888000	0.082765000	1	3.969663000	-0.623127000	-6.102132000
1	1.557641000	5.688461000	-0.104458000	1	2.848397000	-1.965844000	-6.375077000
1	0.246680000	5.786696000	1.074442000	6	5.778049000	-0.403260000	0.099098000
1	-0.104033000	5.928536000	-0.654692000	6	5.874714000	-1.602182000	1.068123000
6	-0.603535000	-3.506454000	2.846102000	1	5.865192000	-1.287669000	2.116021000
6	0.157435000	-4.254299000	1.724396000	1	6.815431000	-2.137704000	0.905440000
1	-0.084239000	-5.321590000	1.754525000	1	5.050859000	-2.304741000	0.915457000
1	1.242300000	-4.162428000	1.826982000	6	6.022482000	-0.922076000	-1.334175000
1	-0.117482000	-3.873114000	0.736424000	1	6.122851000	-0.105845000	-2.056110000
6	-2.104702000	-3.828135000	2.712968000	1	5.210310000	-1.575309000	-1.666990000
1	-2.251679000	-4.912008000	2.739911000	1	6.954991000	-1.494024000	-1.368212000
1	-2.518215000	-3.459241000	1.768159000	6	6.889757000	0.614776000	0.454720000
1	-2.688409000	-3.401577000	3.535042000	1	6.866460000	1.472601000	-0.225564000
6	-0.106219000	-4.015896000	4.221093000	1	7.877434000	0.145267000	0.381003000
1	-0.283997000	-5.092940000	4.312667000	1	6.764508000	0.990190000	1.475794000
1	-0.631338000	-3.512010000	5.039124000	6	2.092313000	1.879791000	0.518637000
1	0.966374000	-3.837331000	4.347438000	6	2.659679000	1.714139000	-0.754677000
6	0.265005000	0.770407000	2.684648000	6	3.819875000	0.942845000	-0.874511000
6	-1.070249000	0.346042000	2.783000000	1	4.250967000	0.839719000	-1.863198000
6	-1.340470000	-1.025310000	2.801194000	6	4.423271000	0.314972000	0.221896000

1	-2.380487000	-1.329167000	2.835956000	6	3.759972000	0.414844000	1.452087000
6	-0.323405000	-1.998321000	2.758939000	1	4.142190000	-0.116573000	2.316028000
6	0.990285000	-1.537591000	2.636985000	6	2.590967000	1.162484000	1.620494000
1	1.797416000	-2.254879000	2.558935000	6	1.129243000	3.946695000	1.304776000
6	1.312029000	-0.178459000	2.554164000	1	1.727209000	3.826344000	2.216483000
6	0.932236000	2.662907000	3.954079000	1	0.117035000	4.243049000	1.599035000
1	1.825207000	2.141890000	4.327614000	6	1.763283000	5.009927000	0.413263000
1	0.117568000	2.496181000	4.673225000	1	1.136899000	5.153779000	-0.474925000
6	1.202372000	4.146141000	3.764862000	1	2.739382000	4.649001000	0.067960000
1	0.299850000	4.616906000	3.357444000	6	1.927363000	6.339009000	1.159865000
1	1.987924000	4.266894000	3.009837000	1	2.372308000	7.099679000	0.512084000
6	1.613433000	4.824333000	5.076091000	1	2.578034000	6.225523000	2.034277000
1	1.801599000	5.890354000	4.919964000	1	0.961483000	6.722635000	1.508511000
1	2.528755000	4.381399000	5.484552000	7	-1.529564000	0.301490000	0.037600000
1	0.829227000	4.732956000	5.835900000	8	-0.445222000	0.541545000	0.131851000
NO⁺@1.2-alternate				NO⁺@1.3-alternate			
8	0.382745000	-0.950183000	1.682518000	8	-1.084319000	2.682470000	0.429962000
8	0.000863000	2.077964000	1.689753000	8	1.414046000	0.301499000	-2.708839000
6	-1.963964000	0.328608000	2.765108000	8	-1.526860000	-2.681163000	-0.525986000
1	-1.001020000	0.556586000	3.216428000	8	1.298247000	-0.633320000	2.646249000
1	-2.731944000	0.390866000	3.542751000	6	0.172380000	1.988828000	2.915556000
6	0.421079000	-3.693192000	0.647072000	1	-0.488045000	2.829947000	3.149692000
1	0.117189000	-4.562467000	0.051800000	1	0.880247000	1.906900000	3.745869000
1	0.824116000	-4.118320000	1.574793000	6	0.316122000	2.872939000	-2.100577000
6	-4.642064000	-3.624337000	1.104795000	1	-0.320553000	3.763106000	-2.087414000
6	-0.788084000	-1.645616000	1.638679000	1	1.075843000	3.046373000	-2.868234000
6	-1.971435000	-1.069323000	2.172666000	6	-0.134487000	-2.110320000	-2.983428000
6	-3.176840000	-1.747174000	2.005997000	1	0.587160000	-2.157679000	-3.804231000
1	-4.075143000	-1.300344000	2.417611000	1	-0.922984000	-2.832539000	-3.214558000
6	-3.273233000	-2.957507000	1.300482000	6	-0.215589000	-3.003269000	-2.035253000
6	-2.075547000	-3.525547000	0.830534000	1	0.486284000	-3.320545000	2.812100000
1	-2.099734000	-4.480569000	0.319047000	1	-0.997097000	-3.767130000	1.987170000
6	-0.832807000	-2.923881000	1.019959000	6	4.636747000	2.753256000	0.584541000
6	-5.603425000	-2.626916000	0.413479000	6	4.880399000	4.258521000	0.864946000
1	-5.763070000	-1.728678000	1.016000000	1	4.418092000	4.561299000	1.810276000
1	-6.580138000	-3.095508000	0.256002000	1	4.458561000	4.879332000	0.067669000
1	-5.213133000	-2.316780000	-0.562183000	1	5.954951000	4.464204000	0.927473000
6	-5.213719000	-4.010535000	2.491644000	6	5.339415000	2.375414000	-0.737002000
1	-4.552322000	-4.715968000	3.004899000	1	6.422072000	2.488750000	-0.623739000
1	-6.193174000	-4.485513000	2.372848000	1	5.037986000	3.021290000	-1.567053000
1	-5.342321000	-3.136371000	3.136972000	1	5.134710000	1.337730000	-1.013832000
6	-4.560016000	-4.894771000	0.237703000	6	5.279352000	1.927828000	1.719478000
1	-4.160705000	-4.681797000	-0.760254000	1	4.926893000	2.236037000	2.708303000
1	-5.562365000	-5.313388000	0.108382000	1	6.364298000	2.071561000	1.710332000
1	-3.941811000	-5.669803000	0.702302000	1	5.078582000	0.860173000	1.597301000
6	-5.282530000	2.391776000	-0.521100000	6	0.293486000	2.544758000	0.432239000
6	-1.237044000	2.133219000	1.114657000	6	0.957241000	2.276252000	1.646006000
6	-1.492796000	2.922466000	-0.037731000	6	2.352382000	2.286406000	1.658130000
6	-2.790473000	2.950196000	-0.539232000	1	2.846479000	2.102698000	2.604346000
1	-2.976165000	3.558888000	-1.419224000	6	3.114484000	2.544476000	0.508617000
6	-3.859511000	2.233959000	0.037680000	6	2.414973000	2.704549000	-0.697209000
6	-3.555464000	1.424045000	1.133581000	1	2.959760000	2.850670000	-1.621896000
1	-4.332516000	0.829702000	1.596675000	6	1.021358000	2.705157000	-0.764270000
6	-2.262051000	1.335059000	1.662320000	6	-1.543659000	4.040645000	0.607945000
6	-6.299957000	1.497159000	0.211201000	1	-1.199649000	4.656615000	-0.234288000
1	-6.051733000	0.435495000	0.109231000	1	-1.102789000	4.458267000	1.523605000
1	-7.295013000	1.645138000	-0.219089000	6	-3.060010000	4.027754000	0.688023000
1	-6.365419000	1.739893000	1.277014000	1	-3.450178000	3.506707000	-0.193145000
6	-5.719942000	3.868067000	-0.354653000	1	-3.364311000	3.437350000	1.557759000
1	-5.711885000	4.160693000	0.700374000	6	-3.642642000	5.442185000	0.774933000
1	-6.735873000	4.006115000	-0.740018000	1	-4.733964000	5.410038000	0.841018000
1	-5.060165000	4.550511000	-0.898944000	1	-3.379574000	6.037387000	-0.106655000
6	-5.309028000	2.018148000	-2.022010000	1	-3.271935000	5.973092000	1.658923000
1	-4.648855000	2.655150000	-2.617794000	6	-4.294444000	0.788887000	-2.799816000
1	-6.322654000	2.135108000	-2.419329000	6	-4.855204000	0.145377000	-1.510264000
1	-5.004775000	0.976443000	-2.172106000	1	-4.482849000	0.670277000	-0.625429000
6	1.252900000	-1.099335000	2.822653000	1	-4.558336000	-0.903964000	-1.427272000
1	1.559679000	-2.149876000	2.918497000	1	-5.949581000	0.192377000	-1.501089000
1	0.712733000	-0.815386000	3.736741000	6	-4.778764000	2.250054000	-2.872748000
6	2.452185000	-0.197543000	2.581099000	1	-4.511966000	2.818831000	-1.976944000
1	2.077617000	0.803797000	2.350538000	1	-5.869822000	2.270420000	-2.952833000
1	2.974166000	-0.551329000	1.686043000	1	-4.369207000	2.768166000	-3.746224000
6	3.396180000	-0.165715000	3.785954000	6	-4.850867000	0.041010000	-4.034601000
1	4.267309000	0.463325000	3.579533000	1	-4.441837000	0.456081000	-4.961430000
1	3.765944000	-1.166283000	4.035413000	1	-5.940712000	0.139791000	-4.068826000

1	2.897599000	0.238244000	4.674684000	1	-4.621527000	-1.028023000	-4.012426000
6	0.533291000	3.245738000	2.361231000	6	0.044145000	0.415882000	-2.697098000
1	0.106812000	4.158464000	1.930997000	6	-0.542776000	1.677118000	-2.467091000
1	1.602044000	3.228678000	2.136379000	6	-1.932649000	1.785473000	-2.515265000
6	0.297770000	3.203990000	3.868222000	1	-2.367878000	2.760109000	-2.333997000
1	0.985549000	3.930571000	4.321413000	6	-2.762475000	0.681279000	-2.761579000
1	0.604767000	2.217697000	4.238356000	6	-2.140456000	-0.570596000	-2.924964000
6	-1.137011000	3.527763000	4.299373000	1	-2.749446000	-1.458117000	-3.053154000
1	-1.231151000	3.510348000	5.389498000	6	-0.758941000	-0.729140000	-2.899890000
1	-1.858436000	2.816042000	3.890901000	6	2.020375000	0.484615000	-4.008021000
1	-1.429987000	4.526377000	3.955538000	1	1.721751000	1.459258000	-4.419031000
8	-0.257183000	1.258228000	-2.171472000	1	1.654637000	-0.289984000	-4.696982000
