

ESI

The preferred conformation of the tetrafluoro-1,3-dithietane ···isopropylamine
complex revealed by rotational spectroscopy

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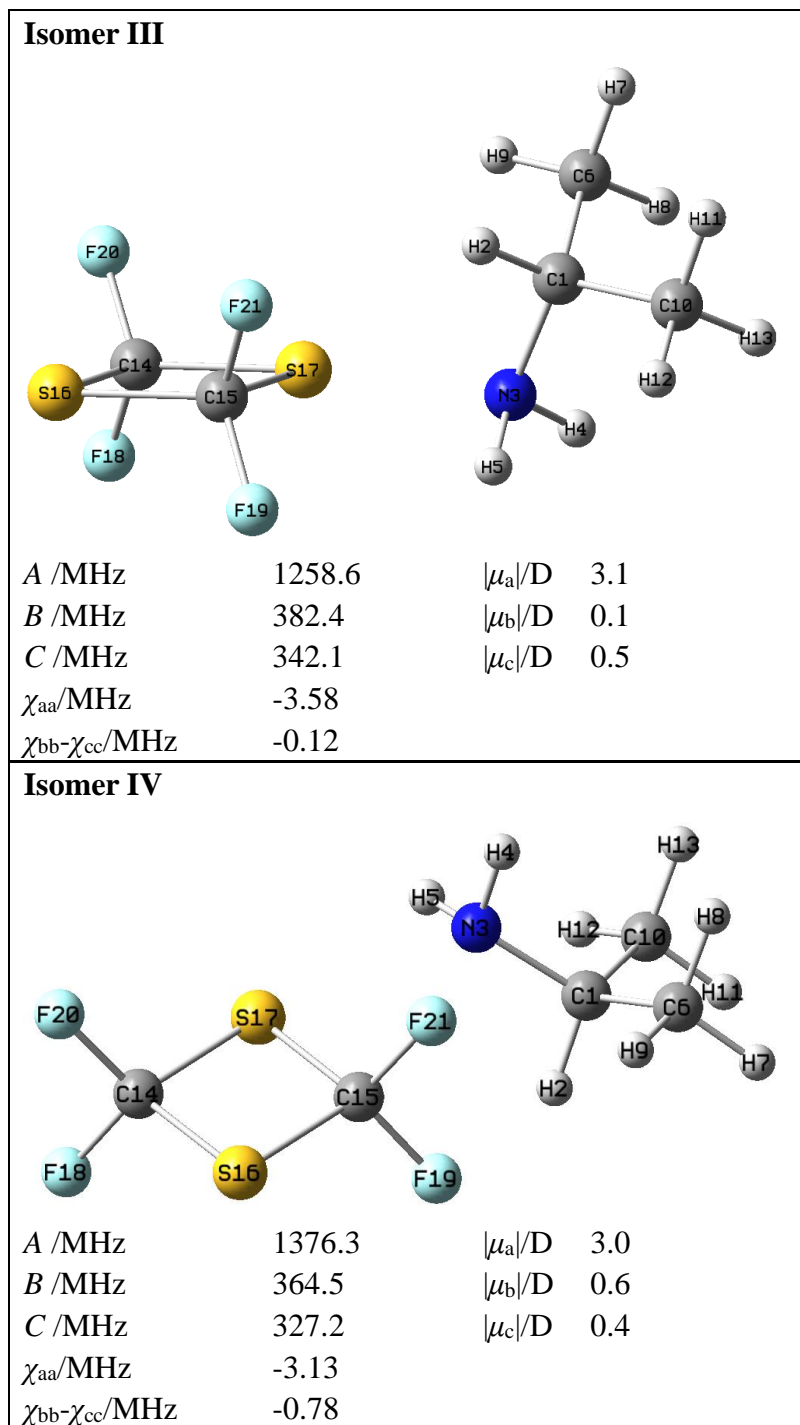
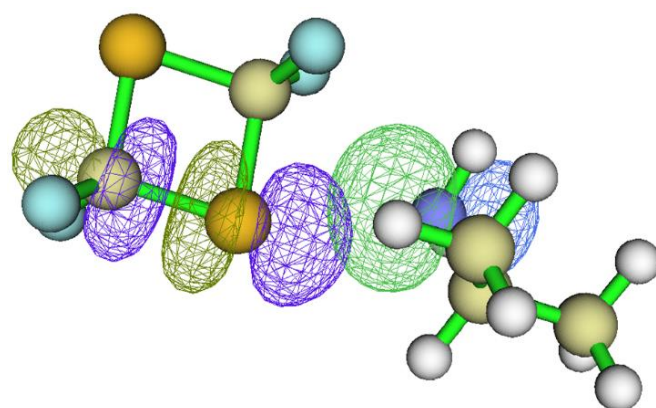
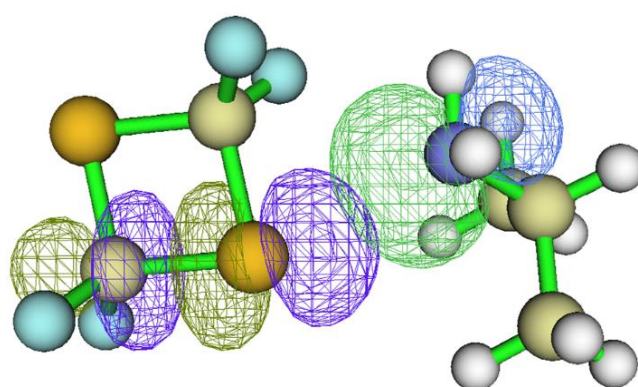


