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Origin of fluorine/sulfur *gauche* effect of β-fluorinated thiol, sulfoxide, sulfone and thionium ion

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Supporting Information

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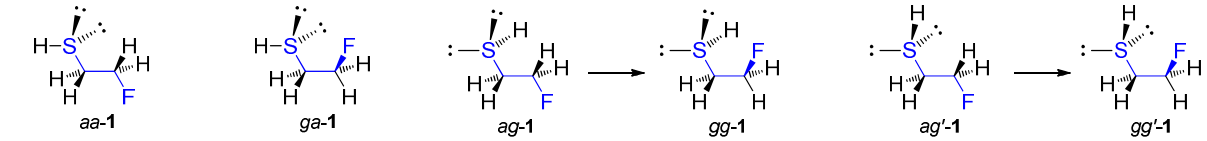
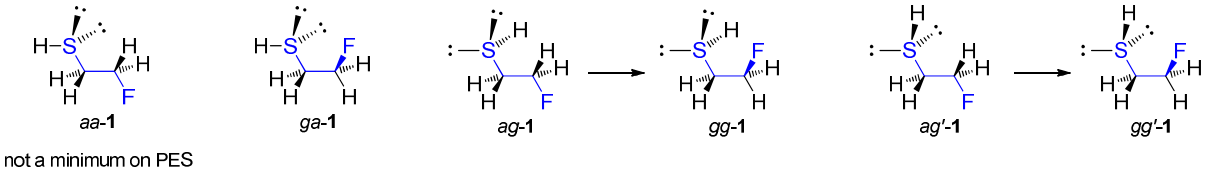
Table S1. Calculated relative electronic energies ΔE, enthalpies ΔH and free energies ΔG of four conformers of **1** and energy changes (in bold) occuring upon conformational isomerization (MP2/6-311++G(d,p) regular, B3LYP/6-311++G(d,p) italic). Values are in kcal/mol.



conformation	gas-phase			in CH_2Cl_2			in Me_2CO			in H_2O		
	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG
ag/g′-**1**	0.24	0.29	0.18	0.11	0.22	0.13	0.11	0.22	0.18	0.10	0.23	0.21
	0.18	*0.27*	*0.10*	*0.18*	*0.28*	*0.17*	*0.19*	*0.28*	*0.16*	*0.20*	*0.28*	*0.15*
ga-**1**	2.29	2.28	1.90	1.58	1.62	1.31	1.47	1.51	1.20	1.39	1.44	1.13
	2.25	*2.23*	*1.72*	*1.53*	*1.55*	*1.20*	*1.42*	*1.42*	*1.01*	*1.34*	*1.34*	*0.87*
gg-**1**	1.85	1.77	1.57	0.83	0.82	0.74	0.67	0.67	0.60	0.57	0.57	0.52
	1.69	*1.63*	*1.38*	*0.72*	*0.73*	*0.66*	*0.56*	*0.57*	*0.52*	*0.46*	*0.47*	*0.42*
gg′-**1**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	0.00	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*
ag-**1** → *gg*-**1**	**1.61**	**1.48**	**1.39**	**0.71**	**0.60**	**0.60**	**0.57**	**0.44**	**0.43**	**0.47**	**0.34**	**0.31**
	1.51	***1.37***	***1.28***	***0.54***	***0.45***	***0.49***	***0.37***	***0.29***	***0.36***	***0.27***	***0.19***	***0.28***
ag′-**1** → *gg′*-**1**	**-0.24**	**-0.29**	**-0.18**	**-0.11**	**-0.22**	**-0.13**	**-0.11**	**-0.22**	**-0.18**	**-0.10**	**-0.23**	**-0.21**
	-0.18	***-0.27***	***-0.10***	***-0.18***	***-0.28***	***-0.17***	***-0.19***	***-0.28***	***-0.16***	***-0.20***	***-0.28***	***-0.15***

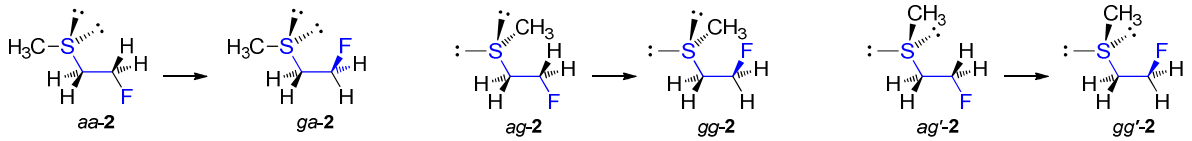
Table S2. Contribution of various energy components to the total binding interactions between two $FCH_2\cdot$ and $\cdot CH_2SH$ fragments and energy changes (ΔΔE values, in bold) occuring upon conformational isomerization.[a] EDA results for 2-fluoroethanol (FE) are included, too.[b] Values are in kcal/mol.



conformation	ΔE_{tot} **ΔE_{iso}**	ΔE_{def} **$\Delta\Delta E_{def}$**	ΔE_{int} **$\Delta\Delta E_{int}$**	ΔE_{elstat} **$\Delta\Delta E_{elstat}$**	ΔE_{ex+rep} **$\Delta\Delta E_{ex+rep}$**	ΔE_{oi} **$\Delta\Delta E_{oi}$**	ΔE_{disp} **$\Delta\Delta E_{disp}$**
ag/g′-**1**	-95.12	13.33	-108.45	-154.61	234.40	-159.04	-29.20
ga-**1**	-93.07	18.71	-111.78	-149.93	226.12	-156.79	-31.18
gg-**1**	-93.50	13.41	-106.91	-153.39	234.46	-158.96	-29.02
gg′-**1**	-95.37	13.86	-109.23	-155.64	235.25	-159.46	-29.38
ag-**1** → *gg*-**1**	**1.61**	**0.07**	**1.54**	**1.22**	**0.06**	**0.08**	**0.18**
ag′-**1** → *gg′*-**1**	**-0.24**	**0.54**	**-0.78**	**-1.03** (63%)	**0.85**	**-0.42** (26%)	**-0.18** (11%)
ag-FE → *gg*-FE	**0.09**	**0.75**	**-0.66**	**-1.28**	**3.86**	**-2.55**	**-0.69**
ag′-FE → *gg′*-FE	**-2.54**	**0.57**	**-3.11**	**-5.34**	**5.77**	**-3.03**	**-0.51**

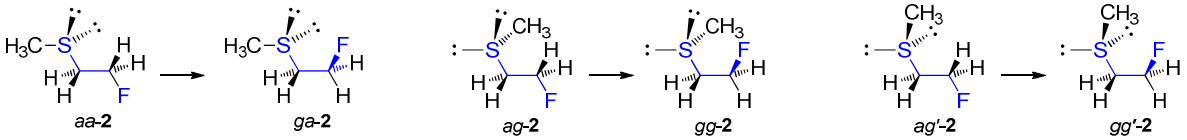
[a] ΔE_{tot} = total binding energy between two radical fragments, ΔE_{def} = deformation energy, ΔE_{int} = interaction energy, ΔE_{elstat} = electrostatic energy, ΔE_{ex+rep} = exchange repulsion energy, ΔE_{oi} = orbital interaction energy, ΔE_{disp} = dispersion energy, ΔE_{iso} = isomerization energy, ΔΔE values represent individual energy changes upon conformational isomerization. Values in parentheses are percentage contribution to all attractive interactions. [b] From ref. 8e.

Table S3. Calculated relative electronic energies ΔE, enthalpies ΔH and free energies ΔG of five conformers of **2** and energy changes (in bold) occuring upon conformational isomerization (MP2/6-311++G(d,p)). Values are in kcal/mol.



conformation	gas-phase			in CH_2Cl_2			in Me_2CO			in H_2O		
	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG
aa-**2**	1.18	1.28	0.94	1.34	1.42	1.17	1.37	1.44	1.17	1.38	1.45	1.17
ag/g′-**2**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
ga-**2**	1.68	1.65	1.48	1.07	1.01	0.92	0.95	0.89	0.77	0.87	0.80	0.67
gg-**2**	1.32	1.17	1.14	0.44	0.35	0.49	0.29	0.19	0.31	0.19	0.09	0.20
gg′-**2**	0.20	0.08	0.21	0.31	0.22	0.43	0.30	0.21	0.41	0.30	0.20	0.39
aa-**2** → *ga*-**2**	**0.50**	**0.37**	**0.54**	**-0.28**	**-0.41**	**-0.25**	**-0.42**	**-0.56**	**-0.40**	**-0.52**	**-0.65**	**-0.50**
ag-**2** → *gg*-**2**	**1.32**	**1.17**	**1.14**	**0.44**	**0.35**	**0.49**	**0.29**	**0.19**	**0.31**	**0.19**	**0.09**	**0.20**
ag′-**2** → *gg′*-**2**	**0.20**	**0.08**	**0.21**	**0.31**	**0.22**	**0.43**	**0.30**	**0.21**	**0.41**	**0.30**	**0.20**	**0.39**