8	0.078751000	-1.794498000	-1.584878000	6	3.528519000	0.403552000	-3.844836000
6	2.193112000	-0.215061000	-2.643359000	1	3.843455000	1.160149000	-3.118587000
1	1.265073000	-0.387213000	-3.185379000	1	3.784144000	-0.568901000	-3.410256000
1	3.013080000	-0.211120000	-3.369435000	6	4.260494000	0.599923000	-5.176497000
6	-0.410323000	3.729178000	-0.738726000	1	4.037518000	1.579482000	-5.614250000
1	-0.195052000	4.636838000	-0.163898000	1	3.974748000	-0.165224000	-5.907073000
1	-0.831032000	4.083044000	-1.686271000	6	4.206226000	-2.886599000	-0.460236000
6	4.650242000	3.409157000	-0.107280000	6	4.673476000	-1.433363000	-0.204501000
6	0.935098000	1.807814000	-1.718691000	1	4.280047000	-1.064007000	0.746852000
6	2.143474000	1.133659000	-1.938747000	1	4.309975000	-0.766904000	-0.991824000
6	3.316705000	1.697174000	-1.430284000	1	5.767683000	-1.377585000	-0.176097000
1	4.248715000	1.167404000	-1.594576000	6	4.750660000	-3.800585000	0.658651000
6	3.330227000	2.894629000	-0.705203000	1	4.495330000	-3.436136000	1.657802000
6	2.102221000	3.539998000	-0.518859000	1	5.843025000	-3.839371000	0.604062000
1	2.057580000	4.474694000	0.027716000	1	4.368870000	-4.822067000	0.559163000
6	0.900264000	3.009851000	-0.999744000	6	4.790587000	-3.381806000	-1.800910000
6	5.175011000	2.358631000	0.903374000	1	5.881087000	-3.440115000	-1.728722000
1	5.366691000	1.393832000	0.423317000	1	4.562706000	-2.707510000	-2.631324000
1	6.111753000	2.700430000	1.357298000	1	4.412917000	-4.377577000	-2.055575000
1	4.445792000	2.191935000	1.703885000	6	-0.144830000	-2.687777000	-0.498339000
6	5.694759000	3.611995000	-1.229517000	6	0.575924000	-2.485477000	-1.695313000
1	5.343657000	4.348674000	-1.959602000	6	1.965157000	-2.582116000	-1.659864000
1	6.639453000	3.972086000	-0.807671000	1	2.502304000	-2.415530000	-2.584707000
1	5.904881000	2.681550000	-1.765469000	6	2.671505000	-2.863471000	-0.481878000
6	4.475737000	4.746707000	0.636534000	6	1.924822000	-3.002818000	0.696389000
1	3.783673000	4.656860000	1.481471000	1	2.430156000	-3.170771000	1.638789000
1	5.439989000	5.073240000	1.038146000	6	0.534448000	-2.915822000	0.718073000
1	4.109901000	5.536617000	-0.027986000	6	-2.130982000	-3.976320000	-0.745328000
6	5.392356000	-2.871610000	0.315091000	1	-1.852029000	-4.652157000	0.074696000
6	1.354162000	-2.059446000	-1.101614000	1	-1.739952000	-4.407824000	-1.676854000
6	1.555963000	-2.963208000	-0.045005000	6	-3.637483000	-3.797305000	-0.814411000
6	2.863396000	-3.194966000	0.382963000	1	-3.973456000	-3.293378000	0.098326000
1	3.013489000	-3.897360000	1.197893000	1	-3.874617000	-3.127606000	-1.649012000
6	3.974960000	-2.553155000	-0.187795000	6	-4.364789000	-5.135377000	-0.986303000
6	3.717009000	-1.618810000	-1.193235000	1	-4.163878000	-5.809069000	-0.145807000
1	4.536383000	-1.082435000	-1.654787000	1	-4.053084000	-5.645005000	-1.904859000
6	2.420540000	-1.333119000	-1.642099000	1	-5.446841000	-4.985538000	-1.040624000
6	6.473034000	-2.072743000	-0.438133000	6	-4.408776000	-0.251212000	2.891700000
1	6.346936000	-0.992420000	-0.305325000	6	-4.965712000	1.140374000	2.524623000
1	7.461268000	-2.336642000	-0.049307000	1	-6.056662000	1.134402000	2.608432000
1	6.471153000	-2.294355000	-1.510632000	1	-4.706470000	1.417150000	1.498595000
6	5.677096000	-4.380033000	0.120307000	1	-4.599715000	1.923596000	3.194961000
1	5.605541000	-4.657268000	-0.936681000	6	-4.702631000	-0.528023000	4.388645000
1	6.686646000	-4.622292000	0.469383000	1	-4.343156000	-1.519404000	4.682970000
1	4.973488000	-5.003319000	0.680625000	1	-5.781405000	-0.485311000	4.575445000
6	5.494704000	-2.516408000	1.817593000	1	-4.214470000	0.213908000	5.028966000
1	4.769981000	-3.072778000	2.420022000	6	-5.145818000	-1.303916000	2.035530000
1	6.494283000	-2.756887000	2.195209000	1	-4.916708000	-2.327059000	2.347420000
1	5.317768000	-1.448568000	1.978507000	1	-4.894990000	-1.201335000	0.976453000
6	-0.661668000	1.664909000	-3.492100000	1	-6.227072000	-1.174210000	2.142694000
1	-0.734793000	2.760518000	-3.535500000	6	-0.071637000	-0.528987000	2.625988000
1	0.099359000	1.355441000	-4.222579000	6	-0.860498000	-1.680578000	2.406494000
6	-2.007444000	1.023567000	-3.788805000	6	-2.246249000	-1.555493000	2.453024000
1	-1.896604000	-0.066564000	-3.747270000	1	-2.837724000	-2.444749000	2.273232000
1	-2.702810000	1.303807000	-2.991538000	6	-2.885683000	-0.328437000	2.703762000
6	-2.564678000	1.446289000	-5.151375000	6	-2.065929000	0.802998000	2.861505000
1	-3.533298000	0.974601000	-5.341350000	1	-2.514796000	1.777024000	3.009060000
1	-2.708240000	2.531518000	-5.201980000	6	-0.674943000	0.732386000	2.820751000
1	-1.889597000	1.161592000	-5.966067000	6	1.855727000	-0.911007000	3.951183000
6	-0.644694000	-2.818856000	-2.299869000	1	1.540543000	-0.130982000	4.658459000
1	-0.424188000	-3.802074000	-1.872875000	1	1.464827000	-1.869444000	4.321179000
1	-1.701645000	-2.601219000	-2.106901000	6	3.368791000	-0.950247000	3.825215000
6	-0.368345000	-2.807835000	-3.802149000	1	3.712332000	0.007597000	3.421952000

1	-1.168237000	-3.394642000	-4.273779000	1	3.641014000	-1.712858000	3.087597000
1	-0.478513000	-1.781598000	-4.170931000	6	4.047636000	-1.241274000	5.167679000
6	0.992758000	-3.384804000	-4.206967000	1	5.135377000	-1.264410000	5.055519000
1	1.088901000	-3.413740000	-5.296541000	1	3.734396000	-2.209910000	5.573218000
1	1.822162000	-2.794000000	-3.812668000	1	3.806593000	-0.473853000	5.911888000
1	1.109273000	-4.408943000	-3.834492000	7	-0.571115000	-0.062738000	-0.025634000
8	-2.336085000	-0.548313000	-0.881648000	8	-1.683526000	0.025238000	-0.044219000
7	-1.337491000	-0.380628000	-0.408700000	1	5.343545000	0.537636000	-5.037055000
NO⁺@Cone (Perpendicular)				NO⁺@Partial cone (Perpendicular)			
8	2.416132000	1.232174000	-0.280253000	8	-1.478955000	-2.851121000	0.004028000
8	0.629337000	2.070548000	-2.768881000	8	-0.141775000	-0.618493000	1.878192000
8	-0.965395000	2.245893000	0.147599000	8	-1.435925000	2.228032000	1.797369000
8	0.815831000	2.075180000	2.639246000	8	-0.765398000	0.813090000	-2.538860000
6	2.471611000	-0.166279000	-2.785287000	6	1.142094000	-3.068826000	1.233996000
1	2.737774000	0.886519000	-2.861569000	1	1.730552000	-3.984264000	1.358598000
1	2.938469000	-0.692220000	-3.624807000	1	0.178720000	-3.224996000	1.718339000
6	-2.238097000	1.773501000	-2.332363000	6	1.167309000	1.704443000	2.972059000
1	-2.991643000	1.868980000	-3.122067000	1	1.771815000	2.319978000	3.646256000
1	-1.669360000	2.702370000	-2.297349000	1	0.200788000	1.541355000	3.448729000
6	-2.027833000	1.573428000	2.728200000	6	-1.824518000	2.964447000	-0.934643000
1	-1.542405000	2.548708000	2.758703000	1	-1.719429000	3.431198000	-1.917289000
1	-2.720237000	1.521889000	3.574949000	1	-2.497085000	3.606783000	-0.357082000
6	2.793101000	-0.028113000	2.287242000	6	-1.946345000	-1.889557000	-2.628280000
1	2.959151000	1.044307000	2.214246000	1	-2.615483000	-2.742950000	-2.481389000
1	3.457407000	-0.426109000	3.062232000	1	-1.890189000	-1.730778000	-3.709237000
6	4.132602000	-4.246886000	-0.272161000	6	3.109315000	-2.293814000	-3.379723000
6	5.410986000	-4.398877000	-1.129563000	6	3.818363000	-3.670662000	-3.386131000
1	6.232718000	-3.808718000	-0.710829000	1	3.156914000	-4.450761000	-3.776692000
1	5.252598000	-4.069977000	-2.161157000	1	4.138471000	-3.968442000	-2.383000000
1	5.724634000	-5.447934000	-1.160004000	1	4.709043000	-3.629249000	-4.021513000
6	2.991404000	-5.091597000	-0.891143000	6	2.758953000	-1.915204000	-4.830794000
1	3.269700000	-6.150810000	-0.911622000	1	2.102863000	-2.655718000	-5.299982000
1	2.771131000	-4.787670000	-1.919423000	1	3.675026000	-1.865624000	-5.426473000
1	2.071310000	-4.992090000	-0.303946000	1	2.275974000	-0.933392000	-4.890375000
6	4.425897000	-4.798647000	1.135813000	6	4.071378000	-1.220202000	-2.816007000
1	5.236154000	-4.250039000	1.627414000	1	3.593007000	-0.235396000	-2.814365000
1	4.734379000	-5.845993000	1.062681000	1	4.968855000	-1.156789000	-3.439545000
1	3.540788000	-4.762915000	1.780871000	1	4.393683000	-1.444533000	-1.794823000
6	2.856080000	-0.072999000	-0.263735000	6	-0.381875000	-2.654894000	-0.781561000
6	3.108017000	-0.710029000	0.960583000	6	-0.562834000	-2.250898000	-2.123472000
6	3.545047000	-2.044299000	0.940465000	6	0.560837000	-2.161018000	-2.955459000
1	3.763298000	-2.514064000	1.892535000	1	0.399114000	-1.877462000	-3.988141000
