

**Electronic Supporting Information for:**

**Modulating the Radical Reactivity of Phenyl Radicals with the Help of Distonic Charges: It is all About Electrostatic Catalysis.**

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Table of Contents

S1. Comparison of the reactivity trends for the radical ions ( <b>1-12</b> ) and their uncharged analogues ( <b>1A-12A</b> ) at different theoretical levels.....	S2-S9
S2. Effect of solvents on radical reactivity.....	S9-S10
S3. Distance-dependent reactivity modulation.....	S10
S4. Note on the connection to the experiment.....	S11-S12
S5. Calculated NBO charges of the distonic radical systems.....	S13
S6. Correlation between the activation barriers and the odd spin densities at the radical sites.....	S13-S14
S7. OEEF model for the ortho- and meta-substituted distonic radical ions.....	S14-S17
S8. Further confirmation of the qualitative Valence Bond reactivity diagram (VBSCD) shown in Fig. 7 .....	S17-S18
S9. Cartesian coordinates of all relevant reactants, intermediates, and transition states.....	S18-S76

**S1. Comparison of the reactivity trends for the radical ions (**1-12**) and their uncharged analogues (**1A-12A**) at different theoretical levels**

Table S1: Reaction energies for the hydrogen abstraction reaction from CH<sub>4</sub> by the distonic radical ions (**1-12**) and their uncharged radical analogues (**1A-12A**) calculated at different levels of theory [L1: ωB97X-D/def2-TZVP, and L2: UB3LYP-D3/def2-TZVP].

Level of theory	charged radical(x)/uncharged radical(xA)				
		ΔE (kcal mol <sup>-1</sup> ) <b>R→RC</b>	ΔE <sup>‡</sup> (kcal mol <sup>-1</sup> ) <b>RC→TS</b>	ΔE (kcal mol <sup>-1</sup> ) <b>TS→P</b>	ΔE (kcal mol <sup>-1</sup> ) <b>R→P</b>
<b>L1</b>	<b>1</b>	-0.9	4.2	-13.6	-10.3
	<b>1A</b>	-0.5	6.9	-15.1	-8.7
<b>L2</b>	<b>1</b>	-1.0	3.4	-13.1	-10.7
	<b>1A</b>	-0.6	6.2	-14.7	-9.1
<b>L1</b>	<b>2</b>	-1.0	4.7	-14.0	-10.3
	<b>2A</b>	-0.7	7.0	-15.1	-8.8
<b>L2</b>	<b>2</b>	-0.9	3.9	-13.6	-10.6
	<b>2A</b>	-0.6	6.2	-14.8	-9.2
<b>L1</b>	<b>3</b>	-0.9	4.7	-13.5	-9.7
	<b>3A</b>	-0.4	6.9	-14.9	-8.4
<b>L2</b>	<b>3</b>	-1.0	3.9	-13.2	-10.3
	<b>3A</b>	-0.6	6.4	-14.5	-8.7
<b>L1</b>	<b>4</b>	-0.8	6.4	-14.4	-8.8
	<b>4A</b>	-0.7	7.3	-14.6	-8.0
<b>L2</b>	<b>4</b>	-0.7	5.5	-14.0	-9.2
	<b>4A</b>	-0.6	6.6	-14.3	-8.3
<b>L1</b>	<b>5</b>	-0.9	4.1	-13.2	-10.0
	<b>5A</b>	-0.6	7.1	-14.8	-8.3
<b>L2</b>	<b>5</b>	-1.1	3.3	-12.8	-10.6
	<b>5A</b>	-0.6	6.3	-14.5	-8.8

<b>L1</b>	<b>6</b>	-0.9	5.1	-13.7	-9.5
	<b>6A</b>	-0.6	7.5	-14.2	-7.3
<b>L2</b>	<b>6</b>	-0.9	4.3	-13.3	-9.9
	<b>6A</b>	-0.6	6.5	-14.0	-8.1
<b>L1</b>	<b>7</b>	-0.9	5.0	-13.9	-9.8
	<b>7A</b>	-0.6	7.0	-14.9	-8.5
<b>L2</b>	<b>7</b>	-0.9	4.1	-13.5	-10.3
	<b>7A</b>	-0.6	6.3	-14.6	-8.9
<b>L1</b>	<b>8</b>	-0.9	4.4	-13.3	-9.8
	<b>8A</b>	-0.6	7.4	-14.5	-7.7
<b>L2</b>	<b>8</b>	-1.0	3.6	-12.8	-10.2
	<b>8A</b>	-0.6	6.7	-14.2	-8.1
<b>L1</b>	<b>9</b>	-0.7	5.4	-14.0	-9.3
	<b>9A</b>	-0.6	7.4	-14.6	-7.8
<b>L2</b>	<b>9</b>	-0.8	4.8	-13.6	-9.6
	<b>9A</b>	-0.6	6.7	-14.2	-8.1
<b>L1</b>	<b>10</b>	-0.9	8.4	-13.8	-6.3
	<b>10A</b>	-0.6	7.4	-14.5	-7.7
<b>L2</b>	<b>10</b>	-0.9	7.7	-13.3	-6.5
	<b>10A</b>	-0.6	6.6	-14.1	-8.1
<b>L1</b>	<b>11</b>	-1.0	8.6	-13.6	-6.0
	<b>11A</b>	-0.6	7.6	-14.3	-7.3
<b>L2</b>	<b>11</b>	-1.0	7.8	-13.0	-6.2
	<b>11A</b>	-0.6	6.8	-14.0	-7.8
<b>L1</b>	<b>12</b>	-1.4	7.0	-13.7	-8.1
	<b>12A</b>	-0.6	7.0	-15.1	-8.7
<b>L2</b>	<b>12</b>	-3.4	8.3	-13.1	-8.2
	<b>12A</b>	-0.6	6.2	-14.7	-9.1
<b>L1</b>	<b>5<sup>m</sup></b>	-0.8	3.5	-13.2	-10.5
	<b>5A<sup>m</sup></b>	-0.6	7.4	-14.4	-7.6
<b>L2</b>	<b>5<sup>m</sup></b>	-1.0	2.8	-12.5	-10.7
	<b>5A<sup>m</sup></b>	-0.6	6.7	-14.0	-7.9

<b>L1</b>	<b>5<sup>o</sup></b>	-1.2	3.3	-12.4	-10.3
	<b>5A<sup>o</sup></b>	-0.8	6.7	-14.3	-8.4
<b>L2</b>	<b>5<sup>o</sup></b>	-1.2	2.3	-11.7	-10.6
	<b>5A<sup>o</sup></b>	-0.7	6.0	-13.8	-8.5
<b>L1</b>	<b>10<sup>m</sup></b>	-1.1	9.1	-13.3	-5.3
	<b>10A<sup>m</sup></b>	-0.7	7.3	-14.7	-8.1
<b>L2</b>	<b>10<sup>m</sup></b>	-1.0	8.4	-12.4	-5.0
	<b>10A<sup>m</sup></b>	-0.6	6.5	-14.2	-8.3
<b>L1</b>	<b>10<sup>o</sup></b>	-2.8	8.9	-14.2	-8.1
	<b>10A<sup>o</sup></b>	-0.9	7.7	-15.3	-8.5
<b>L2</b>	<b>10<sup>o</sup></b>	-3.0	8.2	-13.4	-8.2
	<b>10A<sup>o</sup></b>	-1.3	7.2	-14.8	-8.9

**R** stands for separated reactants; **RC** represents reactant complex; **TS** represents transition state and **P** stands for products.