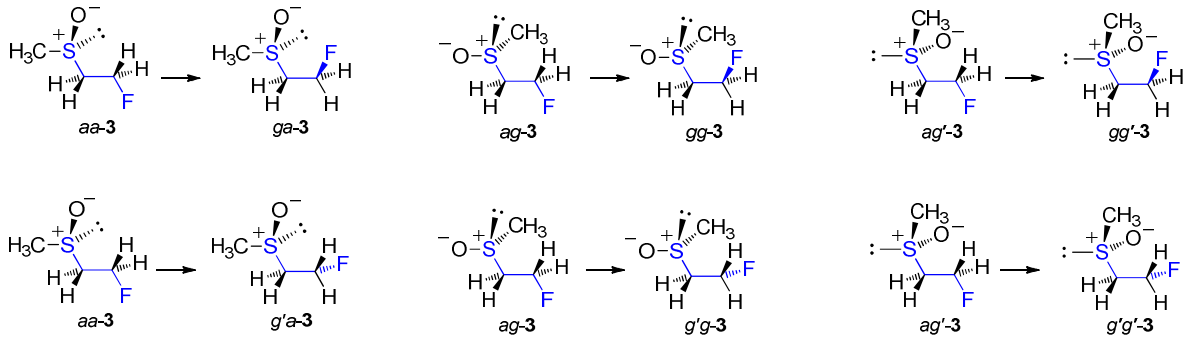
Table S4. Contribution of various energy components to the total binding interactions between two $FCH_2\cdot$ and $\cdot CH_2SCH_3$ fragments and energy changes (ΔΔE values, in bold) occuring upon conformational isomerization.[a] Values are in kcal/mol.



conformation	ΔE_{tot}	ΔE_{def}	ΔE_{int}	ΔE_{elstat}	ΔE_{ex+rep}	ΔE_{oi}	ΔE_{disp}
	$\mathbf{\Delta E_{iso}}$	$\mathbf{\Delta\Delta E_{def}}$	$\mathbf{\Delta\Delta E_{int}}$	$\mathbf{\Delta\Delta E_{elstat}}$	$\mathbf{\Delta\Delta E_{ex+rep}}$	$\mathbf{\Delta\Delta E_{oi}}$	$\mathbf{\Delta\Delta E_{disp}}$
aa-**2**	-92.41	20.25	-112.66	-148.44	221.14	-154.55	-30.81
ag/g′-**2**	-93.59	13.37	-106.96	-157.05	238.86	-160.13	-28.64
ga-**2**	-91.92	20.48	-112.40	-148.38	222.60	-155.47	-31.15
gg-**2**	-92.27	13.60	-105.87	-155.49	238.15	-159.81	-28.72
gg′-**2**	-93.40	13.58	-106.98	-158.19	240.35	-160.74	-28.40
aa-**2** → *ga*-**2**	**0.50**	**0.24**	**0.26**	**0.06**	**1.46**	**-0.92**	**-0.34**
ag-**2** → *gg*-**2**	**1.32**	**0.23**	**1.09**	**1.56**	**-0.71**	**0.32**	**-0.08**
ag′-**2** → *gg′*-**2**	**0.20**	**0.22**	**-0.02**	**-1.14**	**1.49**	**-0.61**	**0.24**

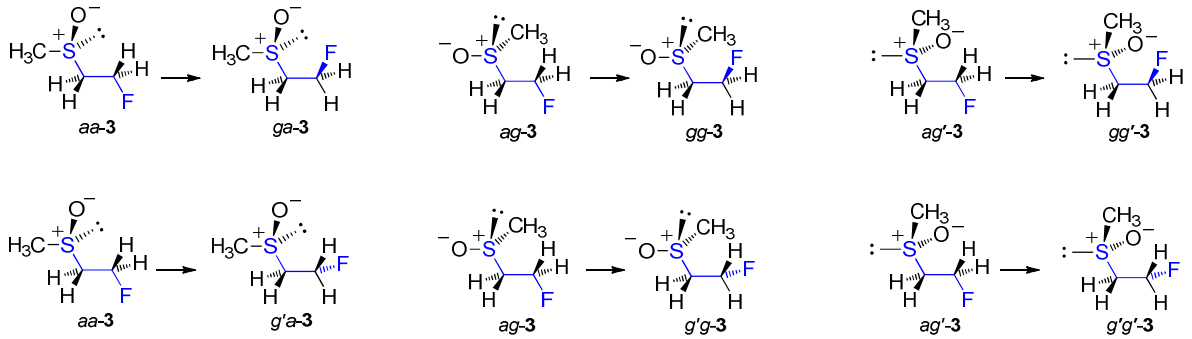
[a] Labeling of various energy terms is the same as in Table S2. Values in parentheses are percentage contribution to all attractive interactions.

Table S5. Calculated relative electronic energies ΔE, enthalpies ΔH and free energies ΔG of nine conformers of **3** and energy changes (in bold) occuring upon conformational isomerization (MP2/6-311++G(d,p)). Values are in kcal/mol.



conformation	gas-phase			in CH_2Cl_2			in Me_2CO			in H_2O		
	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG
aa-**3**	1.29	1.35	0.96	1.48	1.48	1.14	1.43	1.53	1.20	1.48	1.57	1.23
ag-**3**	2.93	3.05	2.75	2.56	2.56	2.60	2.33	2.54	2.59	2.32	2.53	2.58
ag′-**3**	1.95	2.08	1.69	2.15	2.15	2.10	1.96	2.20	2.19	1.99	2.24	2.27
ga-**3**	3.81	3.80	3.44	1.90	1.90	1.94	1.96	1.60	1.62	1.41	1.40	1.39
gg-**3**	2.23	2.27	2.06	1.54	1.54	1.38	1.42	1.51	1.41	1.39	1.47	1.36
gg′-**3**	0.00	0.00	0.00	0.59	0.59	0.70	0.58	0.70	0.80	0.65	0.76	0.85
g′a-**3**	0.29	0.24	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
g′g-**3**	1.14	1.11	0.91	1.08	1.08	0.97	1.11	1.15	1.05	1.17	1.20	1.10
g′g′-**3**	4.75	4.61	4.10	3.13	3.13	3.30	2.85	2.87	3.02	2.67	2.70	2.80
aa-**3** → *ga*-**3**	**2.52**	**2.45**	**2.48**	**0.43**	**0.43**	**0.80**	**0.18**	**0.07**	**0.42**	**-0.06**	**-0.17**	**0.16**
aa-**3** → *g′a*-**3**	**-1.00**	**-1.11**	**-0.95**	**-1.48**	**-1.48**	**-1.14**	**-1.43**	**-1.53**	**-1.20**	**-1.48**	**-1.57**	**-1.23**
ag-**3** → *gg*-**3**	**-0.70**	**-0.78**	**-0.69**	**-1.01**	**-1.01**	**-1.22**	**-0.92**	**-1.03**	**-1.18**	**-0.93**	**-1.05**	**-1.22**
ag-**3** → *g′g*-**3**	**-1.79**	**-1.94**	**-1.84**	**-1.48**	**-1.48**	**-1.63**	**-1.22**	**-1.38**	**-1.54**	**-1.15**	**-1.32**	**-1.48**
ag′-**3** → *gg′*-**3**	**-1.95**	**-2.08**	**-1.69**	**-1.57**	**-1.57**	**-1.39**	**-1.38**	**-1.50**	**-1.39**	**-1.33**	**-1.47**	**-1.42**
ag′-**3**→ *g′g′*-**3**	**2.80**	**2.53**	**2.41**	**0.98**	**0.98**	**1.20**	**0.89**	**0.67**	**0.84**	**0.68**	**0.46**	**0.52**

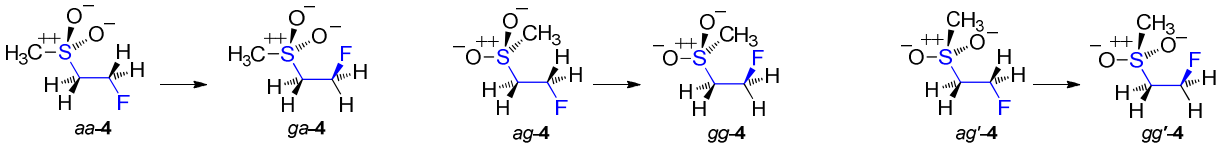
Table S6. Contribution of various energy components to the total binding interactions between two FCH_2· and ·CH_2SOCH_3 fragmentls and energy changes (ΔΔE values, in bold) occuring upon conformational isomerization.[a] Values are in kcal/mol.