6	3.699695000	-2.771468000	-0.243994000	6	1.865940000	-2.384433000	-2.484991000
6	3.393890000	-2.109315000	-1.444627000	6	2.011337000	-2.677599000	-1.113492000
1	3.480768000	-2.643805000	-2.386529000	1	3.004184000	-2.793920000	-0.690933000
6	2.963605000	-0.781989000	-1.477998000	6	0.916875000	-2.817060000	-0.246834000
6	3.398821000	2.215167000	-0.680957000	6	-1.920265000	-4.230610000	0.094025000
1	2.837500000	2.991067000	-1.205095000	1	-1.089082000	-4.856154000	0.447948000
1	4.105375000	1.765213000	-1.390462000	1	-2.204366000	-4.581929000	-0.907918000
6	4.156333000	2.800771000	0.504844000	6	-3.097654000	-4.287707000	1.050918000
1	4.739650000	2.008549000	0.989426000	1	-3.875121000	-3.607137000	0.688666000
1	3.427562000	3.161503000	1.238205000	1	-2.776521000	-3.908060000	2.027589000
6	5.080071000	3.943394000	0.068144000	6	-3.651178000	-5.710345000	1.185778000
1	5.624233000	4.357722000	0.921869000	1	-4.496947000	-5.731533000	1.878730000
1	4.509125000	4.759260000	-0.390646000	1	-2.891526000	-6.401719000	1.567496000
1	5.821622000	3.601682000	-0.663060000	1	-4.001822000	-6.096190000	0.221915000
6	-1.626676000	-3.201916000	-3.039036000	6	5.499009000	-1.021528000	2.862660000
6	-2.495517000	-3.454761000	-1.782120000	6	6.172795000	-1.311413000	1.498888000
1	-2.950798000	-4.448655000	-1.837280000	1	5.971842000	-0.504069000	0.785601000
1	-3.304770000	-2.726171000	-1.679746000	1	5.817008000	-2.248867000	1.059572000
1	-1.886078000	-3.414494000	-0.873023000	1	7.257985000	-1.395141000	1.621577000
6	-2.520587000	-3.256703000	-4.302125000	6	5.793428000	-2.184218000	3.840181000
1	-2.988674000	-4.242893000	-4.385956000	1	6.873178000	-2.284847000	3.994641000
1	-1.931371000	-3.080921000	-5.207973000	1	5.421616000	-3.140919000	3.460694000
1	-3.319703000	-2.509801000	-4.266769000	1	5.324689000	-2.002983000	4.812967000
6	-0.569467000	-4.318334000	-3.130215000	6	6.120132000	0.264462000	3.439904000
1	-1.069207000	-5.289597000	-3.189197000	1	5.975044000	1.122249000	2.773879000
1	0.083446000	-4.337030000	-2.250768000	1	7.198275000	0.126096000	3.566381000
1	0.054539000	-4.218074000	-4.024598000	1	5.703546000	0.512561000	4.421769000
6	0.102175000	0.812884000	-2.793172000	6	1.198767000	-0.722135000	2.200396000
6	0.961030000	-0.305912000	-2.887069000	6	1.881993000	-1.910399000	1.888171000
6	0.393440000	-1.589320000	-2.982997000	6	3.257113000	-1.976102000	2.121509000
1	1.072117000	-2.430307000	-3.051082000	1	3.774408000	-2.900451000	1.879656000
6	-0.992362000	-1.808379000	-2.946019000	6	3.979983000	-0.896370000	2.655714000
6	-1.809389000	-0.674832000	-2.769395000	6	3.261214000	0.265831000	2.961081000

1	-2.881527000	-0.801503000	-2.666122000	1	3.774321000	1.126257000	3.375322000
6	-1.297573000	0.626449000	-2.670021000	6	1.880856000	0.378193000	2.739774000
6	0.634332000	2.746433000	-4.053301000	6	-1.045431000	-0.974023000	2.948213000
1	-0.384220000	2.750591000	-4.465679000	1	-0.849814000	-0.326770000	3.814303000
1	1.279967000	2.187552000	-4.745367000	1	-0.842260000	-2.008907000	3.260884000
6	1.145506000	4.161441000	-3.844349000	6	-2.479122000	-0.821914000	2.474916000
1	0.483191000	4.676558000	-3.139160000	1	-2.629912000	-1.454306000	1.597165000
1	2.134105000	4.111822000	-3.372774000	1	-2.629759000	0.208691000	2.148310000
6	1.223207000	4.935508000	-5.165173000	6	-3.455199000	-1.193589000	3.596645000
1	1.589568000	5.951983000	-4.996740000	1	-4.493387000	-1.078639000	3.275262000
1	0.239580000	5.011822000	-5.642053000	1	-3.313996000	-0.557634000	4.478571000
1	1.903241000	4.449842000	-5.873841000	1	-3.324225000	-2.234066000	3.917544000
6	-6.207387000	-0.073888000	0.256981000	6	3.174855000	3.826080000	-1.212964000
6	-7.227796000	0.882443000	-0.404831000	6	2.954006000	5.297827000	-1.636976000
1	-7.294611000	1.824271000	0.149542000	1	2.848567000	5.943893000	-0.759425000
1	-8.222291000	0.423541000	-0.419855000	1	2.055727000	5.414941000	-2.250738000
1	-6.955803000	1.119037000	-1.438034000	1	3.807579000	5.654725000	-2.223329000
6	-6.708344000	-0.408534000	1.674707000	6	4.493331000	3.740488000	-0.421029000
1	-6.804071000	0.489012000	2.294702000	1	4.466741000	4.363373000	0.479121000
1	-6.045167000	-1.115084000	2.185933000	1	5.319687000	4.096700000	-1.043820000
1	-7.697521000	-0.872670000	1.614045000	1	4.724727000	2.711578000	-0.123618000
6	-6.136837000	-1.392406000	-0.552069000	6	3.312730000	2.941824000	-2.475607000
1	-5.413440000	-2.084730000	-0.106784000	1	3.493152000	1.898504000	-2.195373000
1	-5.843037000	-1.217011000	-1.592042000	1	4.157948000	3.277757000	-3.085758000
1	-7.115531000	-1.884048000	-0.564273000	1	2.415086000	2.975737000	-3.101015000
6	-2.251003000	1.751053000	0.202301000	6	-0.311150000	2.544478000	1.071658000
6	-2.935253000	1.515622000	-1.002236000	6	0.964167000	2.423162000	1.647481000
6	-4.208974000	0.945883000	-0.947315000	6	2.077996000	2.860079000	0.916256000
1	-4.735984000	0.775032000	-1.882059000	1	3.051367000	2.765464000	1.383125000
6	-4.816706000	0.584030000	0.266847000	6	1.967821000	3.348363000	-0.390608000
6	-4.096095000	0.827635000	1.443498000	6	0.683236000	3.352715000	-0.967283000
1	-4.522899000	0.563180000	2.404367000	1	0.560019000	3.672040000	-1.996815000
6	-2.819382000	1.407689000	1.436266000	6	-0.459249000	2.955681000	-0.268562000
6	-0.866177000	3.683591000	0.247067000	6	-1.901790000	3.295431000	2.653099000
1	-1.204712000	4.005746000	1.241192000	1	-2.178696000	4.161826000	2.034827000
1	-1.533842000	4.144713000	-0.495777000	1	-1.088667000	3.610270000	3.322487000
6	0.578553000	4.071185000	0.007150000	6	-3.093771000	2.787007000	3.445829000
1	0.860578000	3.696889000	-0.978590000	1	-3.860522000	2.442765000	2.743860000
1	1.189240000	3.537842000	0.737658000	1	-2.782387000	1.910565000	4.026188000
6	0.799756000	5.582796000	0.098914000	6	-3.665519000	3.865157000	4.372524000
1	1.851667000	5.832265000	-0.074437000	1	-4.521718000	3.480767000	4.934308000
1	0.528752000	5.971719000	1.087024000	1	-4.005283000	4.739372000	3.805698000
1	0.204533000	6.125603000	-0.645045000	1	-2.918201000	4.206708000	5.097582000
6	-0.884849000	-3.377593000	3.240393000	6	-5.812287000	-0.029145000	0.079012000
6	-0.394328000	-4.208203000	2.028866000	6	-6.035664000	-1.484554000	0.545865000
1	-0.683195000	-5.257826000	2.147782000	1	-6.034915000	-2.192909000	-0.288048000
1	0.693399000	-4.173724000	1.916326000	1	-7.010347000	-1.572129000	1.036143000
1	-0.840208000	-3.839675000	1.098497000	1	-5.266718000	-1.793729000	1.259450000
6	-2.412477000	-3.541316000	3.348518000	6	-6.041166000	0.898859000	1.290526000
1	-2.660920000	-4.599874000	3.471884000	1	-6.034987000	1.956257000	1.009289000
1	-2.924717000	-3.183947000	2.448058000	1	-5.279132000	0.743146000	2.059747000
1	-2.818707000	-3.006081000	4.213066000	1	-7.019710000	0.692999000	1.735368000
6	-0.236962000	-3.928164000	4.533419000	6	-6.855116000	0.310883000	-1.014187000
1	-0.518419000	-4.976323000	4.681674000	1	-6.741503000	1.345491000	-1.354579000
1	-0.567524000	-3.358535000	5.408011000	1	-7.872206000	0.187802000	-0.624901000
1	0.855479000	-3.877477000	4.491983000	1	-6.739720000	-0.345256000	-1.883365000
6	0.399013000	0.769086000	2.740791000	6	-1.965275000	0.579362000	-1.873321000
6	-0.974385000	0.485512000	2.866036000	6	-2.503206000	1.606670000	-1.081406000
6	-1.380787000	-0.847858000	3.028558000	6	-3.720239000	1.373213000	-0.431385000
1	-2.444653000	-1.038901000	3.109632000	1	-4.127421000	2.180343000	0.165672000
6	-0.468025000	-1.910010000	3.056537000	6	-4.411685000	0.160399000	-0.529488000
6	0.885690000	-1.589921000	2.864751000	6	-3.794980000	-0.861347000	-1.262272000
1	1.616357000	-2.389595000	2.823961000	1	-4.260410000	-1.838745000	-1.319253000
6	1.339899000	-0.280250000	2.674856000	6	-2.574833000	-0.689193000	-1.921882000
6	1.167385000	2.677848000	3.904626000	6	-0.817514000	0.939500000	-3.975236000
1	2.038421000	2.156284000	4.327469000	1	-1.466524000	0.164501000	-4.399147000
1	0.330072000	2.558804000	4.607414000	1	0.206921000	0.745719000	-4.310737000
6	1.469530000	4.148112000	3.667209000	6	-1.285812000	2.314085000	-4.440589000
1	0.590152000	4.615743000	3.209025000	1	-0.615158000	3.077199000	-4.029434000
1	2.284365000	4.230769000	2.939047000	1	-2.285976000	2.505152000	-4.034313000
6	1.843565000	4.870631000	4.965860000	6	-1.313258000	2.404651000	-5.970941000
1	2.056137000	5.926689000	4.776276000	1	-1.642444000	3.395107000	-6.297490000