Table S2: Activation energies for the hydrogen abstraction reaction from CH<sub>4</sub> by the distonic radical ions and their uncharged radical analogues calculated at different levels of theory [**L1**: U<sub>ω</sub>B97X-D/def2-TZVP, **L2**: UB3LYP-D3/def2-TZVP].

charged radical(x)/uncharged radical(xA)/uncharged radical + OEEF(x <sup>EF</sup> )		
	$\Delta E^\ddagger$ (kcal mol <sup>-1</sup> ) RC → TS (U <sub>ω</sub> B97X-D/def2-TZVP)	$\Delta E^\ddagger$ (kcal mol <sup>-1</sup> ) RC → TS (UB3LYP-D3/def2-TZVP)
<b>1</b>	4.2	3.4
<b>1A</b>	6.9	6.2
<b>1<sup>EF</sup></b>	4.2	3.6
<b>2</b>	4.7	3.9
<b>2A</b>	7.0	6.2

<b>2<sup>EF</sup></b>	4.8	4.1
<b>3</b>	4.7	3.9
<b>3A</b>	6.9	6.4
<b>3<sup>EF</sup></b>	4.0	3.5
<b>4</b>	6.4	5.5
<b>4A</b>	7.3	6.6
<b>4<sup>EF</sup></b>	6.9	6.1
<b>5</b>	4.1	3.3
<b>5A</b>	7.1	6.3
<b>5<sup>EF</sup></b>	4.2	3.4
<b>6</b>	5.1	4.3
<b>6A</b>	7.5	6.5
<b>6<sup>EF</sup></b>	4.4	3.6
<b>7</b>	5.0	4.1
<b>7A</b>	7.0	6.3
<b>7<sup>EF</sup></b>	4.5	3.8
<b>8</b>	4.4	3.6
<b>8A</b>	7.4	6.7
<b>8<sup>EF</sup></b>	3.8	3.8
<b>9</b>	5.4	4.8
<b>9A</b>	7.4	6.7
<b>9<sup>EF</sup></b>	5.7	5.1
<b>10</b>	8.4	7.7
<b>10A</b>	7.4	6.6
<b>10<sup>EF</sup></b>	8.6	7.7
<b>11</b>	8.6	7.8
<b>11A</b>	7.6	6.8
<b>11<sup>EF</sup></b>	8.5	7.7
<b>12</b>	7.0	6.2
<b>12A</b>	7.0	5.9
<b>12<sup>EF</sup></b>	7.7	6.6
<b>5°</b>	3.3	2.3

<b>5A<sup>o</sup></b>	6.7	6.0
<b>5<sup>o</sup>EF</b>	3.7	3.4
<b>5<sup>m</sup></b>	3.5	2.8
<b>5A<sup>m</sup></b>	7.4	6.7
<b>5<sup>m</sup>EF</b>	4.3	3.6
<b>10<sup>o</sup></b>	8.9	8.2
<b>10A<sup>o</sup></b>	7.7	7.2
<b>10<sup>o</sup>EF</b>	8.9	8.1
<b>10<sup>m</sup></b>	9.1	8.4
<b>10A<sup>m</sup></b>	7.3	6.5
<b>10<sup>m</sup>EF</b>	8.6	7.4

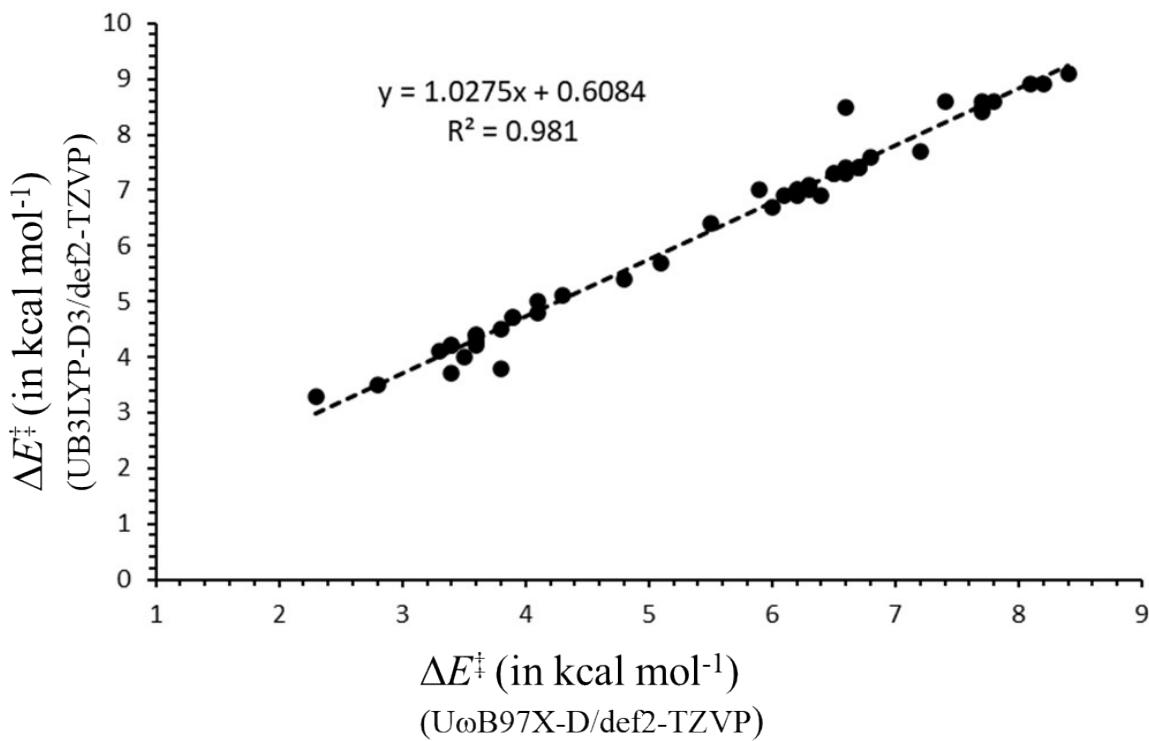


Fig. S1. Correlation between the hydrogen abstraction activation barriers calculated at B3LYP-D3/def2-TZVP and  $\omega$ B97X-D/def2-TZVP levels of theory.

Table S3: Activation energies for the hydrogen abstraction reaction from CH<sub>4</sub> by the distonic radical ions (**1** and **10**) and their uncharged radical analogues (**1A** and **10A**) calculated at different levels of theory [**L1**: UωB97X-D/def2-TZVP, **L2**: UB3LYP-D3/def2-TZVP, **L3**: UPBE0-D3/def2-TZVP and **L4**: UM06-2X/def2-TZVP].

	charged radical(x)/uncharged radical(xA)/uncharged radical + OEEF(x <sup>EF</sup> )			
	$\Delta E^\ddagger$ (kcal mol <sup>-1</sup> ) <b>RC→TS</b> (UωB97X-D/def2-TZVP)	$\Delta E^\ddagger$ (kcal mol <sup>-1</sup> ) <b>RC→TS</b> (UB3LYP-D3/def2-TZVP)	$\Delta E^\ddagger$ (kcal mol <sup>-1</sup> ) <b>RC→TS</b> (UPBE0-D3/def2-TZVP)	$\Delta E^\ddagger$ (kcal mol <sup>-1</sup> ) <b>RC→TS</b> (UM06-2X/def2-TZVP)
<b>1</b>	4.2	3.4	3.0	7.2
<b>1A</b>	6.9	6.2	5.6	9.4
<b>1<sup>EF</sup></b>	4.2	3.6	2.8	7.0
<b>10</b>	8.4	7.7	7.0	10.4
<b>10A</b>	7.4	6.6	6.0	10.0
<b>10<sup>EF</sup></b>	8.6	7.7	7.1	10.7

Table S4: Different activation barriers ( $\Delta E^\ddagger$ ,  $\Delta H^\ddagger$ , and  $\Delta G^\ddagger$ ) for the hydrogen abstraction reaction from CH<sub>4</sub> by the distonic radical ions (**1-12**) and their uncharged radical analogues (**1A-12A**) calculated at different levels of theory [L1: ωB97X-D/def2-TZVP, and L2: UB3LYP-D3/def2-TZVP].

Level of theory		<b>R→TS</b>				<b>RC→TS</b>			
		$\Delta E^\ddagger$ (kcal mol <sup>-1</sup> )	$\Delta H^\ddagger$ (kcal mol <sup>-1</sup> )	$\Delta G^\ddagger$ (kcal mol <sup>-1</sup> )	-TΔS <sup>‡</sup> (kcal mol <sup>-1</sup> )	$\Delta E^\ddagger$ (kcal mol <sup>-1</sup> )	$\Delta H^\ddagger$ (kcal mol <sup>-1</sup> )	$\Delta G^\ddagger$ (kcal mol <sup>-1</sup> )	-TΔS <sup>‡</sup> (kcal mol <sup>-1</sup> )
<b>L1</b>	<b>1</b>	3.3	2.9	11.3	8.4	4.2	3.2	6.4	3.2
	<b>1A</b>	6.4	6.0	14.3	8.3	6.9	5.8	9.0	3.2
<b>L2</b>	<b>1</b>	2.4	2.1	10.4	8.3	3.4	2.4	5.7	3.3
	<b>1A</b>	5.6	5.3	13.2	7.9	6.2	5.2	8.4	3.2
<b>L1</b>	<b>2</b>	3.7	3.5	12.0	8.5	4.7	4.3	5.8	1.5