Fig. S1 B3LYP-D3(BJ)/6-311++G(d,p) calculated spectroscopic parameters of isomers **III** and **IV** of the $C_2S_2F_4$ -IPA complex.



Isomer I



Isomer II

Fig. S2 Overlap of the n donor orbital with the C-S anti-bonding orbital.

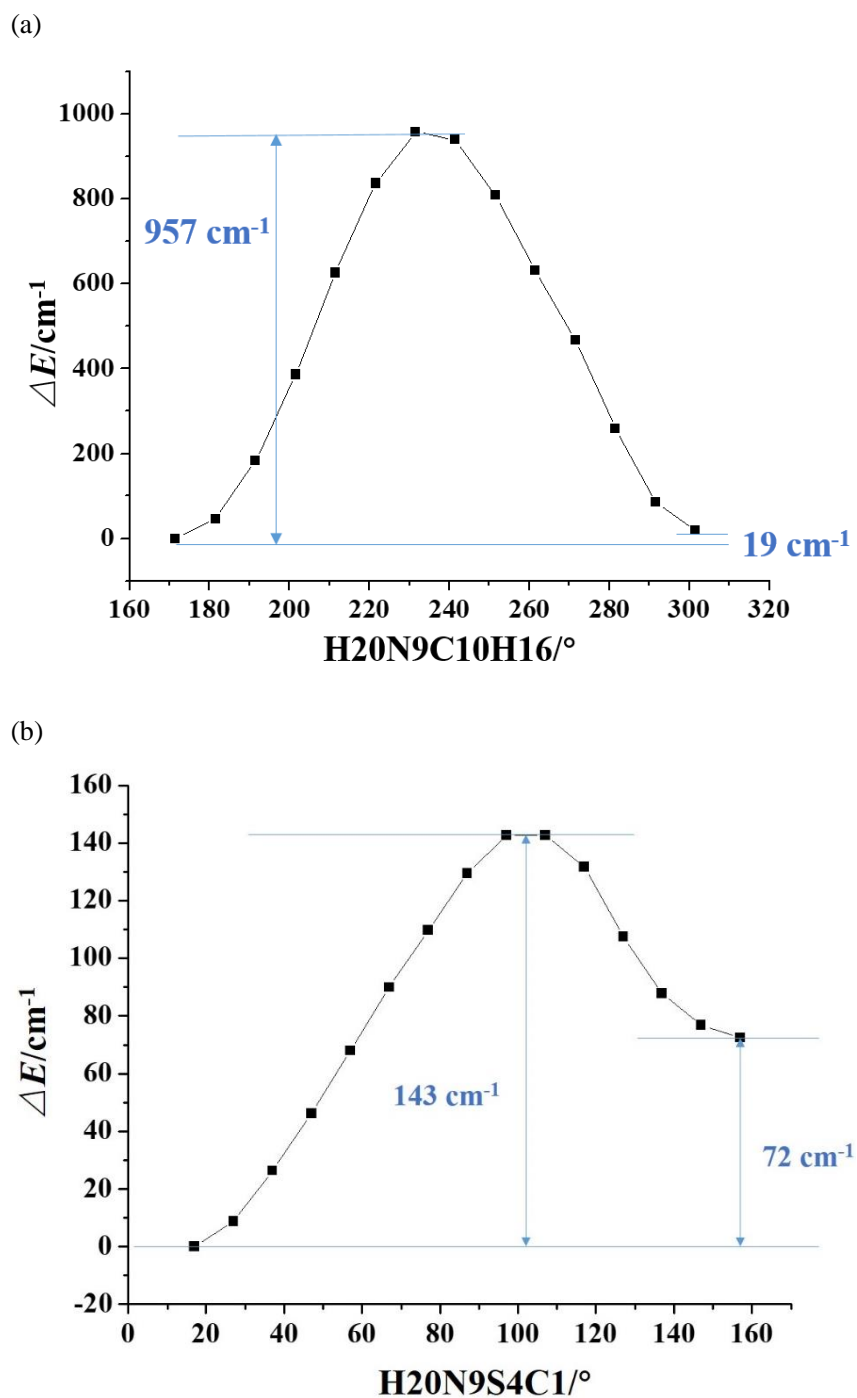
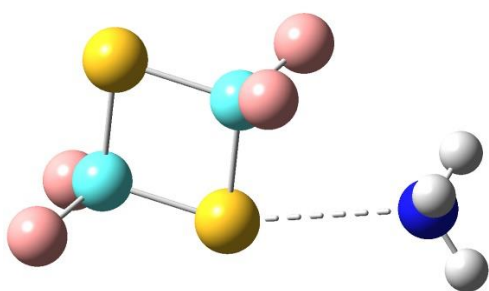
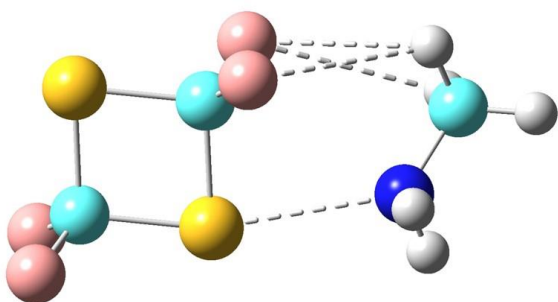