conformation	ΔE_{tot} **ΔE_{iso}**	ΔE_{def} **$\Delta\Delta E_{def}$**	ΔE_{int} **$\Delta\Delta E_{int}$**	ΔE_{elstat} **$\Delta\Delta E_{elstat}$**	ΔE_{ex+rep} **$\Delta\Delta E_{ex+rep}$**	ΔE_{oi} **$\Delta\Delta E_{oi}$**	ΔE_{disp} **$\Delta\Delta E_{disp}$**
aa-**3**	-99.36	15.42	-114.78	-144.94	214.69	-153.47	-31.06
ag-**3**	-97.72	14.30	-112.02	-144.49	217.66	-154.70	-30.49
ag′-**3**	-98.70	13.83	-112.53	-146.92	220.52	-155.82	-30.31
ga-**3**	-96.83	15.34	-112.17	-144.62	218.73	-154.92	-31.36
gg-**3**	-98.42	14.74	-113.16	-146.85	219.82	-155.87	-30.26
gg′-**3**	-100.65	14.46	-115.11	-150.53	223.69	-157.59	-30.68
g′a-**3**	-100.35	15.40	-115.75	-147.30	218.25	-155.33	-31.37
g′g-**3**	-99.50	15.10	-114.60	-148.99	220.40	-155.96	-30.05
g′g′-**3**	-95.89	15.69	-111.58	-141.99	215.34	-153.70	-31.23
aa-**3** → *ga*-**3**	**2.52**	**-0.09**	**2.61**	**0.32**	**4.04**	**-1.45**	**-0.30**
aa-**3** → *g′a*-**3**	**-1.00**	**-0.03**	**-0.97**	**-2.36** (52%)	**3.56**	**-1.86** (41%)	**-0.31** (7%)
ag-**3** → *gg*-**3**	**-0.70**	**0.44**	**-1.14**	**-2.36** (67%)	**2.16**	**-1.17** (33%)	**0.23**
ag-**3** → *g′g*-**3**	**-1.79**	**0.79**	**-2.58**	**-4.50** (78%)	**2.74**	**-1.26** (22%)	**0.44**
ag′-**3** → *gg′*-**3**	**-1.95**	**0.63**	**-2.58**	**-3.61** (63%)	**3.17**	**-1.77** (31%)	**-0.38** (6%)
ag′-**3**→ *g′g′*-**3**	**2.80**	**1.85**	**0.95**	**4.93**	**-5.18**	**2.12**	**-0.92**

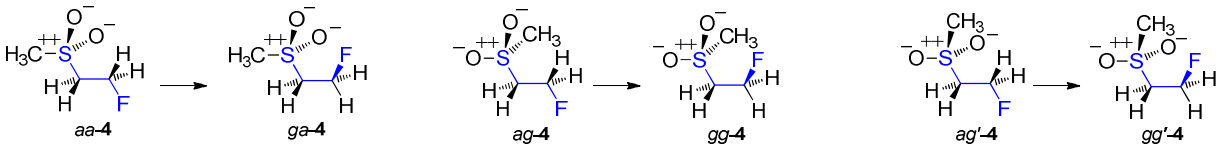
[a] Labeling of various energy terms is the same as in Table S2. Values in parentheses are percentage contribution to all attractive interactions.

Table S7. Calculated relative electronic energies ΔE, enthalpies ΔH and free energies ΔG of five conformers of **4** and energy changes (in bold) occuring upon conformational isomerization (MP2/6-311++G(d,p)). Values are in kcal/mol.



conformation	gas-phase			in CH_2Cl_2			in Me_2CO			in H_2O		
	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG
aa-**4**	2.13	2.36	1.63	2.15	2.21	1.14	2.13	2.21	1.33	2.11	2.21	1.49
ag/g′-**4**	2.34	2.47	2.16	2.04	2.15	1.95	1.97	2.09	1.84	1.94	2.05	1.74
ga-**4**	3.46	3.54	3.27	1.70	1.71	1.57	1.34	1.36	1.27	1.11	1.13	1.03
gg-**4**	4.59	4.52	4.47	2.55	2.66	2.76	2.05	1.95	1.75	1.80	1.72	1.47
gg′-**4**	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
aa-**4** → *ga*-**4**	**1.33**	**1.18**	**1.64**	**-0.45**	**-0.51**	**0.44**	**-0.78**	**-0.84**	**-0.06**	**-1.00**	**-1.08**	**-0.45**
ag-**4** → *gg*-**4**	**2.25**	**2.05**	**2.31**	**0.51**	**0.51**	**0.81**	**0.07**	**-0.13**	**-0.08**	**-0.13**	**-0.33**	**-0.27**
ag′-**4** → *gg′*-**4**	**-2.34**	**-2.47**	**-2.16**	**-2.04**	**-2.15**	**-1.95**	**-1.97**	**-2.09**	**-1.84**	**-1.94**	**-2.05**	**-1.74**

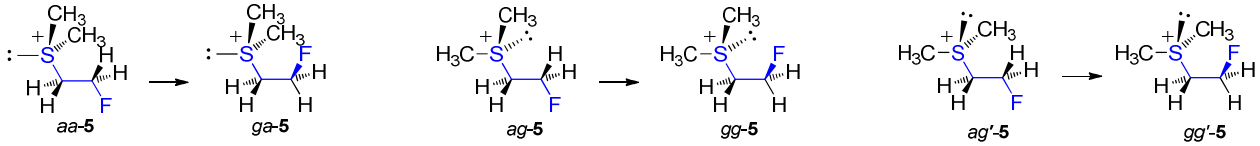
Table S8. Contribution of various energy components to the total binding interactions between two $FCH_2\cdot$ and $\cdot CH_2SO_2CH_3$ fragments and energy changes (ΔΔE values, in bold) occuring upon conformational isomerization.[a] Values are in kcal/mol.



conformation	ΔE_{tot} **ΔE_{iso}**	ΔE_{def} **$\Delta\Delta E_{def}$**	ΔE_{int} **$\Delta\Delta E_{int}$**	ΔE_{elstat} **$\Delta\Delta E_{elstat}$**	ΔE_{ex+rep} **$\Delta\Delta E_{ex+rep}$**	ΔE_{oi} **$\Delta\Delta E_{oi}$**	ΔE_{disp} **$\Delta\Delta E_{disp}$**
aa-**4**	-100.95	13.97	-114.92	-139.54	207.51	-152.08	-30.81
ag/g′-**4**	-100.74	13.07	-113.81	-141.24	210.96	-153.33	-30.20
ga-**4**	-99.62	14.58	-114.20	-139.36	210.87	-154.16	-31.55
gg-**4**	-98.49	13.92	-112.41	-140.88	214.04	-154.15	-31.42
gg′-**4**	-103.07	13.27	-116.34	-146.37	216.19	-156.15	-30.01
aa-**4** → *ga*-**4**	**1.33**	**0.61**	**0.72**	**0.18**	**3.36**	**-2.08**	**-0.74**
ag-**4** → *gg*-**4**	**2.25**	**0.85**	**1.40**	**0.36**	**3.08**	**-0.82**	**-1.22**
ag′-**4** → *gg′*-**4**	**-2.34**	**0.19**	**-2.53**	**-5.13** (65%)	**5.23**	**-2.82** (35%)	**0.19**

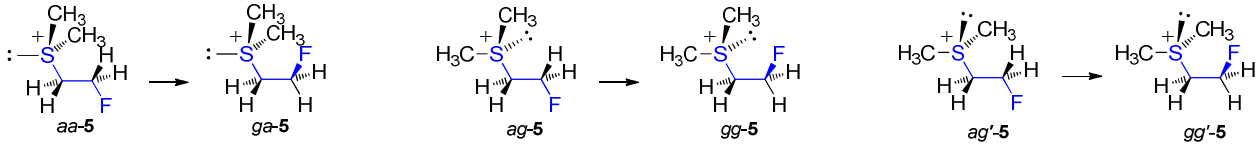
[a] Labeling of various energy terms is the same as in Table S2. Values in parentheses are percentage contribution to all attractive interactions.