	<b>2A</b>	6.3	5.4	16.1	10.7	7.0	5.3	11.7	6.4
<b>L2</b>	<b>2</b>	3.0	2.7	10.3	7.6	3.9	2.9	5.5	2.6
	<b>2A</b>	5.6	5.3	13.2	7.9	6.2	5.2	8.4	3.2
<b>L1</b>	<b>3</b>	3.8	3.5	12.0	8.5	4.7	3.7	7.6	3.9
	<b>3A</b>	6.5	6.3	14.0	7.7	6.9	6.0	8.3	2.3
<b>L2</b>	<b>3</b>	2.9	2.7	11.2	8.5	3.9	2.9	6.8	3.9
	<b>3A</b>	5.8	5.5	13.9	8.4	6.4	5.3	9.0	3.7
<b>L1</b>	<b>4</b>	5.6	5.3	13.9	8.6	6.4	5.3	9.7	4.4
	<b>4A</b>	6.6	6.4	14.8	8.4	7.3	6.3	9.8	3.5
<b>L2</b>	<b>4</b>	4.8	4.6	12.2	7.6	5.5	4.5	7.3	2.8
	<b>4A</b>	6.0	5.7	13.3	7.6	6.6	5.5	8.4	2.9
<b>L1</b>	<b>5</b>	3.2	2.8	11.0	8.2	4.2	3.1	6.1	3.0
	<b>5A</b>	6.5	5.5	17.6	12.1	7.1	5.4	12.3	6.9
<b>L2</b>	<b>5</b>	2.2	1.4	12.2	10.8	3.3	1.7	8.0	6.3
	<b>5A</b>	5.7	4.7	16.0	11.3	6.3	4.6	5.0	0.4
<b>L1</b>	<b>6</b>	4.2	3.9	12.5	8.6	5.1	4.7	5.8	1.1
	<b>6A</b>	6.9	6.5	15.1	8.6	7.5	6.4	10.3	3.9
<b>L2</b>	<b>6</b>	3.4	3.1	10.7	7.6	4.3	3.3	6.2	2.9
	<b>6A</b>	5.9	5.6	14.0	8.4	6.5	5.4	9.2	3.8
<b>L1</b>	<b>7</b>	4.1	3.7	11.4	7.7	5.0	4.5	5.3	0.8
	<b>7A</b>	6.4	6.1	14.8	8.7	7.0	6.5	8.5	2.0
<b>L2</b>	<b>7</b>	3.2	2.3	13.3	11.0	4.1	2.5	8.7	6.2
	<b>7A</b>	5.7	5.3	13.9	8.6	6.3	5.2	9.0	3.8
<b>L1</b>	<b>8</b>	3.5	3.2	11.6	8.4	4.4	3.4	7.2	3.8
	<b>8A</b>	6.8	6.0	16.5	10.5	7.4	5.8	11.9	6.1
<b>L2</b>	<b>8</b>	2.6	2.3	9.9	7.6	3.6	2.6	5.6	3.0
	<b>8A</b>	6.1	5.8	14.1	8.3	6.7	5.6	9.2	3.6
<b>L1</b>	<b>9</b>	4.7	4.4	13.1	8.7	5.4	4.5	7.8	3.3
	<b>9A</b>	6.8	6.4	15.2	8.8	7.4	6.3	10.5	4.2
<b>L2</b>	<b>9</b>	4.0	3.6	11.9	8.3	4.8	3.7	7.2	3.5
	<b>9A</b>	6.1	5.8	13.8	8.0	6.7	5.7	9.0	3.3
<b>L1</b>	<b>10</b>	7.5	7.3	15.4	8.1	8.4	7.4	11.6	4.2

	<b>10A</b>	6.8	6.5	15.1	8.6	7.4	6.3	11.0	4.7
<b>L2</b>	<b>10</b>	6.8	6.4	14.6	8.2	7.7	6.6	10.8	4.2
	<b>10A</b>	6.0	5.7	13.4	7.7	6.6	5.5	8.5	3.0
<b>L1</b>	<b>11</b>	7.6	7.3	15.8	8.5	8.6	7.5	11.7	4.2
	<b>11A</b>	7.0	6.6	15.1	8.5	7.6	6.5	10.7	4.2
<b>L2</b>	<b>11</b>	6.8	6.5	14.5	8.0	7.8	6.7	11.4	4.7
	<b>11A</b>	6.2	5.9	13.9	8.0	6.8	5.7	9.0	3.3
<b>L1</b>	<b>12</b>	5.6	5.2	13.8	8.6	7.0	5.9	10.1	4.2
	<b>12A</b>	6.4	5.9	14.3	8.4	7.0	5.8	9.7	3.9
<b>L2</b>	<b>12</b>	4.9	4.6	12.5	7.9	6.2	5.2	9.2	4.0
	<b>12A</b>	5.6	5.3	13.6	8.3	5.9	4.6	13.9	9.3

## S2. Effect of solvents on radical reactivity

To examine the influence of the solvent, we focused on two solvents with different polarities, *viz.* toluene and DCM. The calculated results showed exactly the same trends as in the gas phase, though – as one could logically expect – we observe some screening of the charges and thus a moderate attenuation of the charge-effect (cf. Tables S5).

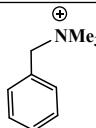
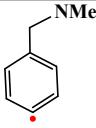
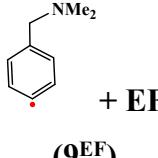
Table S5: Activation energies for the hydrogen abstraction reaction from CH<sub>4</sub> by the distonic radical ions (**1** and **10**) and their uncharged radical analogues (**1A** and **10A**) calculated at different conditions [L1: ωB97X-D(PCM=solvent)/def2-TZVP and L2: UB3LYP-D3(PCM=solvent)/def2-TZVP level of theory.]

		charged radical(x)/uncharged radical(xA)/uncharged radical + OEEF(x <sup>EF</sup> )		
		$\Delta E^\ddagger$ (kcal mol <sup>-1</sup> ) <b>RC→TS</b> <b>(Gas phase)</b>	$\Delta E^\ddagger$ (kcal mol <sup>-1</sup> ) <b>RC→TS</b> <b>(Toluene)</b>	$\Delta E^\ddagger$ (kcal mol <sup>-1</sup> ) <b>RC→TS</b> <b>(Dichloromethane)</b>
<b>L1</b>	<b>1</b>	4.2	4.7	5.9
	<b>1A</b>	6.9	6.9	7.0
	<b>1<sup>EF</sup></b>	4.2	3.5	3.0

<b>L2</b>	<b>1</b>	3.4	4.0	5.4
	<b>1A</b>	6.2	6.3	6.3
	<b>1<sup>EF</sup></b>	3.6	3.1	2.5
<b>L1</b>	<b>10</b>	8.4	7.9	7.8
	<b>10A</b>	7.4	7.2	7.2
	<b>10<sup>EF</sup></b>	8.6	8.5	8.6
<b>L2</b>	<b>10</b>	7.7	7.0	7.2
	<b>10A</b>	6.6	6.5	6.5
	<b>10<sup>EF</sup></b>	7.7	7.8	7.9

### S3. Distance-dependent reactivity modulation

Table S6: Activation energies for the hydrogen abstraction reaction from CH<sub>4</sub> by the distonic radical ion (**9**) and its uncharged radical analogue (**9A**) calculated at different levels of theory.

charged radical(x)/uncharged radical(xA)/uncharged radical + OEEF(x <sup>EF</sup> )		
	$\Delta E^\ddagger$ (kcal mol <sup>-1</sup> ) <b>RC→TS</b> <b>(UB3LYP-D3/def2-TZVP)</b>	$\Delta E^\ddagger$ (kcal mol <sup>-1</sup> ) <b>RC→TS</b> <b>(UωB97X-D/def2-TZVP)</b>
 <b>(9)</b>	4.8	5.4
 <b>(9A)</b>	6.7	7.4
 <b>(9<sup>EF</sup>)</b>	5.1	5.7

#### S4. Note on the connection to the experiment

Note that in the main text, the barrier from the reactant complex (RC) to the transition state (TS) was consistently considered as a reference for evaluating the charge-induced modification of the reaction barrier. From Table S4 and Fig. S2, one can infer that using the individual reactants as a reference for the barrier leads to the exact same trends. Hence, we can unequivocally conclude that remote positive charges indeed reduce the height of the potential energy hill in the potential energy surface (PES), whereas a remote negative charge increases the energy hill.

This realization, *i.e.*, that the PES modification can be observed irrespective of the reference used, is important for connecting our results to the actual (gas-phase) experiments. As pointed out to us by Prof. Chen, in the actual mass spectroscopy experiments featured in Ref. 13 in the main text, the chemical system is best described as a microcanonical ensemble (NVE, *i.e.*, the system cannot exchange energy with its environment during the reaction – the energy is conserved) instead of the usual canonical ensemble (NVT, *i.e.*, the system is in thermal equilibrium – the temperature is conserved) encountered in the liquid phase. Irrespective of whether temperature or energy are conserved, the shape of the PES will tell us something about the rate of the reaction: even when the molecular system has a constant energy, a high potential energy hill will be harder to cross than a low energy hill. Hence, the barrier modifications emerging from our calculations can be directly connected to changes in the experimental reaction rates.