1	2.735135000	4.429224000	5.425313000	1	-2.001264000	1.667998000	-6.400954000
1	1.030303000	4.821295000	5.698633000	1	-0.320099000	2.226638000	-6.399383000
7	-0.310780000	-0.660953000	-0.650884000	7	0.930095000	-0.352133000	-1.004871000

8	-0.255756000	-0.702721000	0.459930000	8	1.096111000	0.609069000	-0.475553000
NO⁺@1.2-alternate (Perpendicular)				NO⁺@1.3-alternate (Perpendicular)			
8	0.316487000	0.977344000	-1.577042000	8	1.199094000	0.366554000	-2.615198000
8	-0.038310000	-2.047067000	-1.775876000	8	-1.567218000	2.661069000	0.342015000
6	-2.036273000	-0.237364000	-2.676915000	8	1.397131000	-0.154507000	2.661399000
1	-1.083546000	-0.433999000	-3.163814000	8	-1.195446000	-2.614579000	-0.240419000
1	-2.820040000	-0.256729000	-3.441122000	6	-0.025373000	-2.235877000	-2.777296000
6	0.456860000	3.782848000	-0.640987000	1	0.651267000	-2.239392000	-3.637639000
1	0.159486000	4.647471000	-0.036156000	1	-0.730438000	-3.059617000	-2.933270000
1	0.884272000	4.213868000	-1.555082000	6	-0.262385000	2.833736000	-2.232950000
6	-4.613479000	3.820934000	-1.057491000	1	0.449226000	3.054108000	-3.035100000
6	-0.813707000	1.730548000	-1.568189000	1	-1.031298000	3.610898000	-2.283367000
6	-2.023362000	1.146371000	-2.043589000	6	-0.187349000	2.285610000	2.814835000
6	-3.217311000	1.854263000	-1.864272000	1	-0.995274000	2.994500000	3.020401000
1	-4.137465000	1.395242000	-2.209083000	1	0.525091000	2.380131000	3.640268000
6	-3.261793000	3.123440000	-1.263124000	6	0.302971000	-2.761753000	2.298790000
6	-2.036333000	3.699734000	-0.886834000	1	-0.302290000	-3.660685000	2.455135000
1	-2.025842000	4.688987000	-0.444693000	1	1.114482000	-2.813127000	3.030097000
6	-0.811519000	3.047258000	-1.036052000	6	-4.525949000	0.161135000	-2.988026000
6	-5.518448000	2.916458000	-0.183886000	6	-4.785029000	0.488522000	-4.479278000
1	-5.701250000	1.943739000	-0.650355000	1	-4.303185000	-0.247936000	-5.131105000
1	-6.489882000	3.396733000	-0.029282000	1	-4.390470000	1.476773000	-4.737717000
1	-5.065383000	2.742702000	0.798507000	1	-5.860237000	0.483223000	-4.691691000
6	-5.284544000	4.045271000	-2.435266000	6	-5.252847000	1.204567000	-2.111751000
1	-4.660069000	4.674993000	-3.077096000	1	-6.334691000	1.123276000	-2.258790000
1	-6.249378000	4.545234000	-2.302191000	1	-4.973565000	2.230280000	-2.369426000
1	-5.468889000	3.103372000	-2.960515000	1	-5.040158000	1.044367000	-1.051264000
6	-4.470971000	5.184789000	-0.356418000	6	-5.133426000	-1.220320000	-2.669197000
1	-4.016583000	5.088729000	0.635853000	1	-4.752866000	-2.004948000	-3.330565000
1	-5.460855000	5.630259000	-0.221467000	1	-6.218642000	-1.185990000	-2.806852000
1	-3.874584000	5.888170000	-0.946801000	1	-4.933301000	-1.512390000	-1.633851000
6	-5.278867000	-2.552991000	0.516381000	6	-0.191526000	0.308363000	-2.627659000
6	-1.269042000	-2.160779000	-1.184782000	6	-0.824521000	-0.937276000	-2.736086000
6	-1.492931000	-3.022467000	-0.085807000	6	-2.221388000	-0.968218000	-2.810764000
6	-2.785558000	-3.106271000	0.432789000	1	-2.695765000	-1.935963000	-2.914150000
1	-2.946393000	-3.776509000	1.272287000	6	-3.003474000	0.191897000	-2.758254000
6	-3.868388000	-2.359401000	-0.064705000	6	-2.328361000	1.404911000	-2.560610000
6	-3.586921000	-1.456839000	-1.093103000	1	-2.892076000	2.325803000	-2.464534000
1	-4.373120000	-0.826041000	-1.489831000	6	-0.935999000	1.489784000	-2.481769000
6	-2.303549000	-1.323895000	-1.643440000	6	1.813299000	0.522835000	-3.908534000
6	-6.309470000	-1.604239000	-0.125392000	1	1.421039000	1.425591000	-4.396505000
1	-6.054057000	-0.551579000	0.043441000	1	1.555925000	-0.334249000	-4.546862000
1	-7.294440000	-1.777538000	0.318535000	6	3.316861000	0.620269000	-3.706147000
1	-6.402560000	-1.771441000	-1.203688000	1	3.529006000	1.486580000	-3.069203000
6	-5.730343000	-4.011082000	0.259259000	1	3.651427000	-0.264909000	-3.151468000
1	-5.753246000	-4.228691000	-0.813594000	6	4.074362000	0.736595000	-5.032650000
1	-6.735459000	-4.174080000	0.663093000	1	5.152218000	0.811161000	-4.861893000
1	-5.057702000	-4.731623000	0.734403000	1	3.764122000	1.626428000	-5.591488000
6	-5.264496000	-2.284069000	2.039611000	1	3.897433000	-0.136285000	-5.670975000
1	-4.589602000	-2.961691000	2.570554000	6	4.142567000	3.233863000	0.294481000
1	-6.267028000	-2.425533000	2.456952000	6	4.736211000	1.815490000	0.109281000
1	-4.951143000	-1.256006000	2.253241000	1	4.397382000	1.369307000	-0.832043000
6	1.225208000	1.103943000	-2.695783000	1	4.434534000	1.154772000	0.928578000
1	1.536940000	2.151869000	-2.795935000	1	5.831175000	1.854279000	0.091147000
1	0.701905000	0.811123000	-3.616468000	6	4.623500000	4.135076000	-0.863556000
6	2.417002000	0.202673000	-2.426891000	1	4.400933000	3.707080000	-1.845644000
1	2.041040000	-0.790504000	-2.168624000	1	5.709381000	4.260879000	-0.808812000
1	2.947645000	0.577709000	-1.546675000	1	4.162972000	5.126872000	-0.811163000
6	3.347861000	0.142171000	-3.641962000	6	4.675188000	3.830493000	1.615069000
1	4.229660000	-0.468131000	-3.428617000	1	4.216680000	4.802279000	1.824705000
1	3.702108000	1.138641000	-3.928221000	1	5.758146000	3.973199000	1.546716000
1	2.842527000	-0.295977000	-4.510522000	1	4.493330000	3.175087000	2.472176000
6	0.498210000	-3.172186000	-2.511366000	6	-0.194489000	2.763967000	0.317733000
1	0.049476000	-4.106175000	-2.155344000	6	0.478821000	2.920103000	-0.908230000
1	1.563029000	-3.188273000	-2.266540000	6	1.866579000	3.104585000	-0.882296000
6	0.293006000	-3.019076000	-4.015629000	1	2.372051000	3.226578000	-1.832976000
1	0.976922000	-3.721553000	-4.510614000	6	2.609511000	3.105607000	0.309436000
1	0.621382000	-2.013012000	-4.306323000	6	1.906288000	2.858514000	1.499075000
6	-1.139698000	-3.284624000	-4.491088000	1	2.440946000	2.783302000	2.438409000
1	-1.219159000	-3.174996000	-5.577044000	6	0.520847000	2.664641000	1.525491000
1	-1.856596000	-2.599240000	-4.032310000	6	-2.237028000	3.937857000	0.446844000
1	-1.451206000	-4.303683000	-4.234985000	1	-2.028202000	4.536084000	-0.451722000
8	-0.278690000	-1.424209000	2.155488000	1	-1.838670000	4.490124000	1.310017000
8	0.032293000	1.947608000	1.611381000	6	-3.728046000	3.692970000	0.597059000
6	2.088870000	0.164337000	2.579803000	1	-4.060203000	3.051812000	-0.225008000

1	1.128296000	0.307048000	3.071727000	1	-3.902729000	3.133447000	1.522637000
1	2.866486000	0.153339000	3.351819000	6	-4.524038000	5.002324000	0.612826000
6	-0.378007000	-3.823355000	0.574198000	1	-4.390377000	5.561498000	-0.320199000
1	-0.129898000	-4.697156000	-0.038616000	1	-4.211988000	5.651596000	1.438732000
1	-0.781672000	-4.230485000	1.507799000	6	-4.321663000	-0.657566000	2.882387000
6	4.676862000	-3.351816000	-0.004747000	6	-4.911729000	-0.131793000	1.552640000
6	0.913774000	-1.894782000	1.630041000	1	-4.532996000	-0.707117000	0.701999000
6	2.096288000	-1.170868000	1.841823000	1	-4.641277000	0.914429000	1.386316000
6	3.284539000	-1.684816000	1.315589000	1	-6.005132000	-0.205311000	1.559624000
1	4.201273000	-1.132670000	1.486647000	6	-4.791889000	-2.110228000	3.094991000
6	3.335308000	-2.871442000	0.573997000	1	-4.528734000	-2.760243000	2.255455000
6	2.126189000	-3.544159000	0.362333000	1	-5.882046000	-2.133216000	3.188830000
1	2.109691000	-4.462883000	-0.212279000	1	-4.368151000	-2.539986000	4.009081000
6	0.909276000	-3.069110000	0.862973000	6	-4.867938000	0.189557000	4.055451000
6	5.197315000	-2.287129000	-1.000954000	1	-5.957191000	0.091497000	4.113297000
1	5.345923000	-1.316277000	-0.517910000	1	-4.642819000	1.253433000	3.938600000
1	6.155594000	-2.600196000	-1.430007000	1	-4.444097000	-0.142601000	5.008902000
1	4.484294000	-2.145837000	-1.819770000	6	0.010234000	-0.267063000	2.687210000
6	5.704656000	-3.536627000	1.136208000	6	-0.788524000	0.884382000	2.790419000
1	5.354910000	-4.281612000	1.858457000	6	-2.173198000	0.715346000	2.846160000
1	6.663758000	-3.877149000	0.730877000	1	-2.784636000	1.607895000	2.913641000
1	5.886760000	-2.603430000	1.677668000	6	-2.789022000	-0.544336000	2.810690000
6	4.546641000	-4.689957000	-0.756670000	6	-1.956955000	-1.655551000	2.644784000
1	3.869164000	-4.612409000	-1.614504000	1	-2.387454000	-2.646794000	2.572591000
1	5.525577000	-4.993190000	-1.140769000	6	-0.565179000	-1.537953000	2.557576000
1	4.185722000	-5.490254000	-0.102002000	6	2.027555000	-0.182844000	3.957066000
6	5.398573000	2.818642000	-0.252373000	1	1.753545000	-1.110280000	4.479826000
