

Supplementary data for article:

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

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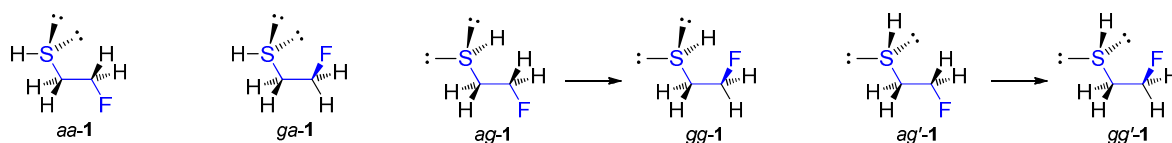
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Supporting Information

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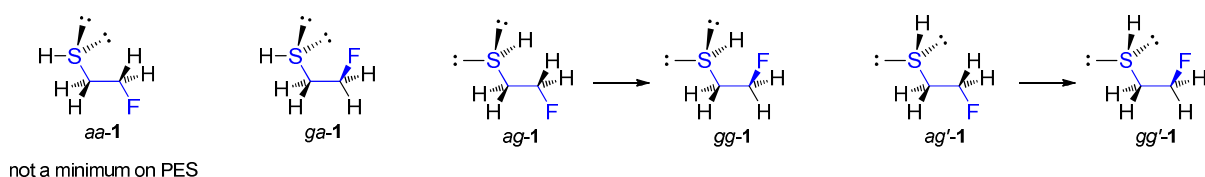
Table S1. Calculated relative electronic energies ΔE , enthalpies ΔH and free energies ΔG of four conformers of **1** and energy changes (in bold) occurring upon conformational isomerization (MP2/6-311++G(d,p) regular, B3LYP/6-311++G(d,p) italic). Values are in kcal/mol.



not a minimum on PES

conformation	gas-phase			in CH ₂ Cl ₂			in Me ₂ CO			in H ₂ O		
	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG
<i>ag/g'-1</i>	0.24	0.29	0.18	0.11	0.22	0.13	0.11	0.22	0.18	0.10	0.23	0.21
	<i>0.18</i>	<i>0.27</i>	<i>0.10</i>	<i>0.18</i>	<i>0.28</i>	<i>0.17</i>	<i>0.19</i>	<i>0.28</i>	<i>0.16</i>	<i>0.20</i>	<i>0.28</i>	<i>0.15</i>
<i>ga-1</i>	2.29	2.28	1.90	1.58	1.62	1.31	1.47	1.51	1.20	1.39	1.44	1.13
	<i>2.25</i>	<i>2.23</i>	<i>1.72</i>	<i>1.53</i>	<i>1.55</i>	<i>1.20</i>	<i>1.42</i>	<i>1.42</i>	<i>1.01</i>	<i>1.34</i>	<i>1.34</i>	<i>0.87</i>
<i>gg-1</i>	1.85	1.77	1.57	0.83	0.82	0.74	0.67	0.67	0.60	0.57	0.57	0.52
	<i>1.69</i>	<i>1.63</i>	<i>1.38</i>	<i>0.72</i>	<i>0.73</i>	<i>0.66</i>	<i>0.56</i>	<i>0.57</i>	<i>0.52</i>	<i>0.46</i>	<i>0.47</i>	<i>0.42</i>
<i>gg'-1</i>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>
<i>ag-1</i> → <i>gg-1</i>	1.61	1.48	1.39	0.71	0.60	0.60	0.57	0.44	0.43	0.47	0.34	0.31
	<i>1.51</i>	<i>1.37</i>	<i>1.28</i>	<i>0.54</i>	<i>0.45</i>	<i>0.49</i>	<i>0.37</i>	<i>0.29</i>	<i>0.36</i>	<i>0.27</i>	<i>0.19</i>	<i>0.28</i>
<i>ag'-1</i> → <i>gg'-1</i>	-0.24	-0.29	-0.18	-0.11	-0.22	-0.13	-0.11	-0.22	-0.18	-0.10	-0.23	-0.21
	<i>-0.18</i>	<i>-0.27</i>	<i>-0.10</i>	<i>-0.18</i>	<i>-0.28</i>	<i>-0.17</i>	<i>-0.19</i>	<i>-0.28</i>	<i>-0.16</i>	<i>-0.20</i>	<i>-0.28</i>	<i>-0.15</i>