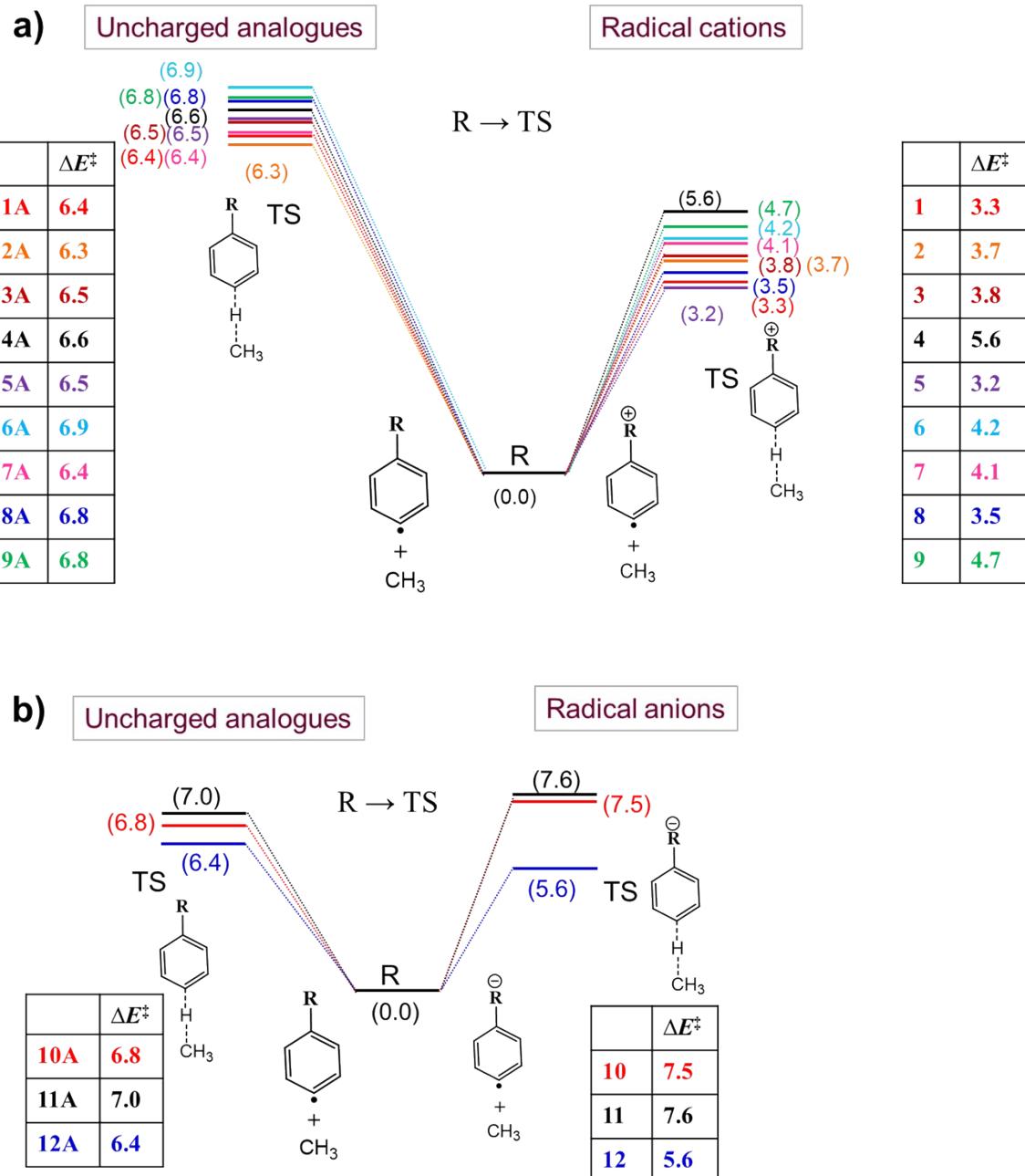


Fig. S2. Energy diagrams related to the H-abstraction reactions involving a) radical cations (**1-9**) and their uncharged analogues (**1A-9A**), and b) radical anions (**10-12**) and their neutral analogues (**10A-12A**). The presented energy values ( $R \rightarrow TS$ , in kcal mol<sup>-1</sup>) consist of electronic energies + zero-point energies.

## S5. Calculated NBO charges of the distonic radical systems

Table S7: NBO charges on different fragments of the distonic radical systems (**1/1A-11/12A**).

Radical systems (x/xA)	xA			X		
	q (uncharged substituent)	q (radical site)	q (rest phenyl ring)	q (charged substituent)	q (radical site)	q (rest phenyl ring)
<b>1/1A</b>	-0.040	0.133	-0.093	0.690	0.243	0.067
<b>2/2A</b>	-0.032	0.129	-0.097	0.710	0.234	0.056
<b>3/3A</b>	0.199	0.159	-0.358	0.978	0.256	0.022
<b>4/4A</b>	0.004	0.172	-0.176	0.943	0.208	-0.151
<b>5/5A</b>	0.166	0.162	-0.328	0.899	0.269	-0.168
<b>6/6A</b>	0.292	0.182	-0.474	1.167	0.249	-0.416
<b>7/7A</b>	-0.132	0.157	-0.025	0.692	0.234	0.074
<b>8/8A</b>	0.257	0.185	-0.442	1.063	0.271	-0.334
<b>9/9A</b>	0.049	0.172	-0.221	0.932	0.229	-0.161
<b>10/10A</b>	0.004	0.203	-0.207	-0.787	0.124	-0.337
<b>11/11A</b>	0.314	0.205	-0.519	-0.553	0.112	-0.559
<b>12/12A</b>	-0.174	0.143	0.031	-0.769	0.004	-0.235

## S6. Correlation between the activation barriers and the odd spin densities at the radical sites

It is important to point out that even though the spin-density values on the radical site fluctuate barely for the investigated systems, these values do, in fact, correlate nicely with the corresponding calculated barrier heights: a high spin density corresponds to a low activation energy and vice versa (cf. Fig. S3). However, it should be evident from our discussion above that this observed correlation does not imply causation in any way: the charge-induced fluctuations in the spin-density values are simply far too small to account for the significant

shifts in barrier height observed (note that the range of activation energies in the plots in Fig. S3 exceeds 5 kcal mol<sup>-1</sup>).

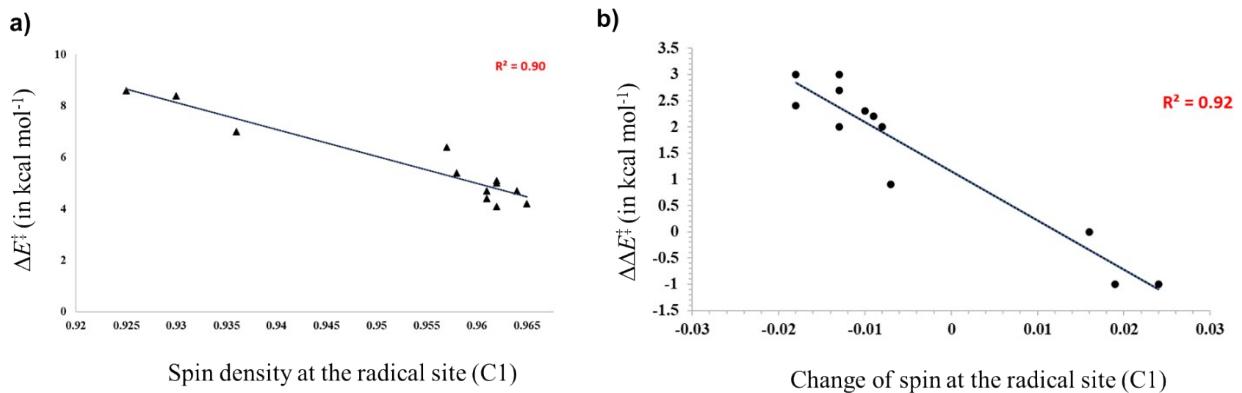


Fig. S3. a) Correlation between the activation barriers with the odd spin densities at the radical sites (C1) for the distonic radical ions **1-12**, b) the change in the activation barrier with respect to the spin density differences at the radical sites for **1-12** relative to phenyl•.