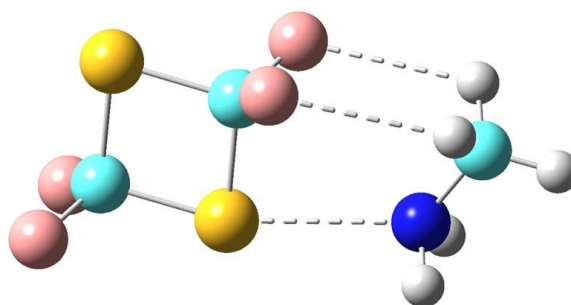
Fig. S3 The potential energy curves connecting conformational interconversion between (a) isomers I and II, and (b) isomers I and III.



a) The most stable isomer of the $C_2F_4S_2-NH_3$ complex.

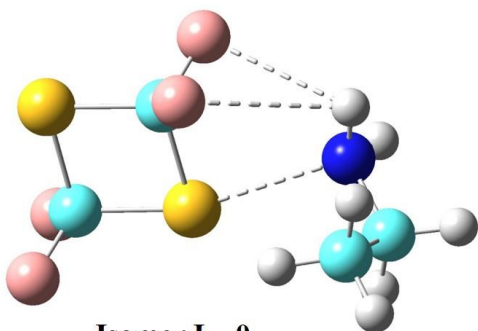


Isomer I 0

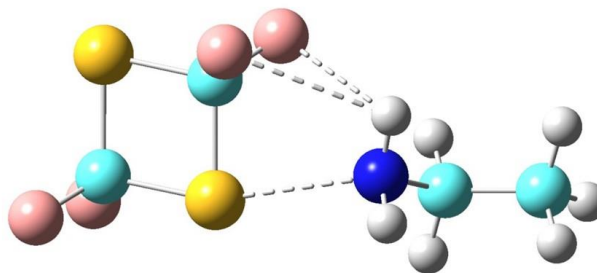


Isomer I +14 cm^{-1}

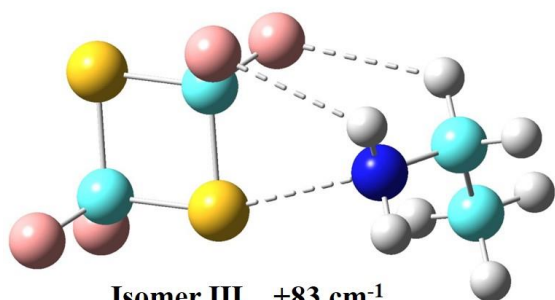
b) Two isomers of the $C_2F_4S_2-MA$ complex in a relative energy window of 300 cm^{-1} .



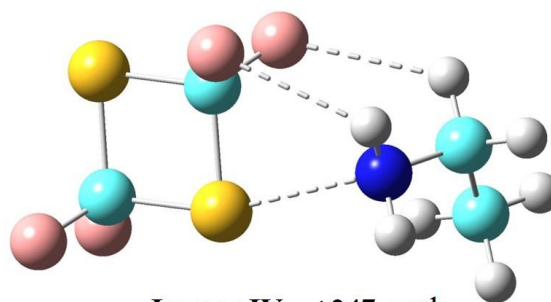
Isomer I 0



Isomer II +56 cm^{-1}



Isomer III +83 cm^{-1}



Isomer IV +247 cm^{-1}

c) Four isomers of the $C_2F_4S_2-EA$ complex in a relative energy window of 300 cm^{-1} .

Fig. S4 molecular sketch of the $C_2F_4S_2$ complexes with NH_3 , MA and EA.

Table S1. Experimental transitions frequencies of isomer I of the C₂F₄S₂-IPA complex.

$J'_{Ka'Kc'}$	F'	$J''_{Ka''Kc''}$	F''	$V_{obs.}/\text{MHz}$	$Obs.-calc./\text{MHz}$
8 0 8	9	7 0 7	8	5722.3801	0.0003
8 0 8	8	7 0 7	7	5722.3768	-0.0001
8 0 8	7	7 0 7	6	5722.3547	-0.0034
8 1 8	9	7 1 7	8	5646.3428	0.0008
8 1 8	8	7 1 7	7	5646.3229	0.0017
8 1 8	7	7 1 7	6	5646.3264	0.0025
8 1 7	9	7 1 6	8	5938.9012	0.0000