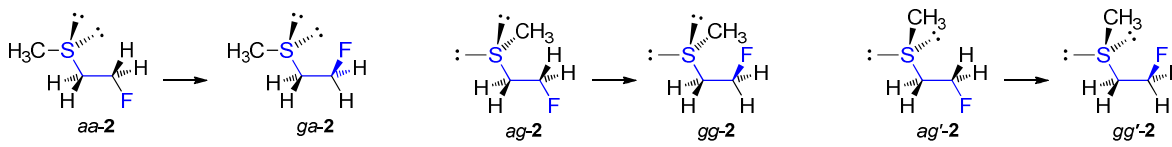
Table S2. Contribution of various energy components to the total binding interactions between two FCH₂· and ·CH₂SH fragments and energy changes ($\Delta\Delta E$ values, in bold) occurring upon conformational isomerization.^a EDA results for 2-fluoroethanol (FE) are included, too.^b Values are in kcal/mol.



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

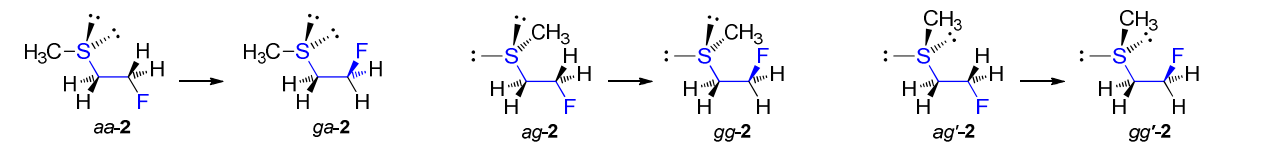
^a ΔE_{tot} = total binding energy between two radical fragments, ΔE_{def} = deformation energy, ΔE_{int} = interaction energy, ΔE_{elstat} = electrostatic energy, $\Delta E_{\text{ex+rep}}$ = exchange repulsion energy, ΔE_{oi} = orbital interaction energy, ΔE_{disp} = dispersion energy, ΔE_{iso} = isomerization energy, $\Delta\Delta E$ 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) occurring upon conformational isomerization (MP2/6-311++G(d,p)). Values are in kcal/mol.



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

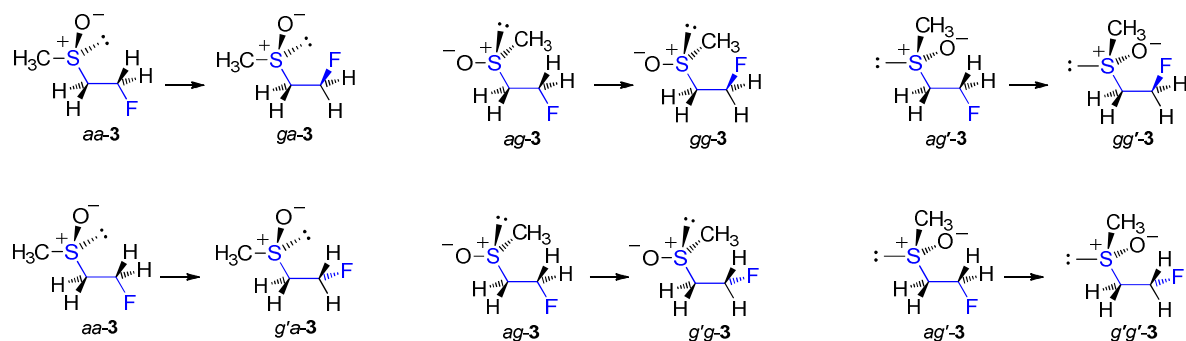
Table S4. Contribution of various energy components to the total binding interactions between two FCH₂[•] and [•]CH₂SCH₃ fragments and energy changes ($\Delta\Delta E$ values, in bold) occurring upon conformational isomerization.^a Values are in kcal/mol.