The (noncausal) correlation in Fig. S3 is presumably the root cause for the unjustified attribution of charge-induced reactivity modulation to electron-withdrawal/donation in distonic radical ions in the past: the minor through-bond effects point in the same direction as the dominant through-space (electrostatic) effects and are thus equally indicative of the observed reactivity trend. Only a careful analysis can properly resolve the two contributions and identify the main driver of the reactivity modulation.

#### S7. OEEF model for the ortho- and meta-substituted distonic radical ions

The qualitative correspondence between the impact of the remote charged functional group and the OEEF model for each of the isomers considered clearly appears in Table 2 (in the main text). The maximum difference between the reaction barrier obtained for the charged species and for the uncharged species with OEEF is calculated to be 0.8 kcal mol<sup>-1</sup>.

A careful analysis reveals that the observed small deviations are not caused by the sudden emergence of significant through-bond effects but are rather due to distinct through-space electrostatic patterns induced by the different positioning of the charged functional groups in the ortho- and meta-isomers compared to the para-isomer (Fig. S4).

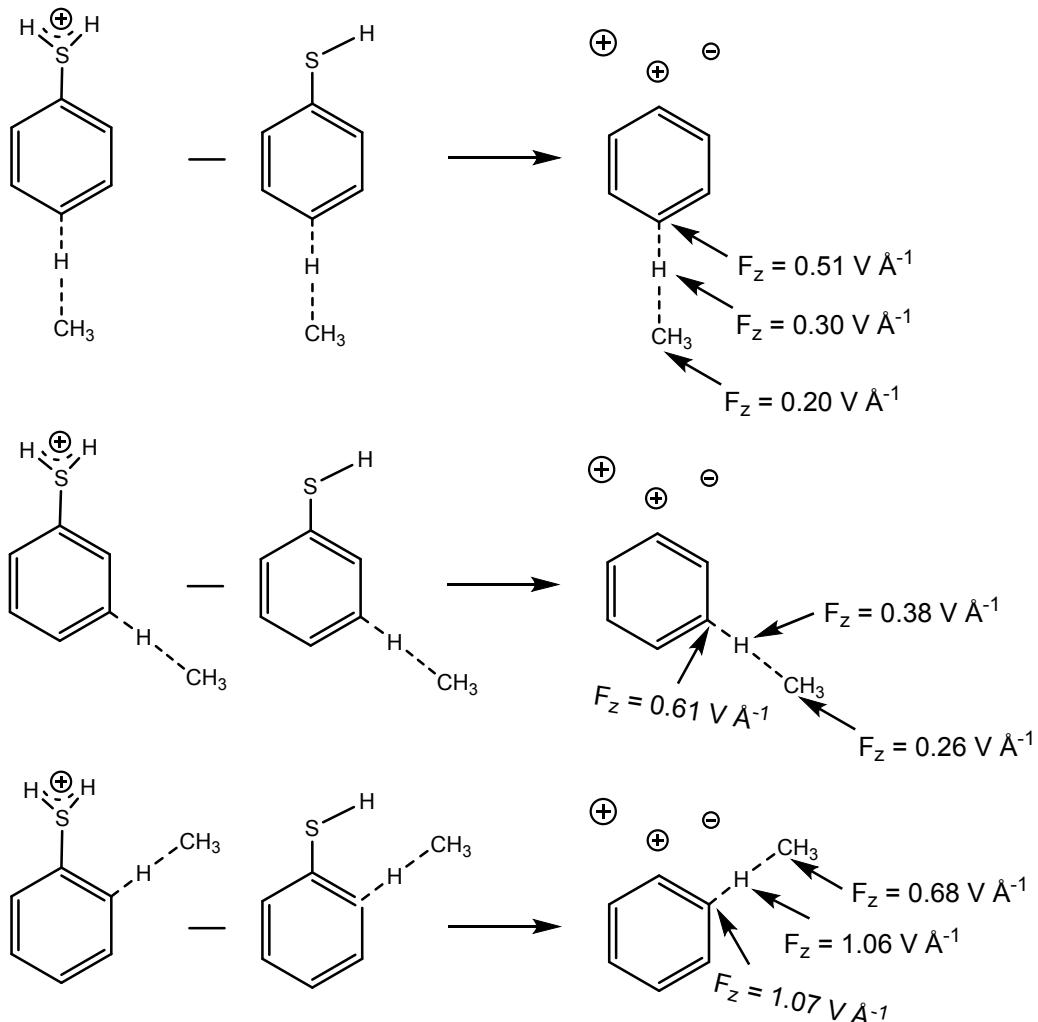


Fig. S4. A schematic representation of the differential charge distribution construction by TITAN.

Additional evidence that the deviations from the OEEF model are caused by distinct through-space electrostatic patterns can be found in Fig. S5. In this figure, the ESP is plotted for an example distonic radical cation, this time with the charged substituent placed in the ortho- and meta-positions, together with the ESP for the neutral analogue with a corresponding

OEEF included. One can clearly observe that the OEEF reproduces the electrostatic potential at the radical site of the molecule. Furthermore, the spin-densities on the radical sites for the neutral species + OEEF agree nicely with those for the distonic radical ions (Table S8, *vide infra*). As such, the observed deviations can only be attributed to different electrostatic patterns further along the C---H---C reaction-axis, not to significant changes in the electronic structure of the phenyl unit of the distonic radical ion.

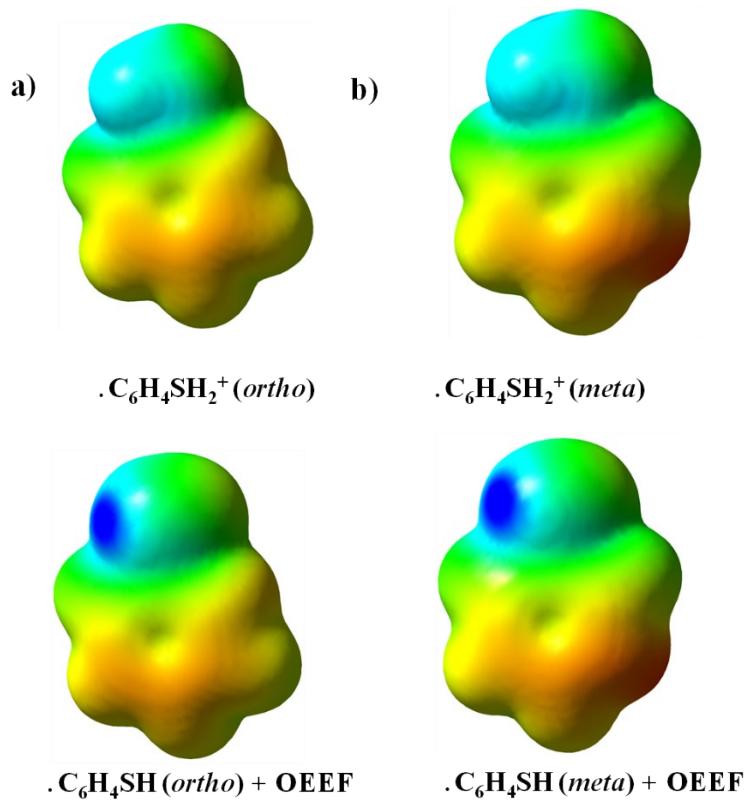


Fig. S5. a) ESP map for ortho isomer of **5** (top) and the corresponding ESP map for (unrelaxed) neutral species + OEEF (bottom); b) ESP map for meta isomer of **5** and the corresponding ESP map for (unrelaxed) neutral species + OEEF (bottom); color range: red (0.10 a.u.) to blue (0.25 a.u.).

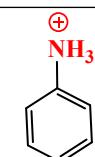
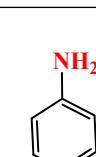
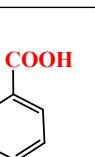
Table S8. Calculated spin densities at the radical sites for the isomeric radical ions and their corresponding neutral species in the presence of oriented external electric fields (OEEFs) [**L1**: U $\omega$ B97X-D/def2-TZVP, **L2**: UB3LYP-D3/def2-TZVP].

spin density at radical site				
	<b>L1</b>		<b>L2</b>	
Isomer	charged radical	neutral radical + OEEF	charged radical	neutral radical + OEEF
<i>para</i> ( <b>5</b> )	0.962	0.965	0.940	0.940
<i>meta</i> ( <b>5<sup>m</sup></b> )	0.961	0.964	0.937	0.939
<i>ortho</i> ( <b>5<sup>o</sup></b> )	0.960	0.963	0.935	0.934
<i>para</i> ( <b>10</b> )	0.936	0.930	0.908	0.904
<i>meta</i> ( <b>10<sup>m</sup></b> )	0.926	0.927	0.884	0.897
<i>ortho</i> ( <b>10<sup>o</sup></b> )	0.953	0.941	0.911	0.905

**S8. Further confirmation of the qualitative Valence Bond reactivity diagram (VBSCD) shown in Fig. 7**

In order to verify our VB understanding, we consider an H-abstraction reaction from nitrobenzene by a prototypical distonic radical cation (**1/1A**), and a prototypical anion (**10/10A**). The H-abstraction barrier calculated for the cationic distonic radical **1** (6.9 kcal mol<sup>-1</sup>, Table S9) is higher than the uncharged radical **1A** (5.3 kcal mol<sup>-1</sup>, Table S9), which is entirely opposite as we observed for H-abstraction from CH<sub>4</sub>. Similarly, the anionic distonic radical **10** (2.0 kcal mol<sup>-1</sup>, Table S9) exhibits a lower H-abstraction barrier than its uncharged analogue **10A** (6.7 kcal mol<sup>-1</sup>, Table S9) when nitrobenzene is selected as a hydrogen donor. In this respect, this finding clearly underlines that our detailed VB analysis enables productive predictions about distonic radical ions.