6	1.318213000	2.108917000	1.109090000	1	1.661646000	0.656203000	4.564449000
6	1.563150000	3.014985000	0.059165000	6	3.530946000	-0.093359000	3.753959000
6	2.879355000	3.207502000	-0.359856000	1	3.847657000	-0.927074000	3.115573000
1	3.059093000	3.912315000	-1.166803000	1	3.755588000	0.826079000	3.201199000
6	3.964134000	2.527439000	0.217589000	6	4.296148000	-0.116571000	5.081154000
6	3.661859000	1.576972000	1.194149000	1	4.101651000	-1.040018000	5.637948000
1	4.459679000	1.007482000	1.652774000	1	4.008617000	0.725177000	5.720887000
6	2.352079000	1.316868000	1.624242000	1	5.374724000	-0.051214000	4.911349000
6	6.445326000	1.991428000	0.517995000	6	4.494768000	-3.158776000	-0.541298000
1	6.303293000	0.915151000	0.370092000	6	5.022178000	-3.150696000	-1.988450000
1	7.447633000	2.240699000	0.156492000	1	6.101490000	-3.328426000	-1.983523000
1	6.420518000	2.201320000	1.592574000	1	4.854089000	-2.186942000	-2.480730000
6	5.711869000	4.318886000	-0.039571000	1	4.562007000	-3.937522000	-2.595352000
1	5.622394000	4.589953000	1.017665000	6	4.841651000	-4.526695000	0.096199000
1	6.734121000	4.541474000	-0.363903000	1	4.544150000	-4.577282000	1.147824000
1	5.035210000	4.961857000	-0.610751000	1	5.922235000	-4.696131000	0.049492000
6	5.525702000	2.472521000	-1.755021000	1	4.345413000	-5.344587000	-0.436176000
1	4.824503000	3.047502000	-2.367895000	6	5.204064000	-2.027978000	0.241801000
1	6.537430000	2.696109000	-2.110063000	1	4.902723000	-2.006455000	1.293129000
1	5.331483000	1.409597000	-1.927680000	1	4.979146000	-1.049691000	-0.194358000
6	-0.595559000	-1.899713000	3.475869000	1	6.288727000	-2.173298000	0.210496000
1	-0.647330000	-2.997741000	3.471161000	6	0.163995000	-2.662919000	-0.273809000
1	0.201678000	-1.608561000	4.174915000	6	0.932503000	-2.803521000	0.912663000
6	-1.931078000	-1.297237000	3.880352000	6	2.319022000	-2.959406000	0.774708000
1	-1.838610000	-0.203901000	3.870525000	1	2.902907000	-3.075788000	1.681985000
1	-2.671271000	-1.561742000	3.118287000	6	2.975370000	-2.947054000	-0.472779000
6	-2.392498000	-1.777731000	5.259575000	6	2.186459000	-2.700482000	-1.607316000
1	-3.354595000	-1.331479000	5.528070000	1	2.648430000	-2.621869000	-2.583786000
1	-2.514336000	-2.866578000	5.280055000	6	0.795292000	-2.529102000	-1.533272000
1	-1.671010000	-1.508812000	6.039124000	6	-1.864986000	-3.887093000	-0.047640000
6	-0.527036000	3.049925000	2.373639000	1	-1.420534000	-4.632111000	-0.721032000
1	-0.049803000	3.987766000	2.069783000	1	-1.715765000	-4.231832000	0.982626000
1	-1.581430000	3.096587000	2.082114000	6	-3.340932000	-3.686082000	-0.339917000
6	-0.390495000	2.843085000	3.879806000	1	-3.469070000	-3.471064000	-1.404633000
1	-1.118256000	3.508578000	4.363565000	1	-3.673822000	-2.794460000	0.200098000
1	-0.701657000	1.818495000	4.117012000	6	-4.176866000	-4.904647000	0.062554000
6	1.007835000	3.129268000	4.438683000	1	-5.232117000	-4.744346000	-0.175987000
1	1.026640000	2.991880000	5.524111000	1	-4.105406000	-5.100151000	1.138612000
1	1.764642000	2.473146000	4.004209000	1	-3.851180000	-5.808500000	-0.464477000
1	1.306388000	4.162424000	4.227892000	7	1.703123000	-0.568102000	-0.112024000
8	-1.931596000	-0.038339000	0.770277000	8	1.538246000	0.513707000	0.060002000
7	-1.932911000	1.040911000	0.503117000	1	-5.593464000	4.805489000	0.731465000

Coordinates of NO@3 complexes	
NO@Cone	NO@ Partial cone

8	0.212297000	-1.864834000	-0.367928000	8	-2.002311000	1.876129000	0.918851000
8	2.596169000	-0.361362000	1.019420000	8	-1.559093000	-1.104579000	0.006456000
8	-0.234200000	1.232997000	1.385566000	8	1.127134000	-2.420516000	0.994634000
8	-2.667987000	-0.458531000	0.566205000	8	2.369709000	1.723331000	-0.595154000
6	2.847767000	-1.737618000	-1.512242000	6	-3.469287000	0.620188000	-1.224673000
1	2.830558000	-2.196539000	-0.524374000	1	-4.406294000	0.946416000	-1.690231000
1	3.729015000	-2.121210000	-2.038497000	1	-3.650613000	0.519297000	-0.154088000
6	2.296198000	2.506312000	1.278016000	6	-0.488586000	-3.490525000	-1.140737000
1	3.081479000	3.209156000	1.579826000	1	-0.463211000	-4.495895000	-1.576331000
1	2.198535000	1.757947000	2.065149000	1	-0.656212000	-3.599492000	-0.068694000
6	-2.736192000	2.421272000	0.715394000	6	3.351683000	-0.673574000	0.635771000
1	-2.825983000	1.723222000	1.548063000	1	4.242481000	-0.172722000	0.248822000
1	-3.588054000	3.108767000	0.765758000	1	3.700510000	-1.398467000	1.379771000
6	-2.215252000	-1.942758000	-1.878292000	6	0.333194000	3.464364000	0.585174000
1	-2.249251000	-2.335118000	-0.863736000	1	-0.285736000	3.999928000	1.313079000
1	-2.970622000	-2.469416000	-2.473157000	1	1.059350000	4.193703000	0.213943000
6	0.325544000	-2.072405000	-1.723425000	6	-1.647354000	2.194720000	-0.380234000
6	-0.845699000	-2.186983000	-2.493770000	6	-0.528987000	3.022330000	-0.586441000
6	-0.710865000	-2.441472000	-3.865411000	6	-0.229936000	3.409850000	-1.894885000
1	-1.605769000	-2.558328000	-4.471685000	1	0.631311000	4.047217000	-2.075235000
6	0.546721000	-2.548621000	-4.459577000	6	-1.008513000	2.970949000	-2.969487000
6	1.694195000	-2.358386000	-3.687338000	6	-2.067859000	2.092282000	-2.745590000
1	2.674402000	-2.397727000	-4.156352000	1	-2.628484000	1.692077000	-3.586036000
6	1.604558000	-2.101211000	-2.314309000	6	-2.391730000	1.672214000	-1.450189000
6	0.539452000	-2.989915000	0.463851000	6	-3.010446000	2.729916000	1.477329000
1	1.023853000	-2.572543000	1.348943000	1	-3.891640000	2.747830000	0.818229000
1	1.263247000	-3.641164000	-0.044542000	1	-2.630727000	3.761278000	1.545850000
6	-0.695599000	-3.796735000	0.853619000	6	-3.378882000	2.194855000	2.852919000
1	-1.126584000	-4.255732000	-0.044574000	1	-2.471115000	2.142878000	3.464978000
1	-1.444119000	-3.104964000	1.252067000	1	-3.737646000	1.165000000	2.742180000
6	-0.360002000	-4.874359000	1.890211000	6	-4.440318000	3.059814000	3.540198000
1	-1.247779000	-5.454272000	2.162327000	1	-4.696607000	2.657450000	4.525217000
1	0.039363000	-4.425436000	2.807750000	1	-5.362246000	3.104214000	2.948506000
1	0.391168000	-5.576488000	1.508919000	1	-4.086342000	4.087752000	3.682081000
6	2.755418000	0.410270000	-0.121798000	6	-2.107051000	-1.527595000	-1.184197000
6	2.969658000	-0.226640000	-1.357638000	6	-3.071856000	-0.723206000	-1.817224000
6	3.228122000	0.569118000	-2.478575000	6	-3.597669000	-1.155120000	-3.041121000
1	3.382613000	0.089831000	-3.441274000	1	-4.348928000	-0.547188000	-3.539608000
6	3.252099000	1.960592000	-2.382126000	6	-3.167108000	-2.346726000	-3.627185000
6	2.968750000	2.573019000	-1.161367000	6	-2.182192000	-3.111170000	-2.999193000
1	2.918113000	3.656339000	-1.098613000	1	-1.829588000	-4.028094000	-3.465388000
6	2.702010000	1.813269000	-0.017788000	6	-1.631594000	-2.712422000	-1.774893000
6	3.831111000	-0.602048000	1.711328000	6	-2.227147000	-1.567076000	1.190697000
1	4.318671000	0.356790000	1.944503000	1	-2.237128000	-2.668323000	1.205221000
1	4.513866000	-1.170009000	1.060112000	1	-3.276125000	-1.231246000	1.180282000
6	3.533631000	-1.375750000	2.986958000	6	-1.485810000	-1.010628000	2.392758000
1	2.848535000	-0.785464000	3.606650000	1	-1.470527000	0.076751000	2.308766000
1	3.004403000	-2.299563000	2.724301000	1	-0.447301000	-1.338019000	2.331514000
6	4.810823000	-1.700602000	3.769193000	6	-2.119405000	-1.447933000	3.715226000
1	4.580215000	-2.253615000	4.685058000	1	-1.566832000	-1.033116000	4.565182000
1	5.344086000	-0.787049000	4.057121000	1	-2.120485000	-2.539911000	3.823631000
1	5.497535000	-2.313286000	3.173529000	1	-3.159228000	-1.107640000	3.799933000
6	-0.235414000	2.584580000	1.128395000	6	1.558466000	-2.216578000	-0.304816000
6	0.991467000	3.269460000	1.108967000	6	0.848578000	-2.798254000	-1.368012000
6	0.976783000	4.644879000	0.845738000	6	1.366086000	-2.658715000	-2.660785000
1	1.914860000	5.194747000	0.837461000	1	0.825796000	-3.095688000	-3.496237000
6	-0.222689000	5.312405000	0.589455000	6	2.529604000	-1.924841000	-2.890062000
6	-1.424569000	4.601221000	0.570713000	6	3.166923000	-1.281283000	-1.825870000
1	-2.355235000	5.116895000	0.346369000	1	4.032545000	-0.652729000	-2.013414000
6	-1.450448000	3.226076000	0.833400000	6	2.688258000	-1.407303000	-0.519280000
6	-0.420133000	0.886816000	2.764794000	6	1.630541000	-3.621069000	1.596200000
1	-1.417635000	1.209057000	3.102135000	1	2.726068000	-3.560861000	1.689917000
1	0.321049000	1.415341000	3.385147000	1	1.402852000	-4.484537000	0.952874000