Table S9. Calculated relative electronic energies ΔE, enthalpies ΔH and free energies ΔG of five conformers of **5** and energy changes (in bold) occuring upon conformational isomerization (MP2/6-311++G(d,p) regular, B3LYP/6-311++G(d,p) italic). Values are in kcal/mol.



conformation	gas-phase			in CH_2Cl_2			in Me_2CO			in H_2O		
	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG
aa-**5**	6.05	6.09	5.62	3.48	3.25	3.95	3.25	2.85	3.29	3.11	2.56	2.90
	5.96	*6.05*	*5.61*	*3.46*	*3.62*	*2.35*	*3.21*	*3.32*	*2.16*	*3.07*	*3.12*	*1.78*
ag/g′-**5**	5.03	5.01	4.50	2.53	2.79	2.86	2.31	2.45	2.25	2.18	2.24	1.95
	4.88	*4.92*	*4.35*	*2.48*	*2.73*	*2.44*	*2.23*	*2.49*	*2.37*	*2.08*	*2.34*	*2.41*
ga-**5**	0.75	0.73	1.12	0.92	0.96	1.25	0.97	1.02	1.29	1.01	1.06	1.47
	0.84	*0.89*	*1.02*	*1.06*	*1.12*	*1.01*	*1.08*	*1.13*	*1.09*	*1.10*	*1.09*	*0.91*
gg-**5**	0.00	0.00	0.00	0.00	0.00	0.11	0.00	0.00	0.00	0.00	0.00	0.00
	0.00	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*
gg′-**5**	1.61	1.65	1.52	0.65	0.51	0.00	0.53	0.48	0.26	0.47	0.38	0.19
	1.90	*1.90*	*1.61*	*0.57*	*0.71*	*0.55*	*0.45*	*0.56*	*0.49*	*0.38*	*0.46*	*0.48*
aa-**5** → *ga*-**5**	**-5.30**	**-5.36**	**-4.50**	**-2.57**	**-2.29**	**-2.69**	**-2.28**	**-1.84**	**-2.00**	**-2.10**	**-1.50**	**-1.43**
	-5.12	***-5.16***	***-4.59***	***-2.40***	***-2.50***	***-1.34***	***-2.13***	***-2.19***	***-1.07***	***-1.97***	***-2.03***	***-0.87***
ag-**5** → *gg*-**5**	**-5.03**	**-5.01**	**-4.50**	**-2.53**	**-2.79**	**-2.75**	**-2.31**	**-2.45**	**-2.25**	**-2.18**	**-2.24**	**-1.95**
	-4.88	***-4.92***	***-4.35***	***-2.48***	***-2.73***	***-2.44***	***-2.23***	***-2.49***	***-2.37***	***-2.08***	***-2.34***	***-2.41***
ag′-**5** → *gg′*-**5**	**-3.42**	**-3.36**	**-2.98**	**-1.88**	**-2.28**	**-2.86**	**-1.78**	**-1.97**	**-1.99**	**-1.71**	**-1.86**	**-1.77**
	-2.98	***-3.02***	***-2.74***	***-1.91***	***-2.02***	***-1.89***	***-1.79***	***-1.93***	***-1.89***	***-1.70***	***-1.88***	***-1.92***

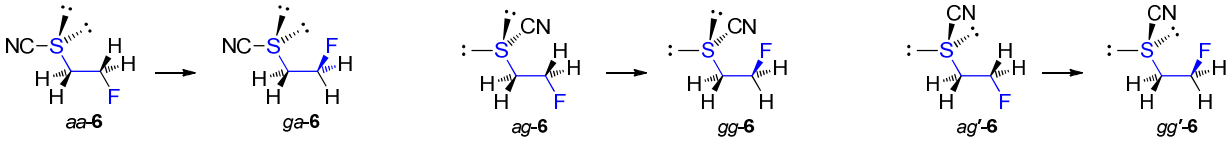
Table S10. Contribution of various energy components to the total binding interactions between two $FCH_2\cdot$ and $\cdot CH_2S(CH_3)_2^+$ fragments and energy changes ($\Delta\Delta E$ values, in bold) occuring upon conformational isomerization.[a] Values are in kcal/mol.



conformation	ΔE_{tot} **ΔE_{iso}**	ΔE_{def} **$\Delta\Delta E_{def}$**	ΔE_{int} **$\Delta\Delta E_{int}$**	ΔE_{elstat} **$\Delta\Delta E_{elstat}$**	ΔE_{ex+rep} **$\Delta\Delta E_{ex+rep}$**	ΔE_{oi} **$\Delta\Delta E_{oi}$**	ΔE_{disp} **$\Delta\Delta E_{disp}$**
aa-**5**	-95.58	13.06	-108.64	-132.10	207.69	-152.81	-31.42
ag/*g′*-**5**	-96.61	14.63	-111.24	-130.67	202.32	-151.29	-31.60
ga-**5**	-100.90	14.41	-115.31	-140.93	212.79	-155.79	-31.38
gg-**5**	-101.65	15.16	-116.81	-139.70	209.19	-154.94	-31.36
gg′-**5**	-100.03	15.24	-115.27	-135.99	206.63	-153.82	-32.09
aa-**5** → *ga*-**5**	**-5.30**	**1.37**	**-6.67**	**-8.83** (75%)	**5.10**	**-2.98** (25%)	**0.04**
ag-**5** → *gg*-**5**	**-5.03**	**0.54**	**-5.57**	**-9.03** (71%)	**6.87**	**-3.65** (29%)	**0.24**
ag′-**5** → *gg′*-**5**	**-3.42**	**0.61**	**-4.03**	**-5.32** (64%)	**4.31**	**-2.53** (30%)	**-0.49** (6%)

[a] Labeling of various energy terms is the same as in Table S2. Values in parentheses are percentage contribution to all attractive interactions.

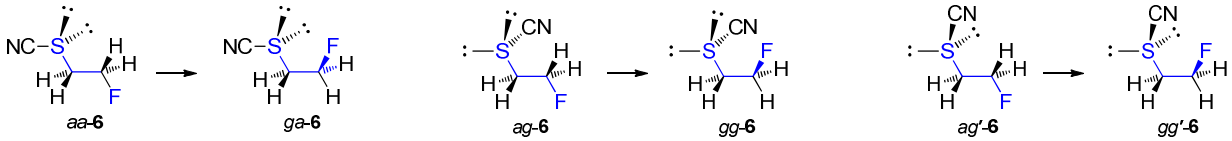
Table S11. Calculated relative electronic energies ΔE, enthalpies ΔH and free energies ΔG of five conformers of **6** and energy changes (in bold) occuring upon conformational isomerization (MP2/6-311++G(d,p) regular, B3LYP/6-311++G(d,p) italic). Values are in kcal/mol.



conformation	gas-phase			in CH_2Cl_2			in Me_2CO			in H_2O		
	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG
aa-**6**[a]	2.51	2.61	2.07	2.67	2.86	2.44	/	/	/	/	/	/
	2.02	*2.17*	*0.86*	*1.81*	*1.86*	*1.34*	*1.79*	*1.85*	*1.44*	*1.78*	*1.84*	*1.49*
ag/g′-**6**	0.00	0.00	0.00	0.35	0.45	0.39	0.41	0.52	0.46	0.46	0.56	0.51
	0.01	*0.12*	*0.09*	*0.57*	*0.70*	*0.73*	*0.64*	*0.77*	*0.80*	*0.68*	*0.82*	*0.84*
ga-**6**	1.50	1.50	1.22	1.39	1.44	1.03	1.40	1.46	1.09	1.41	1.47	1.12
	0.96	*0.99*	*0.60*	*0.95*	*0.99*	*0.63*	*0.95*	*1.00*	*0.63*	*0.96*	*1.00*	*0.60*
gg-**6**	0.16	0.06	0.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	0.00	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*
gg′-**6**	1.66	1.50	1.51	0.45	0.41	0.41	0.29	0.26	0.28	0.19	0.16	0.20
	1.46	*1.43*	*1.39*	*0.44*	*0.43*	*0.39*	*0.27*	*0.27*	*0.34*	*0.16*	*0.17*	*0.28*
aa-**6** → *ga*-**6**	**-1.01**	**-1.11**	**-0.85**	**-1.28**	**-1.42**	**-1.41**	/	/	/	/	/	/
	-1.06	***-1.19***	***-0.25***	***-1.43***	***-1.56***	***-1.44***	***-1.48***	***-1.62***	***-1.61***	***-1.51***	***-1.66***	***-1.74***
ag-**6** → *gg*-**6**	**0.16**	**0.06**	**0.07**	**-0.35**	**-0.45**	**-0.39**	**-0.41**	**-0.52**	**-0.46**	**-0.46**	**-0.56**	**-0.51**
	-0.01	***-0.12***	***-0.09***	***-0.57***	***-0.70***	***-0.73***	***-0.64***	***-0.77***	***-0.80***	***-0.68***	***-0.82***	***-0.84***
ag′-**6** → *gg′*-**6**	**1.66**	**1.50**	**1.51**	**0.10**	**-0.04**	**0.03**	**-0.12**	**-0.26**	**-0.19**	**-0.26**	**-0.40**	**-0.32**
	1.46	***1.30***	***1.30***	***-0.13***	***-0.27***	***-0.35***	***-0.37***	***-0.50***	***-0.46***	***-0.52***	***-0.65***	***-0.56***

[a] Optimization of *aa* form in Me_2CO and H_2O converged into *ag* form.