Table S9: Activation energies for the *para*-hydrogen abstraction reaction from nitrobenzene by the distonic radical ions (**1/10**) and their uncharged radical analogues (**1A/10A**) calculated at different levels of theory [**L1**: U $\omega$ B97X-D/def2-TZVP, **L2**: UB3LYP-D3/def2-TZVP].

	$\Delta E^\ddagger$ (kcal mol <sup>-1</sup> ) (R → TS) <sup>a</sup>			
				
<b>L1</b>	6.9	5.3	2.0	6.7
<b>L2</b>	6.0	4.5	0.8	5.9

<sup>a</sup> For nitrobenzene, it was observed that the D3 dispersion correction in conjunction with the charge leads to a profound and anomalous reorganization of the RC geometry, which makes a comparison between the charged and uncharged species difficult. To mitigate this issue, the separated reactants (R) were considered as the reference point for calculating the barrier heights in this table.

### S9. Cartesian coordinates of all relevant reactants, intermediates, and transition states

#### CH<sub>4</sub>

C	-4.343760000	-0.281482000	-0.497229000
H	-3.785139000	0.648832000	-0.587173000
H	-3.826281000	-0.950770000	0.188266000
H	-5.341146000	-0.070429000	-0.114719000
H	-4.422519000	-0.753586000	-1.475260000

#### 1

C	-0.002797000	0.007400000	0.006228000
C	-0.000366000	-0.009794000	2.663219000
C	1.218654000	0.070194000	0.619978000
C	1.217424000	0.061650000	2.011532000
C	-1.219222000	-0.072591000	2.012908000
C	-1.222974000	-0.064325000	0.621224000
H	2.147090000	0.121315000	0.066617000
H	2.152415000	0.109282000	2.558630000
H	-2.153301000	-0.127920000	2.560861000
H	-2.152052000	-0.115542000	0.068952000

N	-0.000091000	0.005206000	4.146966000
H	-0.033229000	0.958540000	4.515773000
H	-0.805996000	-0.500060000	4.518673000
H	0.839005000	-0.443096000	4.518430000

**1<sup>RC</sup>**

C	-0.003388000	0.029396000	0.000572000
C	-0.000600000	0.000504000	2.657365000
C	1.219942000	0.027351000	0.613829000
C	1.218939000	0.012798000	2.005135000
C	-1.221508000	0.002512000	2.007961000
C	-1.225335000	0.017049000	0.616290000
H	2.146618000	0.033378000	0.055192000
H	2.155339000	0.010397000	2.551996000
H	-2.156762000	-0.007726000	2.556630000
H	-2.156184000	0.015456000	0.064611000
N	0.001133000	0.009087000	4.141230000
H	-0.820602000	-0.470955000	4.511611000
H	0.825447000	-0.468234000	4.509433000
C	2.185933000	-0.028259000	-2.799695000
H	3.189403000	0.014607000	-2.376741000
H	1.678536000	-0.930643000	-2.458930000
H	1.619592000	0.853272000	-2.499388000
H	2.259766000	-0.050337000	-3.884968000
H	0.000068000	0.961343000	4.514141000

**1<sup>TS</sup>**

C	0.001875000	0.000379000	0.000018000
C	0.001366000	-0.010569000	2.703606000
C	1.199852000	0.165023000	0.662096000
C	1.206697000	0.160711000	2.050915000
C	-1.203917000	-0.176207000	2.049095000
C	-1.196411000	-0.169848000	0.660423000
H	2.127274000	0.293638000	0.118519000
H	2.134592000	0.287720000	2.597592000
H	-2.131786000	-0.308558000	2.594524000
H	-2.122702000	-0.300292000	0.115323000
C	-0.000009000	0.010882000	-2.678382000
H	0.001401000	0.005147000	-1.416712000
H	-0.296267000	1.015691000	-2.965977000
H	1.017371000	-0.234523000	-2.970342000
H	-0.719329000	-0.748732000	-2.971600000
N	-0.002497000	0.007616000	4.187820000
H	0.884839000	-0.334359000	4.559558000
H	-0.151112000	0.950663000	4.553818000
H	-0.741904000	-0.590740000	4.559065000

**1<sup>P</sup>**

C	0.000004000	-0.000732000	0.007951000
C	-0.000006000	0.001821000	2.737092000

C	1.204449000	-0.000068000	0.695675000
C	1.214429000	0.001581000	2.081800000
C	-1.214453000	0.000738000	2.081791000
C	-1.204458000	-0.000901000	0.695681000
H	2.141473000	-0.003514000	0.155958000
H	2.152715000	0.002144000	2.624075000
H	-2.152729000	0.000650000	2.624080000
H	-2.141474000	-0.004998000	0.155954000
N	-0.000056000	0.027605000	4.221847000
H	-0.002855000	0.984588000	4.581834000
H	-0.822132000	-0.448594000	4.595999000
H	0.824871000	-0.443706000	4.595899000
H	0.000005000	-0.004130000	-1.073666000

### CH<sub>3</sub>

C	-4.343711000	-0.281449000	-0.497134000
H	-3.784710000	0.532183000	-0.933819000
H	-3.827951000	-1.150655000	-0.118131000
H	-5.420104000	-0.224212000	-0.436363000

### 1A

C	0.000010000	-0.002819000	0.004955000
C	-0.000027000	0.002653000	2.739228000
C	1.211613000	-0.001040000	0.641252000
C	1.204307000	0.002690000	2.032652000
C	-1.204342000	0.001534000	2.032620000
C	-1.211611000	-0.002199000	0.641220000
H	2.149486000	-0.002397000	0.099780000
H	2.143619000	0.010023000	2.574645000
H	-2.143674000	0.007965000	2.574591000
H	-2.149469000	-0.004452000	0.099725000
N	-0.000075000	0.061944000	4.132156000
H	0.833389000	-0.288512000	4.573129000
H	-0.833237000	-0.289265000	4.573100000

### 1A<sup>RC</sup>

C	0.264603000	-0.009912000	-0.318881000
C	0.170033000	-0.005442000	2.412816000
C	1.453872000	-0.007998000	0.358325000
C	1.398257000	-0.006641000	1.748370000
C	-1.009301000	-0.008371000	1.665058000
C	-0.968645000	-0.009798000	0.274256000
H	2.408274000	-0.007601000	-0.153371000
H	2.318231000	-0.010960000	2.322657000
H	-1.966806000	-0.014070000	2.174276000
H	-1.887064000	-0.010779000	-0.299575000
N	0.121846000	-0.059219000	3.804737000
H	-0.726740000	0.291071000	4.215826000
H	0.939440000	0.292415000	4.273459000
C	2.616748000	-0.035883000	-3.142521000

H	1.604463000	-0.014464000	-2.739501000
H	3.157526000	0.849356000	-2.809932000
H	3.127707000	-0.930527000	-2.788737000
H	2.577544000	-0.048141000	-4.230719000

### **1A<sup>TS</sup>**

C	-0.000732000	0.002204000	0.001286000
C	-0.003667000	-0.003064000	2.771524000
C	1.198411000	-0.065291000	0.675833000
C	1.197591000	-0.068732000	2.063283000
C	-1.203500000	0.063528000	2.061011000
C	-1.201286000	0.066891000	0.673537000
H	2.137913000	-0.115329000	0.137641000
H	2.135161000	-0.126910000	2.605340000
H	-2.142823000	0.108717000	2.601264000
H	-2.139584000	0.120287000	0.133575000
C	0.000410000	0.006642000	-2.663957000
H	0.001048000	0.006840000	-1.373106000
H	0.789500000	-0.680013000	-2.958788000
H	-0.987770000	-0.338854000	-2.956152000
H	0.196031000	1.032637000	-2.963581000
N	-0.008139000	-0.060475000	4.162836000
H	0.843608000	0.238622000	4.606355000
H	-0.822704000	0.330427000	4.604788000