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

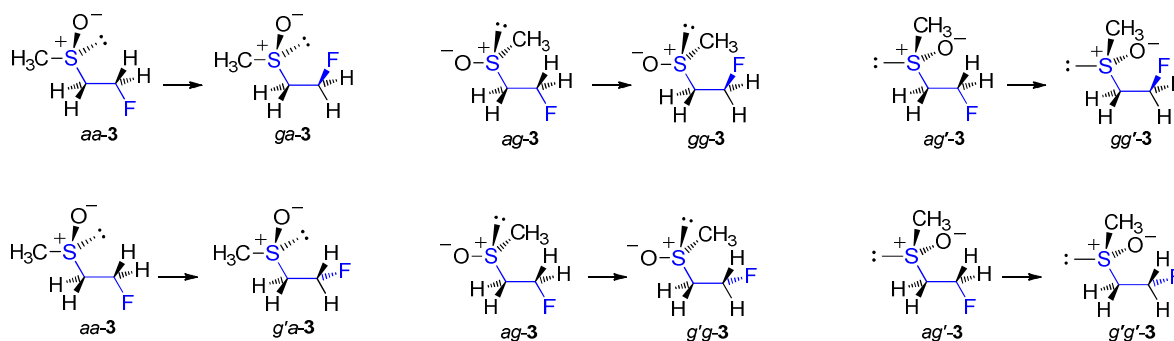
^a Labeling of various energy terms is the same as in Table S2. Values in parentheses are percentage contribution to all attractive interactions.

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



conformation	gas-phase			in CH ₂ Cl ₂			in Me ₂ CO			in H ₂ O		
	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG
<i>aa-3</i>	1.29	1.35	0.96	1.48	1.48	1.14	1.43	1.53	1.20	1.48	1.57	1.23
<i>ag-3</i>	2.93	3.05	2.75	2.56	2.56	2.60	2.33	2.54	2.59	2.32	2.53	2.58
<i>ag'-3</i>	1.95	2.08	1.69	2.15	2.15	2.10	1.96	2.20	2.19	1.99	2.24	2.27
<i>ga-3</i>	3.81	3.80	3.44	1.90	1.90	1.94	1.96	1.60	1.62	1.41	1.40	1.39
<i>gg-3</i>	2.23	2.27	2.06	1.54	1.54	1.38	1.42	1.51	1.41	1.39	1.47	1.36
<i>gg'-3</i>	0.00	0.00	0.00	0.59	0.59	0.70	0.58	0.70	0.80	0.65	0.76	0.85
<i>g'a-3</i>	0.29	0.24	0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<i>g'g-3</i>	1.14	1.11	0.91	1.08	1.08	0.97	1.11	1.15	1.05	1.17	1.20	1.10
<i>g'g'-3</i>	4.75	4.61	4.10	3.13	3.13	3.30	2.85	2.87	3.02	2.67	2.70	2.80
<i>aa-3</i> → <i>ga-3</i>	2.52	2.45	2.48	0.43	0.43	0.80	0.18	0.07	0.42	-0.06	-0.17	0.16
<i>aa-3</i> → <i>g'a-3</i>	-1.00	-1.11	-0.95	-1.48	-1.48	-1.14	-1.43	-1.53	-1.20	-1.48	-1.57	-1.23
<i>ag-3</i> → <i>gg-3</i>	-0.70	-0.78	-0.69	-1.01	-1.01	-1.22	-0.92	-1.03	-1.18	-0.93	-1.05	-1.22
<i>ag-3</i> → <i>g'g-3</i>	-1.79	-1.94	-1.84	-1.48	-1.48	-1.63	-1.22	-1.38	-1.54	-1.15	-1.32	-1.48
<i>ag'-3</i> → <i>gg'-3</i>	-1.95	-2.08	-1.69	-1.57	-1.57	-1.39	-1.38	-1.50	-1.39	-1.33	-1.47	-1.42
<i>ag'-3</i> → <i>g'g'-3</i>	2.80	2.53	2.41	0.98	0.98	1.20	0.89	0.67	0.84	0.68	0.46	0.52