8 1 7	8	7 1 6	7	5938.8788	-0.0023
8 1 7	7	7 1 6	6	5938.8814	-0.0007
8 2 7	9	7 2 6	8	5802.5978	0.0016
8 2 7	8	7 2 6	7	5802.5350	0.0025
8 2 7	7	7 2 6	6	5802.5869	0.0002
8 2 6	9	7 2 5	8	5897.9775	-0.0004
8 2 6	8	7 2 5	7	5897.9071	-0.0019
8 2 6	7	7 2 5	6	5897.9682	-0.0004
9 0 9	9	8 0 8	8	6415.5167	-0.0033
9 0 9	8	8 0 8	7	6415.5015	-0.0033
9 0 9	10	8 0 8	9	6415.5225	0.0008
9 1 8	9	8 1 7	8	6670.8116	0.0034
9 1 8	8	8 1 7	7	6670.8040	-0.0025
9 1 8	10	8 1 7	9	6670.8211	-0.0008
9 1 9	9	8 1 8	8	6346.2104	0.0014
9 1 9	8	8 1 8	7	6346.2104	0.0010
9 1 9	10	8 1 8	9	6346.2210	-0.0030
9 2 7	9	8 2 6	8	6651.8023	-0.0011
9 2 7	8	8 2 6	7	6651.8451	0.0008
9 2 7	10	8 2 6	9	6651.8552	0.0016
9 2 8	9	8 2 7	8	6522.5714	0.0013
9 2 8	8	8 2 7	7	6522.6068	0.0008
9 2 8	10	8 2 7	9	6522.6170	0.0016
9 3 7	9	8 3 6	8	6560.3352	0.0066
9 3 7	8	8 3 6	7	6560.4257	0.0000
9 3 7	10	8 3 6	9	6560.4257	-0.0001
9 3 6	9	8 3 5	8	6572.2354	-0.0003
9 3 6	8	8 3 5	7	6572.3335	-0.0009
9 3 6	10	8 3 5	9	6572.3334	-0.0010
10 0 10	11	9 0 9	10	7105.0986	0.0011
10 0 10	10	9 0 9	9	7105.0925	-0.0038
10 0 10	9	9 0 9	8	7105.0817	-0.0023
10 1 10	11	9 1 9	10	7044.6002	0.0007
10 1 10	10	9 1 9	9	7044.5869	-0.0013
10 1 10	9	9 1 9	8	7044.5869	-0.0004