### **1A<sup>P</sup>**

C	0.000000000	-0.001644000	0.006271000
C	0.000000000	0.002603000	2.808139000
C	1.194320000	-0.000386000	0.711525000
C	1.199814000	0.002335000	2.095559000
C	-1.199814000	0.002541000	2.095558000
C	-1.194320000	-0.000182000	0.711525000
H	2.137463000	-0.001776000	0.178911000
H	2.140705000	0.008196000	2.634143000
H	-2.140704000	0.008564000	2.634142000
H	-2.137462000	-0.001409000	0.178909000
N	0.000004000	0.058330000	4.197710000
H	0.835295000	-0.281874000	4.642649000
H	-0.835345000	-0.281733000	4.642648000
H	0.000001000	-0.004003000	-1.075479000

### **2**

C	0.000204000	-0.000021000	0.013407000
C	-0.000233000	-0.000012000	2.708231000
C	1.212958000	0.000011000	0.637680000
C	1.209366000	0.000016000	2.032262000
C	-1.211368000	-0.000042000	2.024631000
C	-1.218392000	-0.000047000	0.636263000
H	2.148573000	0.000031000	0.094017000
H	2.159788000	0.000040000	2.543125000

H	-2.160075000	-0.000061000	2.544781000
H	-2.152450000	-0.000070000	0.090037000
N	-0.046281000	-0.000006000	4.207335000
C	1.312764000	0.000090000	4.829781000
H	1.183376000	0.000075000	5.908841000
H	1.851142000	-0.894094000	4.528607000
H	1.851012000	0.894357000	4.528618000
C	-0.763014000	1.227265000	4.690270000
H	-1.782642000	1.222917000	4.319703000
H	-0.765871000	1.221624000	5.778016000
H	-0.237909000	2.101805000	4.314799000
C	-0.762846000	-1.227369000	4.690286000
H	-0.237627000	-2.101842000	4.314820000
H	-0.765695000	-1.221718000	5.778032000
H	-1.782478000	-1.223161000	4.319728000

### **2<sup>RC</sup>**

C	-0.000111000	0.000059000	-0.000212000
C	-0.000313000	0.000014000	2.694540000
C	1.218373000	0.000033000	0.622995000
C	1.210959000	0.000005000	2.011102000
C	-1.209810000	0.000042000	2.018613000
C	-1.212933000	0.000080000	0.623934000
H	2.149838000	-0.000117000	0.072367000
H	2.159439000	-0.000036000	2.531733000
H	-2.160394000	0.000037000	2.529062000
H	-2.148565000	0.000100000	0.080293000
N	0.046101000	-0.000070000	4.193827000
C	2.236324000	-0.009053000	-2.785796000
H	3.236416000	0.013600000	-2.353443000
H	1.714988000	-0.910769000	-2.465214000
H	1.677880000	0.872826000	-2.472530000
H	2.318940000	-0.011782000	-3.870723000
C	0.762970000	-1.227349000	4.676229000
H	1.782121000	-1.223270000	4.304353000
H	0.766967000	-1.221641000	5.763989000
H	0.237290000	-2.101770000	4.301309000
C	-1.312449000	-0.000003000	4.817100000
H	-1.850859000	0.894239000	4.516178000
H	-1.851026000	-0.894091000	4.516018000
H	-1.182389000	-0.000118000	5.896087000
C	0.763148000	1.227040000	4.676383000
H	0.237631000	2.101584000	4.301523000
H	0.767097000	1.221228000	5.764142000
H	1.782325000	1.222831000	4.304578000

### **2<sup>TS</sup>**

C	0.004920000	0.002140000	0.011210000
C	0.002322000	0.010622000	2.751433000
C	1.160512000	-0.337263000	0.681960000

C	1.161578000	-0.333641000	2.067517000
C	-1.154023000	0.350242000	2.070354000
C	-1.146411000	0.344034000	0.678770000
H	2.062123000	-0.605125000	0.145534000
H	2.071923000	-0.600968000	2.587762000
H	-2.067121000	0.621382000	2.577362000
H	-2.048244000	0.608784000	0.141029000
C	-0.002240000	-0.004933000	-2.665363000
H	0.002404000	-0.001812000	-1.400613000
H	1.019112000	-0.231837000	-2.958587000
H	-0.708559000	-0.778438000	-2.953531000
H	-0.315708000	0.992993000	-2.958911000
N	0.044835000	0.002193000	4.251187000
C	-1.258951000	0.388871000	4.869977000
H	-2.027955000	-0.316490000	4.568132000
H	-1.137459000	0.355356000	5.949508000
H	-1.521401000	1.397714000	4.564415000
C	1.079304000	0.977057000	4.731291000
H	2.055366000	0.683396000	4.359814000
H	0.822983000	1.963365000	4.353178000
H	1.081467000	0.973832000	5.819135000
C	0.384475000	-1.375812000	4.737764000
H	1.362785000	-1.661533000	4.366019000
H	0.389976000	-1.368689000	5.825577000
H	-0.367284000	-2.066488000	4.364536000

## 2<sup>P</sup>

C	0.000109000	0.000011000	0.014680000
C	-0.000332000	-0.000024000	2.780695000
C	1.194375000	-0.000189000	0.710837000
C	1.203462000	-0.000208000	2.099673000
C	-1.205743000	0.000178000	2.092514000
C	-1.200131000	0.000196000	0.709642000
H	2.136449000	-0.000334000	0.179563000
H	2.155921000	-0.000366000	2.605927000
H	-2.156641000	0.000323000	2.607762000
H	-2.140836000	0.000354000	0.175963000
N	-0.045410000	-0.000044000	4.279893000
C	1.314093000	-0.000252000	4.899905000
H	1.187141000	-0.000251000	5.979305000
H	1.851801000	-0.894184000	4.596899000
H	1.852062000	0.893531000	4.596925000
C	-0.762299000	1.226957000	4.761680000
H	-1.781228000	1.222475000	4.389241000
H	-0.766471000	1.221695000	5.849467000
H	-0.236661000	2.101329000	4.386560000
C	-0.762657000	-1.226855000	4.761629000
H	-0.237266000	-2.101365000	4.386485000
H	-0.766841000	-1.221630000	5.849416000
H	-1.781579000	-1.222066000	4.389174000

H 0.001108000 0.000025000 -1.066852000

**2A**

C 0.000114000 -0.006212000 0.009649000  
C -0.000164000 -0.001537000 2.765220000  
C 1.207811000 -0.004336000 0.651047000  
C 1.204514000 -0.006167000 2.042023000  
C -1.204588000 -0.020226000 2.041799000  
C -1.207644000 -0.018439000 0.650822000  
H 2.148017000 -0.005745000 0.113349000  
H 2.154520000 -0.010293000 2.556374000  
H -2.154581000 -0.035444000 2.555949000  
H -2.147666000 -0.030835000 0.112945000  
N -0.000367000 0.029857000 4.150650000  
C -1.233968000 -0.225958000 4.854177000  
H -1.657078000 -1.214426000 4.627807000  
H -1.051593000 -0.170935000 5.925300000  
H -1.987657000 0.527761000 4.614388000  
C 1.236253000 -0.211310000 4.854025000  
H 1.981073000 0.550991000 4.613647000  
H 1.053506000 -0.157900000 5.925166000  
H 1.670773000 -1.194902000 4.628006000

**2A<sup>RC</sup>**

C 0.044845000 0.008273000 0.005708000  
C 0.015320000 0.001966000 2.760161000  
C 1.245959000 0.012465000 0.659179000  
C 1.227711000 0.005169000 2.049772000  
C -1.181376000 -0.018609000 2.023912000  
C -1.169868000 -0.011394000 0.633034000  
H 2.190156000 0.016970000 0.128653000  
H 2.172207000 0.002810000 2.574145000  
H -2.136643000 -0.039737000 2.527948000  
H -2.104020000 -0.025516000 0.085125000  
N 0.000099000 0.027288000 4.145262000  
C 2.358379000 0.049743000 -2.848792000  
H 2.877702000 -0.850777000 -2.523166000  
H 1.352763000 0.058942000 -2.428996000  
H 2.901689000 0.929118000 -2.505011000  
H 2.301822000 0.061620000 -3.936252000  
C 1.230241000 -0.209067000 4.861576000  
H 1.972717000 0.559465000 4.633970000  
H 1.034820000 -0.162665000 5.930776000  
H 1.673825000 -1.188505000 4.635394000  
C -1.240333000 -0.233251000 4.834912000  
H -1.992633000 0.520664000 4.591216000  
H -1.659692000 -1.221151000 4.599464000  
H -1.068995000 -0.183238000 5.908071000