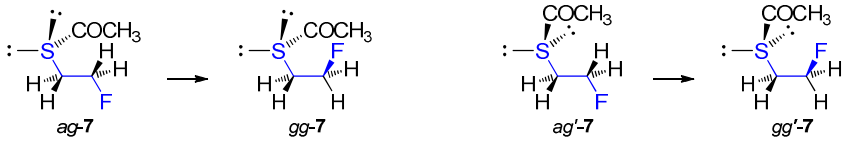
Table S12. Contribution of various energy components to the total binding interactions between two $FCH_2\cdot$ and $\cdot CH_2SCN$ fragments and energy changes (ΔΔE values, in bold) occuring upon conformational isomerization.[a] Values are in kcal/mol.



conformation	ΔE_{tot} **ΔE_{iso}**	ΔE_{def} **$\Delta\Delta E_{def}$**	ΔE_{int} **$\Delta\Delta E_{int}$**	ΔE_{elstat} **$\Delta\Delta E_{elstat}$**	ΔE_{ex+rep} **$\Delta\Delta E_{ex+rep}$**	ΔE_{oi} **$\Delta\Delta E_{oi}$**	ΔE_{disp} **$\Delta\Delta E_{disp}$**
aa-**6**	-94.74	17.18	-111.92	-144.12	217.87	-154.09	-31.58
ag/g′-**6**	-97.25	12.69	-109.94	-148.73	225.88	-156.93	-30.16
ga-**6**	-95.75	17.91	-113.66	-146.52	220.74	-156.06	-31.82
gg-**6**	-97.09	13.23	-110.32	-149.34	226.88	-157.78	-30.08
gg′-**6**	-95.60	12.72	-108.32	-148.87	229.07	-158.34	-30.18
aa-**6** → *ga*-**6**	**-1.01**	**0.73**	**-1.74**	**-2.40**	**2.87**	**-1.97**	**-0.24**
ag-**6** → *gg*-**6**	**0.16**	**0.54**	**-0.38**	**-0.61** (42%)	**1.00**	**-0.85** (58%)	**0.08**
ag′-**6** → *gg′*-**6**	**1.66**	**0.04**	**1.62**	**-0.14**	**3.19**	**-1.41**	**-0.02**

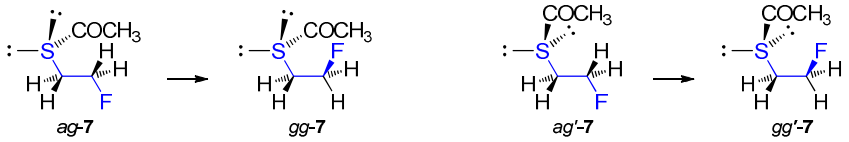
[a] Labeling of various energy terms is the same as in Table S2. Values in parentheses are percentage contribution to all attractive interactions.

Table S13. Calculated relative electronic energies ΔE, enthalpies ΔH and free energies ΔG of three conformers of **7** and energy changes (in bold) occuring upon conformational isomerization (MP2/6-311++G(d,p) regular, B3LYP/6-311++G(d,p) italic). Values are in kcal/mol.



conformation	gas-phase			in CH_2Cl_2			in Me_2CO			in H_2O		
	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG
ag/g′-**7**	0.00	0.00	0.00	0.00	0.05	0.08	0.00	0.06	0.10	0.00	0.06	0.11
	0.00	*0.03*	*0.27*	*0.15*	*0.24*	*0.15*	*0.16*	*0.25*	*0.00*	*0.17*	*0.25*	*0.00*
gg-**7**	0.22	0.11	0.12	0.05	0.00	0.00	0.05	0.00	0.00	0.04	0.00	0.00
	0.07	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*	*0.00*	*0.35*	*0.00*	*0.00*	*0.02*
gg′-**7**	1.45	1.34	1.32	0.78	0.70	0.60	0.66	0.59	0.52	0.58	0.51	0.47
	1.21	*1.11*	*1.40*	*0.55*	*0.53*	*1.07*	*0.42*	*0.40*	*1.21*	*0.33*	*0.31*	*0.75*
ag-**7** → *gg*-**7**	**0.22**	**0.11**	**0.12**	**0.05**	**-0.05**	**-0.08**	**0.05**	**-0.06**	**-0.10**	**0.04**	**-0.06**	**-0.11**
	0.07	***-0.03***	***-0.27***	***-0.15***	***-0.24***	***-0.15***	***-0.16***	***-0.25***	***0.35***	***-0.17***	***-0.25***	***0.02***
ag′-**7** → *gg′*-**7**	**1.45**	**1.34**	**1.32**	**0.78**	**0.65**	**0.52**	**0.66**	**0.53**	**0.42**	**0.58**	**0.45**	**0.36**
	1.21	***1.08***	***1.13***	***0.40***	***0.29***	***0.92***	***0.26***	***0.15***	***1.21***	***0.17***	***0.06***	***0.75***

Table S14. Contribution of various energy components to the total binding interactions between two FCH_2· and ·CH_2SCOCH_3 fragments and energy changes (ΔΔE values, in bold) occuring upon conformational isomerization.[a] Values are in kcal/mol.



conformation	ΔE_{tot} **ΔE_{iso}**	ΔE_{def} **$\Delta\Delta E_{def}$**	ΔE_{int} **$\Delta\Delta E_{int}$**	ΔE_{elstat} **$\Delta\Delta E_{elstat}$**	ΔE_{ex+rep} **$\Delta\Delta E_{ex+rep}$**	ΔE_{oi} **$\Delta\Delta E_{oi}$**	ΔE_{disp} **$\Delta\Delta E_{disp}$**
ag/g′-**7**	-96.34	13.39	-109.73	-151.70	229.01	-157.14	-29.90
gg-**7**	-96.12	13.97	-110.09	-152.33	229.45	-157.67	-29.54
gg′-**7**	-94.91	13.71	-108.63	-151.23	229.95	-157.38	-29.96
ag-**7** → *gg*-**7**	**0.22**	**0.58**	**-0.36**	**-0.63** (54%)	**0.44**	**-0.53** (46%)	**0.36**
ag′-**7** → *gg′*-**7**	**1.45**	**0.34**	**1.11**	**0.47**	**0.94**	**-0.24**	**-0.06**

[a] Labeling of various energy terms is the same as in Table S2. Values in parentheses are percentage contribution to all attractive interactions.

Second-order perturbation analysis of donor-acceptor interactions

The second-order perturbation analysis in NBO basis allows us to quantify stabilizing energy, denoted as E(2), due to charge transfer between an occupied and an empty orbital, as expressed in Eq. 1. In the equation, q_i represents occupancy of donor orbital (~2), $F_{i,j}$ is Fock matrix element between interacting orbitals related to the amount of their overlap and $\Delta E_{i,j}$ is energy difference between the orbitals (for more details, see ref. 35 in the manuscript).

$$E(2) = -q_i(F_{i,j})^2/\Delta E_{i,j} \qquad (1)$$

The interacting orbital energies, their energy difference and Fock matrix element for selected *gauche* conformers of **1** and **3-5** are listed in Table S15. Calculated E(2) values are presented in Table 8, in the manuscript.

Table S15. Orbital energies (E), difference in energy (ΔE) and Fock matrix element (F) between interacting orbtals (HF/6-311++G(d,p)). Values are in a.u.

conformation	$E_{C–H}$	$E_{C–F}^*$	$E_{C–H}$	$E_{C–S}^*$	$\Delta E_{CH/CF}^*$	$\Delta E_{CH/CS}^*$	$F_{CH/CF}^*$	$F_{CH/CS}^*$
gg′-**1**	-0.714	0.483	-0.724	0.370	1.20	1.09	0.075	0.073
g′a-**3**	-0.734	0.484	-0.728	0.332	1.22	1.06	0.072	0.063
g′g-**3**	-0.727	0.463	-0.741	0.334	1.19	1.08	0.077	0.067
gg′-**3**	-0.729	0.479	-0.728	0.332	1.21	1.06	0.072	0.066
gg′-**4**	-0.745	0.462	-0.745	0.321	1.21	1.07	0.073	0.068
ga-**5**	-0.905	0.331	-0.882	0.153	1.24	1.03	0.070	0.077
gg-**5**	-0.910	0.337	-0.878	0.150	1.25	1.03	0.068	0.070
gg′-**5**	-0.914	0.342	-0.879	0.151	1.26	1.03	0.065	0.070

Absolute energies (a.u.) and x, y, z coordinates (Å) of optimized structures at the MP2/6-311++G(d,p) level