10	1	9	11	9	1	8	10	7398.3731	-0.0012
10	1	9	10	9	1	8	9	7398.3651	0.0001
10	1	9	9	9	1	8	8	7398.3574	-0.0042
10	2	9	10	9	2	8	9	7240.7934	0.0005
10	2	9	9	9	2	8	8	7240.8204	0.0030
10	2	9	11	9	2	8	10	7240.8275	0.0013
10	2	8	10	9	2	7	9	7407.2305	-0.0007
10	2	8	9	9	2	7	8	7407.2608	0.0009
10	2	8	11	9	2	7	10	7407.2716	0.0030
10	3	8	10	9	3	7	9	7290.9890	0.0006
10	3	8	9	9	3	7	8	7291.0603	0.0027
10	3	8	11	9	3	7	10	7291.0603	0.0001
10	3	7	10	9	3	6	9	7311.0909	-0.0015
10	3	7	9	9	3	6	8	7311.1663	0.0025
10	3	7	11	9	3	6	10	7311.1663	0.0000
10	4	7	10	9	4	6	9	7287.9518	-0.0010
10	4	7	9	9	4	6	8	7288.0823	0.0000
10	4	7	11	9	4	6	10	7288.0750	-0.0014
10	4	6	10	9	4	5	9	7288.7346	-0.0022
10	4	6	9	9	4	5	8	7288.8648	-0.0016
10	4	6	11	9	4	5	10	7288.8587	-0.0019
11	0	11	11	10	0	10	10	7792.4185	0.0022
11	0	11	10	10	0	10	9	7792.4012	-0.0050
11	0	11	12	10	0	10	11	7792.4185	0.0011
11	1	11	12	10	1	10	11	7741.5564	0.0011
11	1	11	11	10	1	10	10	7741.5448	-0.0018
11	1	11	10	10	1	10	9	7741.5448	-0.0003
11	1	10	11	10	1	9	10	8120.8036	0.0034
11	1	10	10	10	1	9	9	8120.7924	-0.0032
11	1	10	12	10	1	9	11	8120.8107	0.0044
11	2	10	11	10	2	9	10	7957.0555	0.0039
11	2	10	10	10	2	9	9	7957.0671	-0.0016
11	2	10	12	10	2	9	11	7957.0781	0.0015
11	2	9	11	10	2	8	10	8162.5860	-0.0004
11	2	9	10	10	2	8	9	8162.6059	-0.0009
11	2	9	12	10	2	8	11	8162.6157	0.0009
11	3	9	11	10	3	8	10	8021.4693	0.0001
11	3	9	10	10	3	8	9	8021.5195	-0.0005
11	3	9	12	10	3	8	11	8021.5247	0.0009
11	3	8	11	10	3	7	10	8053.4551	-0.0014
11	3	8	10	10	3	7	9	8053.5103	0.0002
11	3	8	12	10	3	7	11	8053.5142	0.0005
11	4	8	11	10	4	7	10	8019.6757	0.0010
11	4	8	10	10	4	7	9	8019.7695	-0.0010