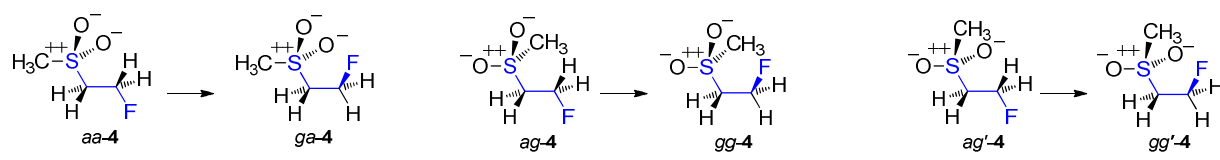
Table S6. Contribution of various energy components to the total binding interactions between two FCH₂[•] and [•]CH₂SOCH₃ fragments and energy changes ($\Delta\Delta E$ values, in bold) occurring upon conformational isomerization.^a Values are in kcal/mol.



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

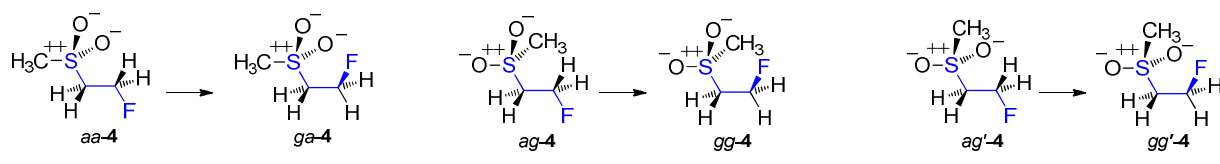
^a Labeling of various energy terms is the same as in Table S2. Values in parentheses are percentage contribution to all attractive interactions.

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



conformation	gas-phase			in CH ₂ Cl ₂			in Me ₂ CO			in H ₂ O		
	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG
<i>aa-4</i>	2.13	2.36	1.63	2.15	2.21	1.14	2.13	2.21	1.33	2.11	2.21	1.49
<i>ag/g'-4</i>	2.34	2.47	2.16	2.04	2.15	1.95	1.97	2.09	1.84	1.94	2.05	1.74
<i>ga-4</i>	3.46	3.54	3.27	1.70	1.71	1.57	1.34	1.36	1.27	1.11	1.13	1.03
<i>gg-4</i>	4.59	4.52	4.47	2.55	2.66	2.76	2.05	1.95	1.75	1.80	1.72	1.47
<i>gg'-4</i>	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
<i>aa-4</i> → <i>ga-4</i>	1.33	1.18	1.64	-0.45	-0.51	0.44	-0.78	-0.84	-0.06	-1.00	-1.08	-0.45
<i>ag-4</i> → <i>gg-4</i>	2.25	2.05	2.31	0.51	0.51	0.81	0.07	-0.13	-0.08	-0.13	-0.33	-0.27
<i>ag'-4</i> → <i>gg'-4</i>	-2.34	-2.47	-2.16	-2.04	-2.15	-1.95	-1.97	-2.09	-1.84	-1.94	-2.05	-1.74

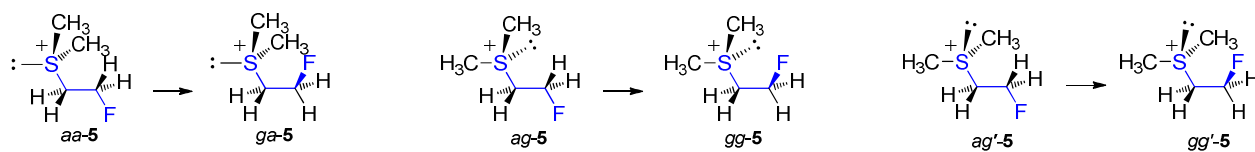
Table S8. Contribution of various energy components to the total binding interactions between two FCH₂[•] and [•]CH₂SO₂CH₃ fragments and energy changes ($\Delta\Delta E$ values, in bold) occurring upon conformational isomerization.^a Values are in kcal/mol.