***ag*-1**

E = -576.4893691 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.018838	0.611892	0.076135
2	1	0	0.106287	1.139073	1.023471
3	1	0	0.092436	1.334559	-0.735337
4	6	0	1.022845	-0.478713	-0.065489
5	1	0	0.938531	-1.215116	0.738655
6	1	0	0.933300	-0.982771	-1.030188
7	9	0	2.297026	0.085138	0.012793
8	16	0	-1.696639	-0.062241	-0.073854
9	1	0	-1.621594	-0.845200	1.006055

***ga*-1**

E = -576.4860491 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.075999	0.872884	-0.280907
2	1	0	-0.347858	1.835553	0.160243
3	1	0	0.059797	0.997003	-1.357461
4	6	0	1.228509	0.435335	0.346586
5	1	0	2.015213	1.167441	0.142475
6	1	0	1.122739	0.290477	1.424491
7	9	0	1.634373	-0.779347	-0.202272
8	16	0	-1.380213	-0.352605	0.066120
9	1	0	-2.390900	0.516022	-0.001305

***gg*-1**

E = -576.4867784 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.071439	0.835487	-0.312012
2	1	0	-0.326694	1.850468	0.006163
3	1	0	0.073209	0.850059	-1.395191
4	6	0	1.225143	0.422132	0.352840
5	1	0	1.997680	1.176974	0.173600
6	1	0	1.097630	0.279165	1.429686
7	9	0	1.681808	-0.776232	-0.180468
8	16	0	-1.459893	-0.291926	-0.008569
9	1	0	-1.542044	-0.045479	1.302085

***gg′*-1**

E = -576.4896925 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.075521	0.862261	-0.315586
2	1	0	-0.349390	1.855535	0.052373
3	1	0	0.057457	0.925024	-1.398162
4	6	0	1.223255	0.446832	0.337968
5	1	0	2.019072	1.162050	0.109392
6	1	0	1.107884	0.340329	1.418882
7	9	0	1.623742	-0.792372	-0.164403
8	16	0	-1.465417	-0.229088	0.095547
9	1	0	-0.888426	-1.340728	-0.365894

***aa*-2**

E = -615.699038 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.345721	0.427416	-0.110240
2	1	0	0.282079	1.180775	0.680550
3	1	0	0.412859	0.928238	-1.080085
4	6	0	1.587560	-0.414794	0.108205
5	1	0	1.598846	-0.854061	1.108159
6	1	0	1.671583	-1.205679	-0.641794
7	9	0	2.713740	0.400462	-0.010188
8	16	0	-1.115060	-0.644066	-0.045092
9	6	0	-2.369456	0.647480	0.076380
10	1	0	-2.254118	1.226553	0.995320
11	1	0	-3.342505	0.152705	0.095003
12	1	0	-2.334395	1.311763	-0.790052

ag-**2**

E = -615.700953 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.398637	-0.549319	0.479670
2	1	0	-0.388066	-0.103508	1.478949
3	1	0	-0.754372	-1.578982	0.571466
4	6	0	-1.324717	0.225134	-0.436639
5	1	0	-0.999811	1.260696	-0.560481
6	1	0	-1.394226	-0.254900	-1.415304
7	9	0	-2.606284	0.256189	0.119866
8	16	0	1.282773	-0.639106	-0.178598
9	6	0	1.821049	1.057512	0.138213
10	1	0	1.335703	1.783900	-0.515216
11	1	0	2.895791	1.088420	-0.052479
12	1	0	1.651004	1.324412	1.184369

ga-**2**

E = -615.6981916 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.278608	0.788116	0.146086
2	1	0	0.078197	1.676408	-0.388867
3	1	0	-0.311047	1.007602	1.218030
4	6	0	-1.677744	0.490632	-0.348688
5	1	0	-2.326345	1.357306	-0.191589
6	1	0	-1.675877	0.217333	-1.407123
7	9	0	-2.223563	-0.575466	0.361919
8	16	0	0.841276	-0.595514	-0.187500
9	6	0	2.391957	0.256556	0.168095
10	1	0	2.559515	1.089321	-0.519492
11	1	0	3.197811	-0.468868	0.039188
12	1	0	2.415765	0.616489	1.199623

***gg*-2**

E = -615.6988463 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.368432	-0.300973	0.908616
2	1	0	0.014777	0.169838	1.822090
3	1	0	-0.830690	-1.251396	1.190343
4	6	0	-1.429327	0.591663	0.296832
5	1	0	-2.183097	0.851476	1.047263
6	1	0	-1.005302	1.508348	-0.121275
7	9	0	-2.081200	-0.077714	-0.732873
8	16	0	1.011125	-0.704754	-0.187457
9	6	0	1.860330	0.888570	-0.172189
10	1	0	1.281039	1.673683	-0.662415
11	1	0	2.790606	0.757024	-0.728849
12	1	0	2.110046	1.190952	0.848461

***gg′*-2**

E = -615.7006776 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.408114	-0.912725	0.532066
2	1	0	0.507045	-2.003746	0.556593
3	1	0	0.376003	-0.558575	1.568021
4	6	0	1.626205	-0.352511	-0.171424
5	1	0	2.544999	-0.697347	0.314108
6	1	0	1.632761	-0.630816	-1.227916
7	9	0	1.623928	1.042243	-0.106317
8	16	0	-1.169758	-0.576726	-0.284319
9	6	0	-1.435662	1.143632	0.204353
10	1	0	-1.392665	1.245145	1.291556
11	1	0	-2.442929	1.406185	-0.126369
12	1	0	-0.716382	1.816207	-0.260006

aa-**3**

E = -690.7491299 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.550758	-0.616967	0.044819
2	1	0	0.475857	-0.909409	1.096668
3	1	0	0.675012	-1.499255	-0.591025
4	6	0	1.709833	0.344384	-0.145891
5	1	0	1.609135	1.209722	0.509937
6	1	0	1.789180	0.675968	-1.185046
7	9	0	2.891914	-0.318436	0.180470
8	16	0	-0.988588	0.222246	-0.435285
9	6	0	-2.097857	-1.036091	0.233152
10	1	0	-3.117441	-0.701265	0.035633
11	1	0	-1.914978	-1.990151	-0.268068
12	1	0	-1.934681	-1.111461	1.310751
13	8	0	-1.096038	1.435985	0.454876

ag-**3**

E = -690.746465 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.574743	-0.546567	0.285813
2	1	0	-0.774101	-1.579536	-0.012777
3	1	0	-0.471527	-0.507466	1.374386
4	6	0	-1.686144	0.349648	-0.227563
5	1	0	-1.665329	0.424250	-1.319212
6	1	0	-1.645013	1.349802	0.208902
7	9	0	-2.911699	-0.206133	0.131439
8	16	0	1.055126	-0.169368	-0.432831
9	6	0	1.215409	1.491232	0.262992
10	1	0	2.236167	1.813300	0.049417
11	1	0	0.509744	2.176081	-0.214373
12	1	0	1.064154	1.446275	1.344635
13	8	0	2.042756	-1.040439	0.297990

ag'-**3**

E = -690.7481091 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.612315	0.009139	0.792763
2	1	0	0.709923	0.898323	1.422869
3	1	0	0.918911	-0.867902	1.369923
4	6	0	1.461199	0.092275	-0.460925
5	1	0	1.312156	1.028578	-1.002108
6	1	0	1.255882	-0.753822	-1.118222
7	9	0	2.804264	0.042267	-0.084778
8	16	0	-1.155144	-0.251270	0.435196
9	6	0	-1.481119	1.348542	-0.348559
10	1	0	-2.552209	1.377091	-0.555305
11	1	0	-1.215189	2.160522	0.333058
12	1	0	-0.933263	1.416935	-1.289893
13	8	0	-1.225831	-1.289944	-0.657515

ga-**3**

E = -690.7449424 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.459094	-0.850585	0.425647
2	1	0	0.433641	-0.573525	1.484916
3	1	0	0.145034	-1.892857	0.299507
4	6	0	1.848213	-0.691361	-0.155853
5	1	0	1.851428	-0.893387	-1.231284
6	1	0	2.547010	-1.370067	0.341790
7	9	0	2.303353	0.605227	0.031806
8	16	0	-0.759392	0.226072	-0.414110
9	6	0	-2.202359	-0.746854	0.082961
10	1	0	-3.080170	-0.177692	-0.227303
11	1	0	-2.192051	-1.719050	-0.416103
12	1	0	-2.204000	-0.854689	1.170566
13	8	0	-0.838810	1.518734	0.350111