11	4	8	12	10	4	7	11	8019.7695	0.0010
11	4	7	11	10	4	6	10	8021.2332	-0.0001
11	4	7	10	10	4	6	9	8021.3246	-0.0049
11	4	7	12	10	4	6	11	8021.3246	-0.0028
12	0	12	12	11	0	11	11	8478.6183	-0.0019
12	0	12	11	11	0	11	10	8478.6081	-0.0041
12	0	12	13	11	0	11	12	8478.6203	-0.0010
12	1	12	11	11	1	11	10	8437.2045	-0.0011
12	1	12	12	11	1	11	11	8437.2045	-0.0030
12	1	12	13	11	1	11	12	8437.2154	0.0011
12	1	11	11	11	1	10	10	8837.4164	0.0001
12	1	11	12	11	1	10	11	8837.4223	0.0007
12	1	11	13	11	1	10	12	8837.4223	-0.0029
12	2	11	11	11	2	10	10	8671.2396	0.0047
12	2	11	12	11	2	10	11	8671.2263	0.0036
12	2	11	13	11	2	10	12	8671.2472	0.0052
12	2	10	11	11	2	9	10	8916.4052	-0.0013
12	2	10	12	11	2	9	11	8916.3905	-0.0015
12	2	10	13	11	2	9	12	8916.4133	-0.0003
13	0	13	12	12	0	12	11	9164.5270	-0.0040
13	0	13	13	12	0	12	12	9164.5378	0.0003
13	0	13	14	12	0	12	13	9164.5378	-0.0009
13	1	13	12	12	1	12	11	9131.7158	0.0012
13	1	13	13	12	1	12	12	9131.7204	0.0038
13	1	13	14	12	1	12	13	9131.7268	0.0048
13	1	12	12	12	1	11	11	9547.7087	0.0020
13	1	12	13	12	1	11	12	9547.7134	0.0007
13	1	12	14	12	1	11	13	9547.7134	-0.0010
13	2	12	12	12	2	11	11	9383.2258	0.0018
13	2	12	13	12	2	11	12	9383.2186	0.0033
13	2	12	14	12	2	11	13	9383.2339	0.0036
13	2	11	12	12	2	10	11	9667.4363	-0.0044
13	2	11	13	12	2	10	12	9667.4274	-0.0032
13	2	11	14	12	2	10	13	9667.4453	-0.0017
14	0	14	15	13	0	13	14	9850.6730	-0.0018
14	0	14	14	13	0	13	13	9850.6730	-0.0004
14	0	14	13	13	0	13	12	9850.6633	-0.0049
14	1	14	13	13	1	13	12	9825.2265	-0.0016
14	1	14	14	13	1	13	13	9825.2265	-0.0036
14	1	14	15	13	1	13	14	9825.2351	0.0006
14	1	13	13	13	1	12	12	10251.4667	0.0010
14	1	13	14	13	1	12	13	10251.4738	0.0017
14	1	13	15	13	1	12	14	10251.4738	0.0013

Table S2. Experimental transitions frequencies of isomer II of the C₂F₄S₂-IPA complex.

$J'_{Ka'Kc'}$	F'	$J''_{Ka''Kc''}$	F''	$V_{obs.}/\text{MHz}$	$Obs.-Calc./\text{MHz}$
8 0 8	9	7 0 7	8	6087.7037	-0.0020
8 0 8	8	7 0 7	7	6087.6925	0.0049
8 0 8	7	7 0 7	6	6087.6978	0.0057
8 1 8	9	7 1 7	8	6024.2254	-0.0005
8 1 8	8	7 1 7	7	6024.2112	0.0044
8 1 8	7	7 1 7	6	6024.2112	-0.0011
8 1 7	9	7 1 6	8	6425.7099	-0.0001
8 1 7	8	7 1 6	7	6425.6987	0.0104
8 1 7	7	7 1 6	6	6425.6987	-0.0014
9 0 9	10	8 0 8	9	6815.6265	0.0004
9 0 9	9	8 0 8	8	6815.6073	-0.0028
9 0 9	8	8 0 8	7	6815.6148	-0.0003
9 1 9	9	8 1 8	8	6765.8932	-0.0004
9 1 9	8	8 1 8	7	6765.8983	0.0002
9 1 9	10	8 1 8	9	6765.9050	-0.0040
9 1 8	9	8 1 7	8	7201.0755	-0.0030
9 1 8	8	8 1 7	7	7201.0900	-0.0002
9 1 8	10	8 1 7	9	7201.0989	0.0006
9 2 7	9	8 2 6	8	7271.2976	0.0042
9 2 7	8	8 2 6	7	7271.3088	-0.0023
9 2 7	10	8 2 6	9	7271.3184	0.0011
10 0 10	11	9 0 9	10	7542.4625	0.0012
10 0 10	10	9 0 9	9	7542.4461	-0.0014
10 0 10	9	9 0 9	8	7542.4533	0.0009
10 1 10	11	9 1 9	10	7505.3592	-0.0008
10 1 10	10	9 1 9	9	7505.3427	-0.0047
10 1 10	9	9 1 9	8	7505.3475	-0.0035
10 1 9	11	9 1 8	10	7965.1859	-0.0036
10 1 9	10	9 1 8	9	7965.1714	0.0004
10 1 9	9	9 1 8	8	7965.1751	-0.0080
10 2 9	10	9 2 8	9	7783.1276	-0.0003
10 2 9	9	9 2 8	8	7783.1480	-0.0020
10 2 9	11	9 2 8	10	7783.1568	0.0013
10 2 8	10	9 2 7	9	8092.3525	0.0006
10 2 8	9	9 2 7	8	8092.3620	-0.0026
10 2 8	11	9 2 7	10	8092.3699	-0.0001
10 3 8	10	9 3 7	9	7888.9873	0.0011
10 3 8	9	9 3 7	8	7889.0326	0.0009
10 3 8	11	9 3 7	10	7889.0326	-0.0007
10 3 7	10	9 3 6	9	7962.3951	0.0015
10 3 7	9	9 3 6	8	7962.4348	0.0029
10 3 7	11	9 3 6	10	7962.4348	0.0008