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

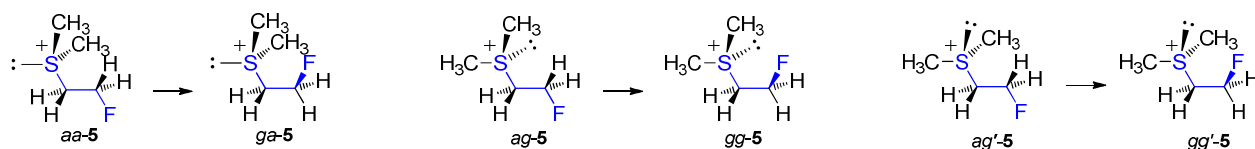
^a Labeling of various energy terms is the same as in Table S2. Values in parentheses are percentage contribution to all attractive interactions.

Table S9. Calculated relative electronic energies ΔE , enthalpies ΔH and free energies ΔG of five conformers of **5** and energy changes (in bold) occurring 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 ₂ Cl ₂			in Me ₂ CO			in H ₂ O		
	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG
<i>aa-5</i>	6.05	6.09	5.62	3.48	3.25	3.95	3.25	2.85	3.29	3.11	2.56	2.90
	<i>5.96</i>	<i>6.05</i>	<i>5.61</i>	<i>3.46</i>	<i>3.62</i>	<i>2.35</i>	<i>3.21</i>	<i>3.32</i>	<i>2.16</i>	<i>3.07</i>	<i>3.12</i>	<i>1.78</i>
<i>ag/g'-5</i>	5.03	5.01	4.50	2.53	2.79	2.86	2.31	2.45	2.25	2.18	2.24	1.95
	<i>4.88</i>	<i>4.92</i>	<i>4.35</i>	<i>2.48</i>	<i>2.73</i>	<i>2.44</i>	<i>2.23</i>	<i>2.49</i>	<i>2.37</i>	<i>2.08</i>	<i>2.34</i>	<i>2.41</i>
<i>ga-5</i>	0.75	0.73	1.12	0.92	0.96	1.25	0.97	1.02	1.29	1.01	1.06	1.47
	<i>0.84</i>	<i>0.89</i>	<i>1.02</i>	<i>1.06</i>	<i>1.12</i>	<i>1.01</i>	<i>1.08</i>	<i>1.13</i>	<i>1.09</i>	<i>1.10</i>	<i>1.09</i>	<i>0.91</i>
<i>gg-5</i>	0.00	0.00	0.00	0.00	0.00	0.11	0.00	0.00	0.00	0.00	0.00	0.00
	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>
<i>gg'-5</i>	1.61	1.65	1.52	0.65	0.51	0.00	0.53	0.48	0.26	0.47	0.38	0.19
	<i>1.90</i>	<i>1.90</i>	<i>1.61</i>	<i>0.57</i>	<i>0.71</i>	<i>0.55</i>	<i>0.45</i>	<i>0.56</i>	<i>0.49</i>	<i>0.38</i>	<i>0.46</i>	<i>0.48</i>
<i>aa-5</i> → <i>ga-5</i>	-5.30	-5.36	-4.50	-2.57	-2.29	-2.69	-2.28	-1.84	-2.00	-2.10	-1.50	-1.43
	<i>-5.12</i>	<i>-5.16</i>	<i>-4.59</i>	<i>-2.40</i>	<i>-2.50</i>	<i>-1.34</i>	<i>-2.13</i>	<i>-2.19</i>	<i>-1.07</i>	<i>-1.97</i>	<i>-2.03</i>	<i>-0.87</i>
<i>ag-5</i> → <i>gg-5</i>	-5.03	-5.01	-4.50	-2.53	-2.79	-2.75	-2.31	-2.45	-2.25	-2.18	-2.24	-1.95
	<i>-4.88</i>	<i>-4.92</i>	<i>-4.35</i>	<i>-2.48</i>	<i>-2.73</i>	<i>-2.44</i>	<i>-2.23</i>	<i>-2.49</i>	<i>-2.37</i>	<i>-2.08</i>	<i>-2.34</i>	<i>-2.41</i>
<i>ag'-5</i> → <i>gg'-5</i>	-3.42	-3.36	-2.98	-1.88	-2.28	-2.86	-1.78	-1.97	-1.99	-1.71	-1.86	-1.77
	<i>-2.98</i>	<i>-3.02</i>	<i>-2.74</i>	<i>-1.91</i>	<i>-2.02</i>	<i>-1.89</i>	<i>-1.79</i>	<i>-1.93</i>	<i>-1.89</i>	<i>-1.70</i>	<i>-1.88</i>	<i>-1.92</i>