***gg*-3**

E = -690.7476138 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.478158	-0.806732	0.582166
2	1	0	-0.605591	-1.827497	0.211789
3	1	0	-0.077664	-0.852239	1.601542
4	6	0	-1.793427	-0.058926	0.552524
5	1	0	-1.713417	0.935382	0.997116
6	1	0	-2.562167	-0.626191	1.083836
7	9	0	-2.218850	0.102547	-0.765362
8	16	0	0.858112	-0.107287	-0.445925
9	6	0	0.874181	1.538777	0.301541
10	1	0	1.774919	2.024682	-0.077854
11	1	0	-0.004148	2.108765	-0.009966
12	1	0	0.940093	1.451152	1.389352
13	8	0	2.109031	-0.807388	0.026233

***gg′*-3**

E = -690.7512777 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.541542	-0.673553	0.896259
2	1	0	0.813988	-0.071567	1.768218
3	1	0	0.429312	-1.717774	1.206003
4	6	0	1.589687	-0.599865	-0.191540
5	1	0	1.178858	-0.949340	-1.142420
6	1	0	2.467760	-1.190466	0.080354
7	9	0	2.012335	0.721729	-0.359772
8	16	0	-1.130981	-0.202862	0.324718
9	6	0	-0.838784	1.557126	0.041840
10	1	0	-1.800454	1.979703	-0.254230
11	1	0	-0.492121	2.029190	0.964398
12	1	0	-0.110566	1.680620	-0.759147
13	8	0	-1.282096	-0.839049	-1.037508

g′a-**3**

E = -690.7507055 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.456927	-0.818879	0.462439
2	1	0	0.056993	-0.994078	1.467607
3	1	0	0.573426	-1.763190	-0.078124
4	6	0	1.781925	-0.096823	0.570347
5	1	0	2.477954	-0.663448	1.193660
6	1	0	1.644313	0.907514	0.977291
7	9	0	2.345422	0.022258	-0.699030
8	16	0	-0.743745	0.235634	-0.415753
9	6	0	-2.177825	-0.802133	-0.052746
10	1	0	-3.046639	-0.318076	-0.501633
11	1	0	-2.035698	-1.791899	-0.494891
12	1	0	-2.306996	-0.861949	1.030733
13	8	0	-0.867300	1.477707	0.433554

g′g-**3**

E = -690.7494256 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.471319	-0.846224	0.537074
2	1	0	-0.217637	-1.911524	0.553697
3	1	0	-0.448826	-0.462827	1.561780
4	6	0	-1.828964	-0.672081	-0.107297
5	1	0	-2.590105	-1.223633	0.449814
6	1	0	-1.823697	-1.004800	-1.148691
7	9	0	-2.198595	0.674914	-0.102203
8	16	0	0.894506	-0.104968	-0.423274
9	6	0	0.782944	1.560473	0.260553
10	1	0	1.568088	2.148610	-0.217388
11	1	0	-0.199696	1.982694	0.045190
12	1	0	0.969046	1.502991	1.336025
13	8	0	2.165266	-0.709907	0.121225

g′g′-**3**

E = -690.7436533 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.497633	-0.752163	0.707556
2	1	0	-0.148307	-1.782742	0.823790
3	1	0	-0.983630	-0.441101	1.635511
4	6	0	-1.493001	-0.608014	-0.433821
5	1	0	-2.053467	-1.536820	-0.570020
6	1	0	-1.010208	-0.320587	-1.371008
7	9	0	-2.407312	0.387519	-0.117823
8	16	0	0.982695	0.313209	0.492069
9	6	0	1.876397	-0.828789	-0.592115
10	1	0	2.772118	-0.300604	-0.923028
11	1	0	2.157546	-1.728963	-0.039775
12	1	0	1.259891	-1.071385	-1.461335
13	8	0	0.579270	1.477122	-0.374568

aa-**4**

E = -765.8415171 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.956984	0.262746	0.000000
2	1	0	-1.286958	0.790033	0.898358
3	1	0	-1.286958	0.790033	-0.898358
4	6	0	-1.486105	-1.164118	0.000000
5	1	0	-1.168707	-1.701764	0.894716
6	1	0	-1.168707	-1.701764	-0.894716
7	9	0	-2.877048	-1.099258	0.000000
8	16	0	0.837705	0.240320	0.000000
9	6	0	1.269920	1.969787	0.000000
10	1	0	2.361267	2.000163	0.000000
11	1	0	0.880257	2.438153	-0.904442
12	1	0	0.880257	2.438153	0.904442
13	8	0	1.269920	-0.338456	1.269406
14	8	0	1.269920	-0.338456	-1.269406

ag-**4**

E = -765.8412539 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.749902	-0.441098	-0.534938
2	1	0	0.865335	-1.528535	-0.527685
3	1	0	0.803552	-0.089706	-1.568593
4	6	0	1.803285	0.218541	0.339016
5	1	0	1.793193	-0.197119	1.346727
6	1	0	1.671938	1.302629	0.388099
7	9	0	3.049584	-0.027343	-0.230311
8	16	0	-0.919060	-0.161853	0.061428
9	6	0	-1.276135	1.522847	-0.409547
10	1	0	-2.290995	1.714118	-0.055567
11	1	0	-0.577537	2.201137	0.081579
12	1	0	-1.234800	1.608987	-1.495874
13	8	0	-1.808367	-1.028921	-0.701575
14	8	0	-0.870918	-0.218269	1.520836

ga-**4**

E = -765.8393992 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.599330	-0.880557	-0.569509
2	1	0	-0.691590	-0.673130	-1.638202
3	1	0	-0.278770	-1.914807	-0.407611
4	6	0	-1.916422	-0.657667	0.149340
5	1	0	-1.780763	-0.698577	1.232193
6	1	0	-2.637402	-1.415396	-0.168784
7	9	0	-2.429704	0.587741	-0.178625
8	16	0	0.707872	0.171536	0.098321
9	6	0	2.188952	-0.645004	-0.473969
10	1	0	3.018377	-0.019248	-0.139268
11	1	0	2.257874	-1.636141	-0.024696
12	1	0	2.173988	-0.691461	-1.563931
13	8	0	0.654837	1.480649	-0.538770
14	8	0	0.650223	0.033587	1.552474

gg-**4**

E = -765.8379012 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.604211	-1.118696	-0.136414
2	1	0	0.696177	-1.670132	0.803579
3	1	0	0.335428	-1.811623	-0.938865
4	6	0	1.903613	-0.419956	-0.487224
5	1	0	1.836982	0.095960	-1.448596
6	1	0	2.708071	-1.158754	-0.536480
7	9	0	2.238972	0.519420	0.476713
8	16	0	-0.831418	-0.050571	0.126982
9	6	0	-0.614510	1.290408	-1.029093
10	1	0	-1.507614	1.907785	-0.914195
11	1	0	0.272989	1.862772	-0.758988
12	1	0	-0.566009	0.898370	-2.046268
13	8	0	-2.001654	-0.817778	-0.291692
14	8	0	-0.746342	0.505207	1.470950

gg′-**4**

E = -765.8451258 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.613755	-0.854330	-0.685686
2	1	0	-0.682991	-0.505093	-1.719107
3	1	0	-0.362273	-1.920284	-0.690567
4	6	0	-1.898701	-0.631133	0.079633
5	1	0	-1.767069	-0.855076	1.139785
6	1	0	-2.700027	-1.242152	-0.342667
7	9	0	-2.283753	0.706540	-0.032668
8	16	0	0.835260	-0.099001	0.072401
9	6	0	0.675899	1.647083	-0.243527
10	1	0	1.559293	2.102192	0.208557
11	1	0	0.675333	1.814707	-1.321109
12	1	0	-0.235119	2.017056	0.224219
13	8	0	0.721426	-0.310664	1.514023
14	8	0	1.993800	-0.583825	-0.672277

aa-**5**

E = -655.2443329 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.771204	-0.700661	0.000000
2	1	0	-1.376593	-0.923733	0.883871
3	1	0	-1.376593	-0.923733	-0.883871
4	6	0	0.509147	-1.531239	0.000000
5	1	0	1.110712	-1.359166	0.895522
6	1	0	1.110712	-1.359166	-0.895522
7	9	0	0.104605	-2.846722	0.000000
8	16	0	-0.571785	1.096551	0.000000
9	6	0	0.509147	1.419929	-1.405194
10	1	0	0.615085	2.503701	-1.478575
11	1	0	1.481632	0.946512	-1.273507
12	1	0	0.004005	1.046658	-2.298009
13	6	0	0.509147	1.419929	1.405194
14	1	0	0.615085	2.503701	1.478575
15	1	0	0.004005	1.046658	2.298009
16	1	0	1.481632	0.946512	1.273507