6	-0.262010000	-0.616642000	2.883369000	6	0.977095000	-3.781523000	2.960727000
1	0.737060000	-0.867405000	2.523443000	1	1.181140000	-2.884784000	3.556945000
1	-0.971344000	-1.075298000	2.192207000	1	-0.109863000	-3.822570000	2.824489000
6	-0.473062000	-1.121505000	4.311992000	6	1.472258000	-5.034225000	3.690578000
1	-0.351623000	-2.209052000	4.363017000	1	0.988506000	-5.136468000	4.667005000
1	-1.479146000	-0.885261000	4.679384000	1	2.555177000	-4.996307000	3.857670000
1	0.246849000	-0.675404000	5.009449000	1	1.256151000	-5.942087000	3.115161000
6	-2.665354000	0.243994000	-0.628032000	6	1.967107000	1.479417000	0.704690000
6	-2.784853000	1.646563000	-0.594722000	6	2.457085000	0.328706000	1.351206000
6	-2.879440000	2.335205000	-1.807578000	6	2.081908000	0.106458000	2.680741000
1	-2.957943000	3.418988000	-1.794338000	1	2.457761000	-0.775938000	3.190703000
6	-2.836071000	1.653626000	-3.024239000	6	1.226262000	0.981608000	3.345948000

6	-2.647151000	0.271705000	-3.035255000	6	0.688240000	2.068047000	2.659086000
1	-2.544508000	-0.250038000	-3.982107000	1	-0.033624000	2.714332000	3.150667000
6	-2.540770000	-0.453536000	-1.843161000	6	1.027071000	2.327103000	1.326353000
6	-3.982383000	-0.839424000	0.998227000	6	3.279851000	2.812355000	-0.799801000
1	-4.401697000	-1.581382000	0.300620000	1	3.011122000	3.665102000	-0.162675000
1	-4.645610000	0.038909000	0.984587000	1	3.136587000	3.110066000	-1.844262000
6	-3.884040000	-1.409889000	2.405165000	6	4.737523000	2.432281000	-0.547921000
1	-3.426257000	-0.655311000	3.055500000	1	4.999527000	1.588302000	-1.196541000
1	-3.203056000	-2.268334000	2.395909000	1	4.841163000	2.090297000	0.488953000
6	-5.253211000	-1.827465000	2.951650000	6	5.680571000	3.612504000	-0.808241000
1	-5.164237000	-2.234536000	3.963732000	1	6.723747000	3.331092000	-0.633153000
1	-5.715011000	-2.597303000	2.322390000	1	5.449239000	4.458189000	-0.149755000
1	-5.941669000	-0.975371000	2.994335000	1	5.599916000	3.964628000	-1.843604000
7	0.204031000	1.605652000	-2.564553000	7	0.667212000	0.458683000	-2.794798000
8	0.130721000	1.055633000	-1.547497000	8	0.272971000	0.189387000	-1.740496000
1	3.455319000	2.564728000	-3.261093000	1	-0.764219000	3.282542000	-3.980450000
1	-2.913274000	2.200440000	-3.959092000	1	2.915665000	-1.818052000	-3.899248000
1	0.632360000	-2.758350000	-5.521724000	1	-3.588318000	-2.671841000	-4.574032000
1	-0.219556000	6.380497000	0.392397000	1	0.945236000	0.793678000	4.378097000
NO@1,2-alternate				NO@1,3-alternate			
8	0.176768000	-1.550807000	0.818480000	8	-2.758671000	-0.000562000	-1.255458000
8	2.918294000	-0.044333000	0.464378000	8	0.000145000	2.605850000	1.383196000
6	1.582825000	-0.323989000	2.941165000	8	2.757053000	0.000679000	-1.258066000
1	2.165948000	-1.066682000	2.401218000	8	0.001352000	-2.606035000	1.382891000
1	2.017048000	-0.229843000	3.943502000	6	-2.549114000	-2.546669000	0.060995000
6	-2.549961000	-2.760849000	1.085667000	1	-3.358277000	-2.645178000	-0.670007000
1	-3.625152000	-2.629548000	1.256401000	1	-2.686537000	-3.359246000	0.783239000
1	-2.355476000	-3.810934000	1.338898000	6	-2.550346000	2.545513000	0.061142000
6	-0.500342000	-1.446212000	2.009585000	1	-3.359485000	2.643651000	-0.669934000
6	0.150438000	-0.804898000	3.085220000	1	-2.688245000	3.358002000	0.783397000
6	-0.547064000	-0.613613000	4.280190000	6	2.549299000	2.546656000	0.058881000
1	-0.051740000	-0.120971000	5.112774000	1	2.687345000	3.359150000	0.781102000
6	-1.872399000	-1.034062000	4.406950000	1	3.357774000	2.645332000	-0.672862000
6	-2.492933000	-1.680623000	3.339114000	6	2.550523000	-2.545526000	0.058436000
1	-3.521307000	-2.018676000	3.444720000	1	2.689051000	-3.358098000	0.780478000
6	-1.822873000	-1.916686000	2.129165000	1	3.358983000	-2.643637000	-0.673399000
6	2.342298000	1.102544000	0.969456000	6	-2.717308000	-0.000613000	0.127930000
6	2.333707000	2.309589000	0.241428000	6	-2.672442000	-1.228304000	0.810305000
6	1.819988000	3.451761000	0.864982000	6	-2.699013000	-1.205217000	2.208302000
1	1.825407000	4.393542000	0.321497000	1	-2.675570000	-2.146383000	2.748949000
6	1.255879000	3.393770000	2.139179000	6	-2.734973000	-0.000702000	2.908852000
6	1.170141000	2.166205000	2.790792000	6	-2.699663000	1.203880000	2.208379000
1	0.676247000	2.095561000	3.756126000	1	-2.676730000	2.145027000	2.749083000
6	1.705143000	1.007068000	2.218715000	6	-2.673095000	1.227057000	0.810389000
6	0.888643000	-2.774105000	0.576550000	6	-4.075578000	-0.000960000	-1.816594000
1	0.203683000	-3.628773000	0.673941000	1	-4.633095000	0.884859000	-1.474432000
1	1.686221000	-2.892752000	1.325675000	1	-4.632528000	-0.887160000	-1.474502000
6	1.464221000	-2.701870000	-0.827666000	6	-3.934947000	-0.000831000	-3.331230000
1	2.098305000	-1.814382000	-0.891089000	1	-3.346486000	0.876054000	-3.624647000
1	0.642073000	-2.554341000	-1.530585000	1	-3.346031000	-0.877364000	-3.624781000
6	2.245612000	-3.966940000	-1.191338000	6	-5.294381000	-0.001137000	-4.037580000
1	2.661260000	-3.888913000	-2.201248000	1	-5.172266000	-0.001049000	-5.125330000
1	1.602475000	-4.855058000	-1.164549000	1	-5.883937000	0.883630000	-3.769052000
1	3.080731000	-4.141042000	-0.500875000	1	-5.883487000	-0.886231000	-3.769145000
6	4.309603000	-0.014402000	0.101666000	6	-0.000563000	2.700596000	0.002575000
1	4.792065000	0.861222000	0.556487000	6	-1.231638000	2.724713000	-0.678808000
1	4.384667000	0.069979000	-0.987722000	6	-1.209226000	2.882587000	-2.067746000
6	4.981847000	-1.302945000	0.563211000	1	-2.148777000	2.895306000	-2.612821000
1	5.952655000	-1.369993000	0.053536000	6	-0.001876000	2.982491000	-2.760842000
1	4.381940000	-2.147783000	0.204629000	6	1.206147000	2.883077000	-2.068843000
6	5.185689000	-1.393568000	2.078571000	1	2.145199000	2.896218000	-2.614766000
1	5.669030000	-2.336117000	2.356551000	6	1.229876000	2.725228000	-0.679929000
1	4.233579000	-1.335250000	2.611156000	6	-0.000057000	3.871711000	2.056466000
1	5.818329000	-0.573121000	2.437910000	1	-0.886221000	4.454037000	1.760301000
8	-0.086058000	1.867573000	-1.260535000	1	0.885179000	4.454894000	1.759198000
8	-2.545426000	-0.192816000	-0.420329000	6	0.001000000	3.623098000	3.557550000
6	-1.407722000	0.063073000	-3.029749000	1	-0.874470000	3.017559000	3.814386000
1	-1.893141000	0.859659000	-2.471073000	1	0.877267000	3.018228000	3.813239000
1	-1.796978000	0.074239000	-4.054637000	6	0.001008000	4.932758000	4.353113000
6	2.780464000	2.385934000	-1.208062000	1	-0.884285000	5.538310000	4.125218000
1	3.862738000	2.240955000	-1.292770000	1	0.885603000	5.538936000	4.124180000
1	2.602320000	3.410774000	-1.555256000	6	2.717483000	0.000589000	0.125354000
6	0.708569000	1.207818000	-2.173730000	6	2.673468000	1.228209000	0.807915000
6	0.095632000	0.318949000	-3.074913000	6	2.701737000	1.204964000	2.205874000
6	0.905285000	-0.338151000	-4.011031000	1	2.678981000	2.146067000	2.746664000

1	0.449687000	-1.014086000	-4.728084000	6	2.738520000	0.000362000	2.906239000
6	2.282888000	-0.134905000	-4.039264000	6	2.702349000	-1.204144000	2.205676000
6	2.872200000	0.732581000	-3.118267000	1	2.680069000	-2.145350000	2.746308000
1	3.947622000	0.891732000	-3.143350000	6	2.674097000	-1.227163000	0.807717000
6	2.103159000	1.415766000	-2.169555000	6	4.073159000	0.001270000	-1.821057000
6	-2.194067000	-1.360838000	-1.055236000	1	4.631298000	-0.884447000	-1.479646000
6	-2.247647000	-2.606446000	-0.394135000	1	4.630454000	0.887569000	-1.479782000
6	-2.002676000	-3.766075000	-1.140288000	6	3.930415000	0.001090000	-3.335495000
1	-2.055558000	-4.731090000	-0.641785000	1	3.341813000	-0.875965000	-3.628109000
6	-1.682803000	-3.707347000	-2.496059000	1	3.340823000	0.877441000	-3.628220000
6	-1.527896000	-2.461985000	-3.098878000	6	5.288872000	0.001806000	-4.043723000
1	-1.230720000	-2.404141000	-4.141584000	1	5.879083000	-0.882761000	-3.775976000
6	-1.737256000	-1.274401000	-2.385318000	1	5.878065000	0.887099000	-3.776136000
6	-0.496904000	3.182254000	-1.654709000	1	5.165254000	0.001635000	-5.131303000
1	0.377316000	3.845973000	-1.730592000	6	0.000705000	-2.700615000	0.002260000
1	-0.967788000	3.141539000	-2.649429000	6	1.231122000	-2.724600000	-0.680302000
6	-1.472713000	3.698882000	-0.611669000	6	1.207384000	-2.882303000	-2.069238000
1	-2.330186000	3.021902000	-0.585183000	1	2.146416000	-2.894965000	-2.615207000