10	4	7	10	9	4	6	9	7892.8162	-0.0012
10	4	7	9	9	4	6	8	7892.9026	0.0014
10	4	7	11	9	4	6	10	7892.8952	-0.0021
10	4	6	10	9	4	5	9	7897.8871	-0.0022
10	4	6	9	9	4	5	8	7897.9733	0.0010
10	4	6	11	9	4	5	10	7897.9679	-0.0006
11	0	11	12	10	0	10	11	8269.6093	0.0004
11	0	11	11	10	0	10	10	8269.5962	-0.0010
11	0	11	10	10	0	10	9	8269.6026	0.0011
11	1	11	12	10	1	10	11	8242.9521	0.0029
11	1	11	11	10	1	10	10	8242.9382	-0.0001
11	1	11	10	10	1	10	9	8242.9473	0.0057
11	1	10	11	10	1	9	10	8717.2870	0.0008
11	1	10	10	10	1	9	9	8717.2977	-0.0012
11	1	10	12	10	1	9	11	8717.3048	0.0005
11	2	10	11	10	2	9	10	8543.9836	0.0016
11	2	10	10	10	2	9	9	8544.0025	0.0030
11	2	10	12	10	2	9	11	8544.0089	0.0045
11	2	9	11	10	2	8	10	8906.7745	0.0000
11	2	9	10	10	2	8	9	8906.7842	-0.0005
11	2	9	12	10	2	8	11	8906.7906	0.0011
11	3	9	11	10	3	8	10	8676.3612	-0.0008
11	3	9	10	10	3	8	9	8676.3991	0.0031
11	3	9	12	10	3	8	11	8676.3991	0.0008
11	3	8	11	10	3	7	10	8788.3327	0.0002
11	3	8	10	10	3	7	9	8788.3554	-0.0024
11	3	8	12	10	3	7	11	8788.3554	-0.0053
11	4	8	11	10	4	7	10	8687.9286	0.0026
11	4	8	10	10	4	7	9	8687.9877	0.0002
11	4	8	12	10	4	7	11	8687.9877	0.0015
11	4	7	11	10	4	6	10	8697.8926	-0.0018
11	4	7	10	10	4	6	9	8697.9529	-0.0017
11	4	7	12	10	4	6	11	8697.9529	-0.0005
12	0	12	11	11	0	11	10	8997.6435	-0.0036
12	0	12	12	11	0	11	11	8997.6389	-0.0046
12	0	12	13	11	0	11	12	8997.6526	-0.0008
12	1	12	12	11	1	11	11	8979.0404	0.0013
12	1	12	11	11	1	11	10	8979.0404	-0.0014
12	1	12	13	11	1	11	12	8979.0520	0.0037
12	1	11	12	11	1	10	11	9458.0320	0.0033
12	1	11	11	11	1	10	10	9458.0404	-0.0013
12	1	11	13	11	1	10	12	9458.0478	0.0015