ag-**5**

E = -655.2459725 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.632469	-0.542400	0.202313
2	1	0	0.548124	-0.522363	1.292575
3	1	0	0.770203	-1.572796	-0.138260
4	6	0	1.804672	0.313600	-0.279412
5	1	0	1.737128	1.343333	0.080273
6	1	0	1.886494	0.301650	-1.369503
7	9	0	2.936152	-0.255795	0.256800
8	16	0	-0.933919	0.006362	-0.518831
9	6	0	-1.255376	1.542256	0.366080
10	1	0	-2.291176	1.820031	0.162287
11	1	0	-1.092748	1.398732	1.435828
12	1	0	-0.593661	2.310210	-0.035556
13	6	0	-2.095075	-1.122557	0.269650
14	1	0	-3.099898	-0.810348	-0.019821
15	1	0	-1.896851	-2.121199	-0.122689
16	1	0	-1.970425	-1.092284	1.353178

ga-**5**

E = -655.2529122 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.699894	-0.110462	1.148997
2	1	0	0.778071	0.869975	1.627635
3	1	0	0.759424	-0.877768	1.926900
4	6	0	1.797701	-0.315374	0.120803
5	1	0	1.770072	-1.312529	-0.322741
6	1	0	2.765314	-0.163236	0.604623
7	9	0	1.655033	0.615296	-0.898189
8	16	0	-1.008778	-0.176732	0.519585
9	6	0	-0.938530	-1.301337	-0.884429
10	1	0	-1.946816	-1.332530	-1.301617
11	1	0	-0.222379	-0.947366	-1.625804
12	1	0	-0.677784	-2.292289	-0.509114
13	6	0	-1.237851	1.422120	-0.281472
14	1	0	-2.229237	1.399324	-0.737761
15	1	0	-1.221446	2.179378	0.504086
16	1	0	-0.457355	1.597410	-1.019267

gg-**5**

E = -655.2539454 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.505401	-0.931264	0.477126
2	1	0	0.428347	-0.617510	1.521925
3	1	0	0.225842	-1.985480	0.383613
4	6	0	1.901149	-0.707435	-0.080696
5	1	0	1.984351	-1.040291	-1.117562
6	1	0	2.630370	-1.231346	0.540481
7	9	0	2.171861	0.653315	-0.040663
8	16	0	-0.720234	-0.000669	-0.491440
9	6	0	-0.721833	1.622699	0.291441
10	1	0	-1.527488	2.195819	-0.170892
11	1	0	-0.882142	1.516281	1.365703
12	1	0	0.240639	2.087004	0.080112
13	6	0	-2.258852	-0.699789	0.131970
14	1	0	-3.074584	-0.087341	-0.255991
15	1	0	-2.346576	-1.713740	-0.260679
16	1	0	-2.256968	-0.697793	1.223247

gg′-**5**

E = -655.2513376 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.505471	-0.923111	0.499036
2	1	0	-0.600081	-1.878837	-0.023326
3	1	0	-0.095751	-1.081251	1.501476
4	6	0	-1.847813	-0.207563	0.559170
5	1	0	-1.807539	0.692512	1.176351
6	1	0	-2.600784	-0.888809	0.960815
7	9	0	-2.207234	0.161739	-0.724783
8	16	0	0.687686	0.031167	-0.484744
9	6	0	2.234096	-0.755970	-0.001726
10	1	0	3.041140	-0.236129	-0.520624
11	1	0	2.366888	-0.705007	1.080040
12	1	0	2.193170	-1.791520	-0.344002
13	6	0	0.779025	1.591833	0.406186
14	1	0	1.651243	2.124358	0.022169
15	1	0	-0.119533	2.163363	0.170791
16	1	0	0.874348	1.415864	1.479272

aa-**6**

E = -668.5481888 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.575542	-0.351595	0.280514
2	1	0	0.684440	-0.595017	1.338280
3	1	0	0.333220	-1.251860	-0.285576
4	6	0	1.855701	0.268526	-0.253801
5	1	0	1.801385	0.415908	-1.334606
6	1	0	2.078004	1.220688	0.236755
7	9	0	2.904588	-0.602169	0.013175
8	16	0	-0.768293	0.871362	0.061389
9	6	0	-2.066134	-0.207955	-0.050099
10	7	0	-2.990902	-0.937978	-0.130763

ag-**6**

E = -668.5522526 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.682767	-0.638172	0.488005
2	1	0	-1.210328	-1.595474	0.513134
3	1	0	-0.607225	-0.249609	1.505025
4	6	0	-1.406293	0.336627	-0.422075
5	1	0	-0.885722	1.295828	-0.469056
6	1	0	-1.516969	-0.074451	-1.428199
7	9	0	-2.677288	0.560107	0.098580
8	16	0	0.975338	-1.035488	-0.149920
9	6	0	1.671687	0.500979	0.018940
10	7	0	2.173524	1.564850	0.125910

ga-**6**

E = -668.549777 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.490336	0.784600	-0.230573
2	1	0	0.539029	0.962172	-1.306410
3	1	0	0.004757	1.629026	0.264623
4	6	0	1.879264	0.615250	0.344630
5	1	0	2.476673	1.508464	0.143155
6	1	0	1.846809	0.422807	1.419691
7	9	0	2.507168	-0.468578	-0.261682
8	16	0	-0.486328	-0.729717	0.094786
9	6	0	-2.023518	-0.026499	0.003487
10	7	0	-3.103862	0.447157	-0.055394

gg-**6**

E = -668.5519936 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.677303	-0.509638	0.872398
2	1	0	-1.354119	-1.366506	0.930882
3	1	0	-0.252463	-0.326892	1.862840
4	6	0	-1.436105	0.708980	0.392282
5	1	0	-2.173351	1.002293	1.145711
6	1	0	-0.765781	1.547374	0.186630
7	9	0	-2.120894	0.405522	-0.776366
8	16	0	0.647652	-1.042186	-0.262644
9	6	0	1.632020	0.325899	-0.099142
10	7	0	2.308522	1.288223	0.010045

gg′-**6**

E = -668.5496034 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.869461	-0.797296	0.612947
2	1	0	0.647481	-0.410287	1.609659
3	1	0	1.324581	-1.787719	0.719316
4	6	0	1.828698	0.111116	-0.126199
5	1	0	2.781003	0.160394	0.411430
6	1	0	1.995332	-0.237970	-1.148311
7	9	0	1.308357	1.394403	-0.192998
8	16	0	-0.689277	-1.106418	-0.278149
9	6	0	-1.484768	0.359862	0.021113
10	7	0	-2.110791	1.340936	0.221159

ag-**7**

E = -728.8382423 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.092436	-0.519788	-0.578192
2	1	0	0.937602	0.188284	-1.394712
3	1	0	1.654160	-1.380740	-0.947727
4	6	0	1.832035	0.142858	0.568308
5	1	0	1.991026	-0.558026	1.391574
6	1	0	1.292665	1.022990	0.922917
7	9	0	3.083813	0.560398	0.115513
8	16	0	-0.515742	-1.138505	-0.033514
9	6	0	-1.435985	0.392623	-0.098370
10	8	0	-0.946455	1.435541	-0.480200
11	6	0	-2.856947	0.263055	0.401136
12	1	0	-3.232149	-0.757565	0.303704
13	1	0	-2.872244	0.543910	1.458801
14	1	0	-3.491100	0.956834	-0.153635

gg-**7**

E = -728.8379098 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.104885	0.057201	-0.938872
2	1	0	0.676052	0.836775	-1.574247
3	1	0	1.754469	-0.581401	-1.542418
4	6	0	1.904059	0.697614	0.176175
5	1	0	1.261177	1.250645	0.863140
6	1	0	2.662479	1.366895	-0.241350
7	9	0	2.569360	-0.286512	0.904008
8	16	0	-0.242501	-0.991830	-0.344661
9	6	0	-1.432687	0.285856	0.002010
10	8	0	-1.214798	1.463841	-0.208450
11	6	0	-2.712256	-0.227897	0.622718
12	1	0	-2.881795	-1.282683	0.397974
13	1	0	-2.635460	-0.106738	1.707673
14	1	0	-3.546750	0.377025	0.263141

gg'-**7**

E = -728.835892 a.u.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.230368	0.628081	0.720028
2	1	0	-1.674554	1.522254	1.166619
3	1	0	-0.908833	-0.047445	1.517593
4	6	0	-2.253894	-0.053499	-0.165872
5	1	0	-2.544519	0.582271	-1.006470
6	1	0	-3.138793	-0.321373	0.419808
7	9	0	-1.724573	-1.226479	-0.690857
8	16	0	0.249122	1.134769	-0.184408
9	6	0	1.327686	-0.240763	0.220174
10	8	0	1.039550	-1.097076	1.026701
11	6	0	2.612352	-0.226510	-0.575594
12	1	0	2.444761	-0.798186	-1.493620
13	1	0	2.908099	0.789057	-0.847444
14	1	0	3.398002	-0.711827	0.005725