1	-0.989705000	3.635462000	0.368257000	6	-0.000622000	-2.982169000	-2.761193000
6	-1.926405000	5.131866000	-0.904219000	6	-1.207987000	-2.882882000	-2.068030000
1	-2.637950000	5.479909000	-0.148438000	1	-2.147560000	-2.895954000	-2.613057000
1	-1.078024000	5.826967000	-0.905815000	6	-1.230390000	-2.725197000	-0.679076000
1	-2.418222000	5.205642000	-1.881731000	6	0.002172000	-3.871980000	2.056005000
6	-3.865223000	-0.139982000	0.158246000	1	-0.883457000	-4.455036000	1.759660000
1	-4.490928000	-0.919398000	-0.297322000	1	0.887944000	-4.454360000	1.758774000
1	-3.790741000	-0.330465000	1.233986000	6	0.002831000	-3.623551000	3.557120000
6	-4.486996000	1.230874000	-0.071728000	1	-0.873186000	-3.018784000	3.813916000
1	-5.435269000	1.247362000	0.482914000	1	0.878552000	-3.017970000	3.812998000
1	-3.844861000	1.985992000	0.391266000	6	0.003849000	-4.933307000	4.352522000
6	-4.736604000	1.569212000	-1.543524000	1	0.004334000	-4.738604000	5.429596000
1	-5.222823000	2.545092000	-1.646500000	1	0.888949000	-5.538739000	4.123561000
1	-3.798717000	1.600667000	-2.103177000	1	-0.880940000	-5.539549000	4.124506000
1	-5.381095000	0.819208000	-2.017452000	8	-0.000936000	0.000091000	-1.303530000
7	-2.369924000	1.656717000	3.041347000	7	-0.001175000	0.000148000	-2.460724000
8	-1.853896000	1.513459000	2.014273000	1	0.001705000	4.737923000	5.430163000
1	0.854820000	4.290754000	2.602109000	1	2.761292000	0.000279000	3.992174000
1	-1.520956000	-4.618823000	-3.063339000	1	-2.756435000	-0.000746000	3.994814000
1	-2.415240000	-0.865087000	5.331927000	1	-0.001133000	-3.094718000	-3.841104000
1	2.895957000	-0.648026000	-4.774527000	1	-0.002389000	3.095168000	-3.840740000

Coordinates of NO ⁺ @3 complexes							
NO ⁺ @Cone				NO ⁺ @Partial Cone			
8	-0.466180000	1.374087000	1.735230000	8	1.922024000	-2.074492000	0.923115000
7	-0.178184000	0.443227000	1.195602000	8	1.531086000	1.036269000	0.154858000
8	0.390174000	-1.999618000	0.114125000	8	-1.226172000	2.464016000	1.024403000
8	-2.523290000	-0.988024000	-0.938467000	8	-2.354208000	-1.615714000	-0.916911000
8	-0.266463000	1.403831000	-1.065611000	6	3.556258000	-0.630567000	-0.974971000
8	2.671410000	0.559934000	-0.731520000	1	4.510193000	-0.972216000	-1.389482000
6	-2.078658000	-2.589059000	1.426108000	1	3.649743000	-0.625132000	0.111650000
1	-2.021597000	-2.923227000	0.391096000	6	0.657835000	3.548249000	-0.882178000
1	-2.803483000	-3.224834000	1.945320000	1	0.661949000	4.572898000	-1.267655000
6	-3.051932000	1.864248000	-0.917298000	1	0.718226000	3.602567000	0.205526000
1	-4.042879000	2.300987000	-1.079448000	6	-3.367132000	0.714227000	0.379430000
1	-2.818434000	1.247356000	-1.786494000	1	-4.254507000	0.290916000	-0.096208000
6	1.803598000	3.306370000	-0.552910000	1	-3.716787000	1.441403000	1.118054000
1	2.091831000	2.776909000	-1.462018000	6	-0.461708000	-3.474671000	0.286250000
1	2.400222000	4.222806000	-0.506223000	1	0.124047000	-4.058511000	1.001862000
6	2.779950000	-1.278577000	1.509141000	1	-1.152949000	-4.175157000	-0.190383000
1	2.850869000	-1.529168000	0.452424000	6	1.632013000	-2.207223000	-0.412282000
1	3.726697000	-1.546869000	1.991038000	6	0.462870000	-2.914384000	-0.779613000
6	0.439288000	-2.261503000	1.461826000	6	0.176840000	-3.074357000	-2.143850000
6	1.641408000	-2.042989000	2.163955000	1	-0.704612000	-3.636081000	-2.435208000
6	1.701741000	-2.438737000	3.506421000	6	0.994748000	-2.508750000	-3.116581000
1	2.633701000	-2.323010000	4.053217000	6	2.097788000	-1.733807000	-2.727824000
6	0.586264000	-2.981757000	4.146236000	1	2.706911000	-1.245844000	-3.483227000
6	-0.631867000	-3.070848000	3.466375000	6	2.437363000	-1.581223000	-1.372449000
1	-1.515136000	-3.433577000	3.985234000	6	2.893425000	-3.008514000	1.446970000
6	-0.730893000	-2.691333000	2.124576000	1	3.820478000	-2.942269000	0.860235000
6	0.389749000	-3.171293000	-0.739749000	1	2.506334000	-4.032398000	1.346089000
1	-0.218258000	-2.902201000	-1.606207000	6	3.139616000	-2.653252000	2.903827000
1	-0.101622000	-4.004719000	-0.222439000	1	2.182715000	-2.682535000	3.437967000
6	1.798329000	-3.568086000	-1.164157000	1	3.494516000	-1.616890000	2.955959000

1	2.38322000	-3.827701000	-0.273371000	6	4.150399000	-3.599269000	3.560797000
1	2.280168000	-2.698970000	-1.626208000	1	4.315579000	-3.325649000	4.606659000
6	1.778002000	-4.746219000	-2.144526000	1	5.119804000	-3.564821000	3.051050000
1	2.792068000	-5.022717000	-2.447031000	1	3.798150000	-4.636638000	3.540302000
1	1.216251000	-4.496492000	-3.052173000	6	2.218454000	1.536075000	-0.917676000
1	1.312814000	-5.631132000	-1.695872000	6	3.265450000	0.768195000	-1.488667000
6	-2.729865000	-0.383121000	0.274867000	6	3.967119000	1.309216000	-2.568431000
6	-2.564862000	-1.145067000	1.460877000	1	4.779189000	0.741879000	-3.014376000
6	-2.832524000	-0.529999000	2.692720000	6	3.640461000	2.570087000	-3.075647000
1	-2.714510000	-1.104106000	3.606493000	6	2.585604000	3.302483000	-2.523943000
6	-3.219388000	0.804330000	2.754532000	1	2.330295000	4.274918000	-2.935511000
6	-3.313346000	1.558161000	1.575642000	6	1.855389000	2.802577000	-1.443223000
1	-3.557617000	2.615069000	1.632638000	6	2.057562000	1.367565000	1.470492000
6	-3.070440000	0.984017000	0.325655000	1	2.081489000	2.460220000	1.575205000
6	-3.715467000	-1.510839000	-1.571258000	1	3.088768000	0.997319000	1.540740000
1	-4.446036000	-0.699572000	-1.697240000	6	1.162777000	0.726641000	2.510579000
1	-4.165022000	-2.273438000	-0.919504000	1	1.139554000	-0.348920000	2.327175000
6	-3.312938000	-2.100989000	-2.912459000	1	0.147304000	1.098864000	2.365731000
1	-2.838753000	-1.316320000	-3.514109000	6	1.648852000	1.022522000	3.932223000
1	-2.551434000	-2.871712000	-2.741791000	1	0.989894000	0.550433000	4.667351000
6	-4.513467000	-2.693941000	-3.658204000	1	1.659957000	2.098614000	4.142154000
1	-4.204838000	-3.112610000	-4.620185000	1	2.661888000	0.639651000	4.103462000
1	-5.275776000	-1.932266000	-3.856375000	6	-1.477127000	2.274617000	-0.311964000
1	-4.984533000	-3.497544000	-3.081312000	6	-0.630691000	2.841057000	-1.273439000
6	-0.655561000	2.701787000	-0.823996000	6	-0.917774000	2.611636000	-2.630402000
6	-2.034555000	2.986345000	-0.772571000	1	-0.264365000	3.035351000	-3.387559000
6	-2.420669000	4.308886000	-0.531289000	6	-2.035325000	1.855883000	-3.018351000
1	-3.477335000	4.560416000	-0.501391000	6	-2.826257000	1.253539000	-2.046509000
6	-1.462378000	5.306561000	-0.332129000	1	-3.655825000	0.617980000	-2.336626000
6	-0.100769000	4.992476000	-0.351795000	6	-2.549174000	1.428039000	-0.681627000
1	0.635707000	5.773070000	-0.181772000	6	-1.757367000	3.682737000	1.592746000
6	0.329003000	3.682899000	-0.592989000	1	-2.853844000	3.673077000	1.515897000
6	-0.013465000	1.094815000	-2.468636000	1	-1.389205000	4.545798000	1.020313000
1	0.850907000	1.680911000	-2.802238000	6	-1.306419000	3.753597000	3.042211000
1	-0.888689000	1.413795000	-3.049377000	1	-1.653675000	2.852894000	3.561801000
6	0.235596000	-0.389285000	-2.616888000	1	-0.2110354000	3.726428000	3.069068000
1	-0.641989000	-0.913026000	-2.237652000	6	-1.828528000	5.012245000	3.743264000
1	1.076543000	-0.657550000	-1.977141000	1	-1.491957000	5.045510000	4.783263000
6	0.512369000	-0.770791000	-4.074094000	1	-2.923851000	5.041740000	3.747316000
1	0.692546000	-1.847063000	-4.162213000	1	-1.470968000	5.922437000	3.248822000
1	1.397156000	-0.256892000	-4.466729000	6	-2.076838000	-1.487002000	0.434243000
1	-0.333195000	-0.524083000	-4.726772000	6	-2.593686000	-0.371011000	1.117076000
6	2.458659000	1.075395000	0.520031000	6	-2.353005000	-0.265795000	2.491010000
6	2.109457000	2.433638000	0.654367000	1	-2.756118000	0.583684000	3.034102000
6	1.925243000	2.946744000	1.940027000	6	-1.595341000	-1.224189000	3.161928000
1	1.634578000	3.987246000	2.055956000	6	-1.004809000	-2.263464000	2.444662000
6	2.095680000	2.141412000	3.076349000	1	-0.350797000	-2.966529000	2.951958000
6	2.393626000	0.792555000	2.927949000	6	-1.212445000	-2.401193000	1.067833000
1	2.475966000	0.159490000	3.804928000	6	-3.291913000	-2.651798000	-1.289035000
6	2.549797000	0.222697000	1.653292000	1	-3.050305000	-3.582216000	-0.761201000
6	4.054145000	0.554433000	-1.161352000	1	-3.120033000	-2.811656000	-2.358184000
1	4.647746000	-0.062355000	-0.472059000	6	-4.747328000	-2.277811000	-1.027103000
1	4.446262000	1.580433000	-1.122134000	1	-4.993283000	-1.371310000	-1.592617000