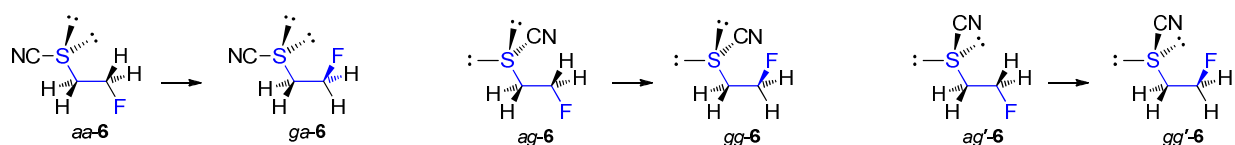
Table S10. Contribution of various energy components to the total binding interactions between two $\text{FCH}_2\cdot$ and $\cdot\text{CH}_2\text{S}(\text{CH}_3)_2^+$ fragments and energy changes ($\Delta\Delta\text{E}$ values, in bold) occurring upon conformational isomerization.^a Values are in kcal/mol.



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

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

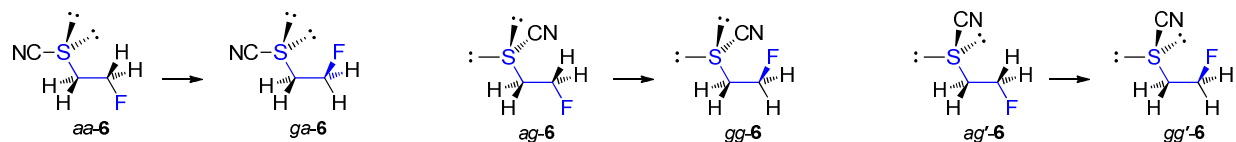
Table S11. Calculated relative electronic energies ΔE , enthalpies ΔH and free energies ΔG of five conformers of **6** and energy changes (in bold) occurring upon conformational isomerization (MP2/6-311++G(d,p) regular, B3LYP/6-311++G(d,p) italic). Values are in kcal/mol.



conformation	gas-phase			in CH ₂ Cl ₂			in Me ₂ CO			in H ₂ O		
	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG
<i>aa-6^a</i>	2.51	2.61	2.07	2.67	2.86	2.44	/	/	/	/	/	/
	<i>2.02</i>	<i>2.17</i>	<i>0.86</i>	<i>1.81</i>	<i>1.86</i>	<i>1.34</i>	<i>1.79</i>	<i>1.85</i>	<i>1.44</i>	<i>1.78</i>	<i>1.84</i>	<i>1.49</i>
<i>ag/g'-6</i>	0.00	0.00	0.00	0.35	0.45	0.39	0.41	0.52	0.46	0.46	0.56	0.51
	<i>0.01</i>	<i>0.12</i>	<i>0.09</i>	<i>0.57</i>	<i>0.70</i>	<i>0.73</i>	<i>0.64</i>	<i>0.77</i>	<i>0.80</i>	<i>0.68</i>	<i>0.82</i>	<i>0.84</i>
<i>ga-6</i>	1.50	1.50	1.22	1.39	1.44	1.03	1.40	1.46	1.09	1.41	1.47	1.12
	<i>0.96</i>	<i>0.99</i>	<i>0.60</i>	<i>0.95</i>	<i>0.99</i>	<i>0.63</i>	<i>0.95</i>	<i>1.00</i>	<i>0.63</i>	<i>0.96</i>	<i>1.00</i>	<i>0.60</i>
<i>gg-6</i>	0.16	0.06	0.07	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>
<i>gg'-6</i>	1.66	1.50	1.51	0.45	0.41	0.41	0.29	0.26	0.28	0.19	0.16	0.20
	<i>1.46</i>	<i>1.43</i>	<i>1.39</i>	<i>0.44</i>	<i>0.43</i>	<i>0.39</i>	<i>0.27</i>	<i>0.27</i>	<i>0.34</i>	<i>0.16</i>	<i>0.17</i>	<i>0.28</i>
<i>aa-6</i> → <i>ga-6</i>	-1.01	-1.11	-0.85	-1.28	-1.42	-1.41	/	/	/	/	/	/
	<i>-1.06</i>	<i>-1.19</i>	<i>-0.25</i>	<i>-1.43</i>	<i>-1.56</i>	<i>-1.44</i>	<i>-1.48</i>	<i>-1.62</i>	<i>-1.61</i>	<i>-1.51</i>	<i>-1.66</i>	<i>-1.74</i>
<i>ag-6</i> → <i>gg-6</i>	0.16	0.06	0.07	-0.35	-0.45	-0.39	-0.41	-0.52	-0.46	-0.46	-0.56	-0.51
	<i>-0.01</i>	<i>-0.12</i>	<i>-0.09</i>	<i>-0.57</i>	<i>-0.70</i>	<i>-0.73</i>	<i>-0.64</i>	<i>-0.77</i>	<i>-0.80</i>	<i>-0.68</i>	<i>-0.82</i>	<i>-0.84</i>
<i>ag'-6</i> → <i>gg'-6</i>	1.66	1.50	1.51	0.10	-0.04	0.03	-0.12	-0.26	-0.19	-0.26	-0.40	-0.32
	<i>1.46</i>	<i>1.30</i>	<i>1.30</i>	<i>-0.13</i>	<i>-0.27</i>	<i>-0.35</i>	<i>-0.37</i>	<i>-0.50</i>	<i>-0.46</i>	<i>-0.52</i>	<i>-0.65</i>	<i>-0.56</i>

^a Optimization of *aa* form in Me₂CO and H₂O converged into *ag* form.

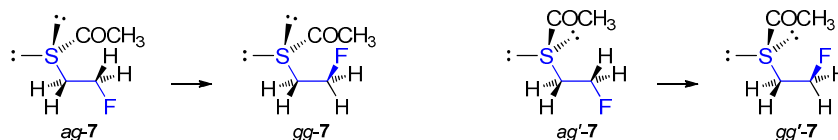
Table S12. Contribution of various energy components to the total binding interactions between two FCH₂· and ·CH₂SCN fragments and energy changes ($\Delta\Delta E$ values, in bold) occurring upon conformational isomerization.^a Values are in kcal/mol.



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

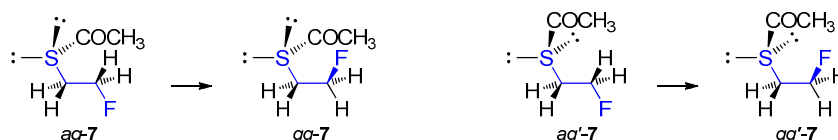
^a Labeling of various energy terms is the same as in Table S2. Values in parentheses are percentage contribution to all attractive interactions.