6	4.102824000	0.001383000	-2.575478000	1	-4.869787000	-2.042930000	0.036918000
1	3.468995000	0.624824000	-3.217204000	6	-5.694377000	-3.416518000	-1.424797000
1	3.661413000	-1.001963000	-2.576727000	1	-6.736435000	-3.138073000	-1.244363000
6	5.534283000	-0.044832000	-3.120890000	1	-5.488471000	-4.324533000	-0.847007000
1	5.548767000	-0.443485000	-4.139144000	1	-5.596025000	-3.665219000	-2.487695000
1	6.175814000	-0.684213000	-2.504248000	7	0.337530000	0.263691000	-2.230297000
1	5.983772000	0.954006000	-3.148519000	8	-0.207055000	-0.139404000	-1.347676000
1	-1.777446000	6.329870000	-0.153342000	1	4.203877000	2.979149000	-3.908519000
1	-3.429777000	1.268793000	3.712780000	1	-2.257405000	1.717988000	-4.071688000
1	1.973963000	2.568549000	4.066732000	1	0.768140000	-2.640003000	-4.169798000
1	0.656661000	-3.305308000	5.179889000	1	-1.427030000	-1.135749000	4.230583000
NO*@I.2-alternate				NO*@I.3-alternate			
8	0.204143000	-2.066478000	0.370948000	8	-0.001206000	2.787410000	-1.235593000
8	2.544817000	-0.363691000	-0.653850000	8	2.920742000	0.001094000	1.338258000
6	2.467852000	-1.396623000	1.987576000	8	0.001297000	-2.786903000	-1.236133000
1	2.621614000	-1.977146000	1.080685000	8	-2.921046000	-0.001434000	1.338093000
1	3.217117000	-1.702369000	2.724726000	6	-2.555538000	2.526733000	0.066479000
6	-2.486405000	-2.627994000	1.404550000	1	-2.620798000	3.365545000	-0.631681000
1	-3.409396000	-2.455083000	1.970363000	1	-3.369663000	2.646696000	0.786509000
1	-2.385077000	-3.719785000	1.369301000	6	2.553320000	2.528931000	0.066640000
6	-0.012366000	-1.954512000	1.711453000	1	2.617916000	3.367776000	-0.631536000
6	1.082699000	-1.640923000	2.559814000	1	3.367306000	2.649571000	0.786718000

6	0.834869000	-1.437371000	3.920687000	6	2.555495000	-2.526885000	0.066189000
1	1.661494000	-1.211024000	4.586453000	1	3.369578000	-2.647018000	0.786238000
6	-0.461100000	-1.504561000	4.429287000	1	2.620769000	-3.365544000	-0.632150000
6	-1.529858000	-1.835194000	3.586668000	6	-2.553359000	-2.528972000	0.066033000
1	-2.531246000	-1.914681000	4.000685000	1	-3.367388000	-2.649685000	0.786048000
6	-1.328738000	-2.101082000	2.233013000	1	-2.617996000	-3.367698000	-0.632285000
6	2.603721000	0.561782000	0.345046000	6	-0.001168000	2.635958000	0.136473000
6	2.577513000	1.956647000	0.073490000	6	-1.235802000	2.552145000	0.822384000
6	2.658674000	2.835697000	1.153196000	6	-1.209866000	2.427951000	2.212660000
1	2.638632000	3.905062000	0.961553000	1	-2.147225000	2.354017000	2.752278000
6	2.755773000	2.376559000	2.472261000	6	-0.001128000	2.381476000	2.907478000
6	2.737587000	1.008866000	2.725077000	6	1.207603000	2.429018000	2.212741000
1	2.794322000	0.651299000	3.747953000	1	2.144992000	2.355911000	2.752417000
6	2.627942000	0.085967000	1.679046000	6	1.233502000	2.553215000	0.822460000
6	0.486851000	-3.371632000	-0.179184000	6	-0.001905000	4.156760000	-1.705142000
1	-0.357826000	-4.045064000	0.018019000	1	0.883483000	4.676123000	-1.314362000
1	1.378449000	-3.788648000	0.309668000	1	-0.888074000	4.675073000	-1.314728000
6	0.700302000	-3.186096000	-1.671400000	6	-0.001630000	4.142311000	-3.224249000
1	1.516137000	-2.470717000	-1.812178000	1	0.877632000	3.587947000	-3.572650000
1	-0.200047000	-2.725149000	-2.090401000	1	-0.879834000	3.586424000	-3.572895000
6	1.003290000	-4.512321000	-2.374720000	6	-0.002754000	5.560719000	-3.805651000
1	1.153228000	-4.356831000	-3.447096000	1	-0.002465000	5.532654000	-4.898846000
1	0.179419000	-5.225476000	-2.256038000	1	0.881859000	6.123302000	-3.487061000
1	1.910695000	-4.981939000	-1.977514000	1	-0.888515000	6.121727000	-3.487481000
6	3.637689000	-0.485645000	-1.600408000	6	2.788430000	0.001134000	-0.028459000
1	4.184951000	0.459949000	-1.671251000	6	2.708641000	1.235629000	-0.712319000
1	3.152717000	-0.676648000	-2.560201000	6	2.653090000	1.213938000	-2.105347000
6	4.585006000	-1.621502000	-1.227974000	1	2.582267000	2.150179000	-2.648497000
1	5.188422000	-1.842913000	-2.118429000	6	2.643825000	0.001328000	-2.802595000
1	3.987684000	-2.520149000	-1.029575000	6	2.654179000	-1.211404000	-2.105552000
6	5.513028000	-1.311115000	-0.048451000	1	2.584190000	-2.147598000	-2.648889000
1	6.182701000	-2.152309000	0.154420000	6	2.709748000	-1.233313000	-0.712535000
1	4.955058000	-1.101887000	0.867719000	6	4.295600000	0.001577000	1.796764000
1	6.135061000	-0.434438000	-0.262183000	1	4.810446000	0.888242000	1.401159000
8	-0.277544000	2.271089000	-0.557735000	1	4.811036000	-0.884821000	1.401322000
8	-2.299265000	0.187369000	0.549771000	6	4.299106000	0.001689000	3.316050000
6	-2.345574000	1.043966000	-2.160810000	1	3.749395000	0.880239000	3.672602000
1	-2.550720000	1.707927000	-1.323580000	1	3.749512000	-0.876900000	3.672690000
1	-3.032947000	1.305424000	-2.972180000	6	5.725472000	0.001833000	3.877871000
6	2.461456000	2.528377000	-1.330706000	1	6.282941000	0.887125000	3.552086000
1	3.428849000	2.459417000	-1.840177000	1	6.283015000	-0.883506000	3.552346000
1	2.272184000	3.602613000	-1.226652000	6	0.001114000	-2.635969000	-1.360250000
6	0.066558000	1.812259000	-1.823442000	6	1.235702000	-2.552446000	0.822018000
6	-0.916277000	1.239918000	-2.643790000	6	1.209704000	-2.428821000	2.212356000
6	-0.541113000	0.819392000	-3.927314000	6	2.147030000	-2.355157000	2.752070000
1	-1.290537000	0.392723000	-4.587011000	6	0.000928000	-2.382624000	2.907103000
6	0.772009000	0.950311000	-4.371972000	6	-1.207770000	-2.429884000	2.212263000
6	1.739196000	1.491099000	-3.523229000	1	-2.145194000	-2.357025000	2.751916000
1	2.765823000	1.586475000	-3.866220000	6	-1.233596000	-2.553538000	0.821933000
6	1.405718000	1.921070000	-2.235607000	6	0.001709000	-4.156083000	-1.706146000
6	-2.546356000	-0.795469000	-0.400558000	1	-0.884052000	-4.675262000	-1.315963000
6	-2.655180000	-2.145562000	-0.023451000	1	0.887496000	-4.674870000	-1.315493000
6	-2.935533000	-3.084518000	-1.021369000	6	0.002091000	-4.141161000	-3.225251000
1	-3.036695000	-4.131682000	-0.749050000	1	-0.876653000	-3.586093000	-3.573835000
6	-3.074090000	-2.701347000	-2.355552000	1	0.880813000	-3.585783000	-3.573398000
6	-2.893325000	-1.366835000	-2.710229000	6	0.002495000	-5.559400000	-3.807078000
1	-2.982103000	-1.069928000	-3.750547000	1	-0.882656000	-6.121457000	-3.489058000
6	-2.605166000	-0.393975000	-1.744893000	1	0.887719000	-6.121118000	-3.488665000
6	-0.691605000	3.653419000	-0.513595000	1	0.002728000	-5.531011000	-4.900265000
1	0.096857000	4.285611000	-0.943736000	6	-2.788572000	-0.001209000	-0.028684000
1	-1.591924000	3.783135000	-1.130351000	6	-2.708538000	-1.235518000	-0.712709000
6	-0.960160000	4.037514000	0.932806000	6	-2.652690000	-1.213594000	-2.105747000
1	-1.725376000	3.366444000	1.340662000	1	-2.581757000	-2.149748000	-2.649037000
1	-0.046104000	3.875452000	1.515579000	6	-2.643411000	-0.000893000	-2.802820000
6	-1.420384000	5.494002000	1.057983000	6	-2.653804000	1.211671000	-2.105541000
1	-1.607760000	5.756907000	2.103001000	1	-2.583726000	2.147993000	-2.648653000
1	-0.662694000	6.184844000	0.671971000	6	-2.709661000	1.233293000	-0.712493000
1	-2.346341000	5.668681000	0.498917000	6	-4.295934000	-0.001901000	1.796397000
6	-3.308398000	0.511077000	1.533500000	1	-4.811297000	0.884561000	1.400995000
1	-3.847865000	-0.393593000	1.828817000	1	-4.810790000	-0.888495000	1.400626000
1	-2.744769000	0.863405000	2.405104000	6	-4.299659000	-0.002227000	3.315684000
6	-4.280595000	1.590262000	1.061126000	1	-3.750157000	0.876331000	3.672549000
1	-4.788857000	1.968013000	1.958481000	1	-3.749946000	-0.880807000	3.672170000
1	-3.704363000	2.430410000	0.656627000	6	-5.726097000	-0.002531000	3.877321000
6	-5.326353000	1.111145000	0.048184000	1	-5.712585000	-0.002815000	4.970792000

1	-6.028962000	1.915987000	-0.187466000	1	-6.283460000	-0.887823000	3.551356000
1	-4.871513000	0.779598000	-0.887608000	1	-6.283660000	0.882804000	3.551814000
1	-5.904435000	0.271808000	0.450937000	7	0.001332000	0.000313000	-0.498115000
8	-0.302973000	1.187839000	2.235423000	8	0.000355000	0.000232000	-1.612808000
7	-0.151827000	0.523971000	1.352560000	1	5.711802000	0.001999000	4.971339000
1	1.042406000	0.633247000	-5.374358000	1	0.000850000	-2.293138000	3.988910000
1	-3.304580000	-3.442539000	-3.114115000	1	-0.001122000	2.291507000	3.989244000
1	2.843414000	3.084599000	3.290281000	1	2.597043000	0.001395000	-3.887153000
1	-0.640694000	-1.326177000	5.484945000	1	-2.596455000	-0.000783000	-3.887371000