Table S13. Calculated relative electronic energies ΔE , enthalpies ΔH and free energies ΔG of three conformers of **7** and energy changes (in bold) occurring 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 ₂ Cl ₂			in Me ₂ CO			in H ₂ O		
	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG	ΔE	ΔH	ΔG
<i>ag/g'-7</i>	0.00	0.00	0.00	0.00	0.05	0.08	0.00	0.06	0.10	0.00	0.06	0.11
	<i>0.00</i>	<i>0.03</i>	<i>0.27</i>	<i>0.15</i>	<i>0.24</i>	<i>0.15</i>	<i>0.16</i>	<i>0.25</i>	<i>0.00</i>	<i>0.17</i>	<i>0.25</i>	<i>0.00</i>
<i>gg-7</i>	0.22	0.11	0.12	0.05	0.00	0.00	0.05	0.00	0.00	0.04	0.00	0.00
	<i>0.07</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.00</i>	<i>0.35</i>	<i>0.00</i>	<i>0.00</i>	<i>0.02</i>
<i>gg'-7</i>	1.45	1.34	1.32	0.78	0.70	0.60	0.66	0.59	0.52	0.58	0.51	0.47
	<i>1.21</i>	<i>1.11</i>	<i>1.40</i>	<i>0.55</i>	<i>0.53</i>	<i>1.07</i>	<i>0.42</i>	<i>0.40</i>	<i>1.21</i>	<i>0.33</i>	<i>0.31</i>	<i>0.75</i>
<i>ag-7 → gg-7</i>	0.22	0.11	0.12	0.05	-0.05	-0.08	0.05	-0.06	-0.10	0.04	-0.06	-0.11
	<i>0.07</i>	<i>-0.03</i>	<i>-0.27</i>	<i>-0.15</i>	<i>-0.24</i>	<i>-0.15</i>	<i>-0.16</i>	<i>-0.25</i>	<i>0.35</i>	<i>-0.17</i>	<i>-0.25</i>	<i>0.02</i>
<i>ag'-7 → gg'-7</i>	1.45	1.34	1.32	0.78	0.65	0.52	0.66	0.53	0.42	0.58	0.45	0.36
	<i>1.21</i>	<i>1.08</i>	<i>1.13</i>	<i>0.40</i>	<i>0.29</i>	<i>0.92</i>	<i>0.26</i>	<i>0.15</i>	<i>1.21</i>	<i>0.17</i>	<i>0.06</i>	<i>0.75</i>

Table S14. Contribution of various energy components to the total binding interactions between two FCH₂· and ·CH₂SCOCH₃ fragments and energy changes ($\Delta\Delta E$ values, in bold) occurring upon conformational isomerization.^a Values are in kcal/mol.



conformation	ΔE_{tot}	ΔE_{def}	ΔE_{int}	ΔE_{elstat}	$\Delta E_{\text{ex+rep}}$	ΔE_{oi}	ΔE_{disp}
	ΔE_{iso}	$\Delta\Delta E_{\text{def}}$	$\Delta\Delta E_{\text{int}}$	$\Delta\Delta E_{\text{elstat}}$	$\Delta\Delta E_{\text{ex+rep}}$	$\Delta\Delta E_{\text{oi}}$	$\Delta\Delta E_{\text{disp}}$
<i>ag/g'-7</i>	-96.34	13.39	-109.73	-151.70	229.01	-157.14	-29.90
<i>gg-7</i>	-96.12	13.97	-110.09	-152.33	229.45	-157.67	-29.54
<i>gg'-7</i>	-94.91	13.71	-108.63	-151.23	229.95	-157.38	-29.96
<i>ag-7 → gg-7</i>	0.22	0.58	-0.36	-0.63	0.44	-0.53	0.36
				(54%)		(46%)	
<i>ag'-7 → gg'-7</i>	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).

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

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 orbitals (HF/6-311++G(d,p)). Values are in a.u.

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