**2A<sup>TS</sup>**

C	-0.071917000	0.026397000	-0.008090000
C	-0.020287000	0.004438000	2.782484000
C	1.138150000	0.019215000	0.647404000
C	1.168622000	0.003931000	2.034063000
C	-1.235973000	-0.003390000	2.078581000
C	-1.256783000	0.011948000	0.691663000
H	2.070718000	0.020900000	0.094694000
H	2.128500000	-0.007936000	2.529687000
H	-2.176873000	-0.021118000	2.609152000
C	-0.127063000	0.047032000	-2.672774000
H	-0.097416000	0.036493000	-1.382212000
H	0.537176000	0.851161000	-2.978025000
H	0.219412000	-0.933483000	-2.987991000
H	-1.163943000	0.234213000	-2.939696000
N	0.005366000	0.020434000	4.166353000
C	-1.216573000	-0.228788000	4.892026000
H	-1.968048000	0.533146000	4.671904000
H	-1.652890000	-1.211601000	4.666695000
H	-1.013032000	-0.183436000	5.959811000
C	1.254801000	-0.221969000	4.846078000
H	1.993084000	0.544648000	4.599182000
H	1.090615000	-0.178732000	5.920704000
H	1.688336000	-1.201964000	4.603783000
H	-2.209135000	0.007876000	0.173800000

### 2A<sup>P</sup>

C	-0.000065000	0.003841000	0.010818000
C	0.000066000	0.002283000	2.833541000
C	1.190196000	0.003682000	0.720342000
C	1.199927000	0.007499000	2.104089000
C	-1.199781000	0.017066000	2.104204000
C	-1.190219000	0.013186000	0.720457000
H	2.135627000	0.005018000	0.191413000
H	2.151598000	0.014251000	2.614728000
H	-2.151316000	0.031352000	2.614948000
H	-2.135663000	0.022057000	0.191624000
N	-0.000022000	-0.024145000	4.215635000
C	1.237869000	0.199720000	4.922286000
H	1.682134000	1.179859000	4.701778000
H	1.053166000	0.142859000	5.992927000
H	1.975515000	-0.568299000	4.677799000
C	-1.235991000	0.210243000	4.922250000
H	-1.979924000	-0.551883000	4.678331000
H	-1.051658000	0.152603000	5.992911000
H	-1.672238000	1.193831000	4.701131000
H	-0.000119000	0.002871000	-1.070896000

### 3

C	-0.001222000	-0.000061000	0.013303000
C	-0.004408000	0.000149000	2.685758000

C	1.220989000	-0.000312000	0.624735000
C	1.215724000	-0.000197000	2.016847000
C	-1.225872000	0.000392000	2.014998000
C	-1.227526000	0.000289000	0.627676000
H	2.151001000	-0.000582000	0.071508000
H	2.149057000	-0.000387000	2.566580000
H	-2.167994000	0.000663000	2.549681000
H	-2.155732000	0.000465000	0.071272000
S	0.091828000	0.000274000	4.447983000
C	-0.907046000	-1.395197000	4.965088000
H	-0.919851000	-1.397133000	6.054077000
H	-1.915216000	-1.316564000	4.564629000
H	-0.413188000	-2.292896000	4.598554000
C	-0.906257000	1.396413000	4.964821000
H	-0.919067000	1.398572000	6.053808000
H	-0.411886000	2.293759000	4.598110000
H	-1.914466000	1.318270000	4.564366000

### **3<sup>RC</sup>**

C	0.033431000	0.030626000	0.001163000
C	0.008256000	-0.009667000	2.673094000
C	1.248738000	-0.045562000	0.621649000
C	1.232113000	-0.066388000	2.013276000
C	-1.205968000	0.067406000	1.993688000
C	-1.196053000	0.088482000	0.606544000
H	2.179134000	-0.087873000	0.070759000
H	2.159388000	-0.125830000	2.569996000
H	-2.150790000	0.110906000	2.521756000
H	-2.118388000	0.147738000	0.043615000
C	2.244615000	-0.049733000	-2.790548000
H	3.245183000	-0.075310000	-2.359585000
H	1.686286000	-0.933399000	-2.482001000
H	1.724643000	0.850966000	-2.464572000
H	2.325869000	-0.040905000	-3.875522000
S	0.089830000	-0.041550000	4.435618000
C	-0.834996000	1.399074000	4.967367000
H	-1.842651000	1.382137000	4.558373000
H	-0.856554000	1.385470000	6.056164000
H	-0.289660000	2.273643000	4.618212000
C	-0.988033000	-1.388032000	4.924094000
H	-0.541185000	-2.305803000	4.547007000
H	-1.009696000	-1.405927000	6.012828000
H	-1.987136000	-1.248200000	4.517682000

### **3<sup>TS</sup>**

C	-0.005316000	0.012615000	-0.025046000
C	-0.001300000	0.032472000	2.694570000
C	1.202261000	0.106641000	0.630144000
C	1.210683000	0.117348000	2.018957000
C	-1.218226000	-0.062742000	2.024643000

C	-1.213706000	-0.072496000	0.640512000
H	2.133875000	0.171406000	0.082233000
H	2.143772000	0.190414000	2.564096000
H	-2.157290000	-0.128524000	2.560725000
H	-2.146536000	-0.145998000	0.095540000
C	-0.009412000	-0.012303000	-2.702351000
H	-0.009418000	0.000057000	-1.436642000
H	0.843187000	0.593059000	-2.997297000
H	0.088951000	-1.056855000	-2.984000000
H	-0.960404000	0.423028000	-2.996564000
S	0.098080000	0.052997000	4.455697000
C	-0.795925000	-1.407597000	4.985643000
H	-0.810760000	-1.401811000	6.074567000
H	-1.806158000	-1.406736000	4.582748000
H	-0.237143000	-2.269578000	4.626729000
C	-1.001351000	1.374213000	4.964667000
H	-1.016343000	1.382706000	6.053572000
H	-0.574882000	2.303426000	4.592171000
H	-2.000063000	1.218887000	4.562986000

### **3P**

C	-0.001410000	-0.000053000	0.014226000
C	-0.004390000	0.000098000	2.760088000
C	1.202277000	-0.000174000	0.699934000
C	1.209753000	-0.000099000	2.086384000
C	-1.220133000	0.000221000	2.084476000
C	-1.209435000	0.000142000	0.702724000
H	2.139140000	-0.000327000	0.159726000
H	2.145352000	-0.000196000	2.631016000
H	-2.164636000	0.000373000	2.613824000
H	-2.144841000	0.000234000	0.159721000
S	0.090274000	0.000188000	4.523664000
C	-0.911701000	-1.394830000	5.035994000
H	-0.931299000	-1.396801000	6.124836000
H	-1.917139000	-1.315972000	4.628831000
H	-0.415981000	-2.292651000	4.672360000
C	-0.911269000	1.395584000	5.035817000
H	-0.930883000	1.397694000	6.124659000
H	-0.415260000	2.293205000	4.672080000
H	-1.916724000	1.316992000	4.628645000
H	-0.003049000	-0.000113000	-1.067794000

### **3A**

C	-0.003631000	-0.000436000	0.010198000
C	-0.002051000	0.000374000	2.735258000
C	1.213013000	-0.000441000	0.641052000
C	1.204178000	-0.000017000	2.029966000
C	-1.206681000	0.000353000	2.038716000
C	-1.213505000	-0.000052000	0.642713000
H	2.149317000	-0.000744000	0.097409000

H	2.143350000	0.000019000	2.571364000
H	-2.152523000	0.000646000	2.562760000
H	-2.151443000	-0.000058000	0.101533000
S	0.129219000	0.000840000	4.494703000
C	-1.579903000	0.001706000	5.044060000
H	-1.537381000	0.002253000	6.132233000
H	-2.107892000	0.895872000	4.713672000
H	-2.108529000	-0.892429000	4.714607000

### 3A<sup>RC</sup>

C	-0.046273000	0.297078000	0.036823000
C	-0.015964000	0.093418000	2.753023000
C	1.173708000	0.343233000	0.659305000
C	1.179394000	0.238578000	2.044134000
C	-1.224518000	0.053233000	2.064471000
C	-1.246219000	0.157091000	0.672453000
H	2.099705000	0.455750000	0.109823000
H	2.121454000	0.269904000	2.579574000
H	-2.161847000	-0.058350000	2.591885000
H	-2.187036000	0.125676000	0.137247000
C	2.182883000	0.726422000	-2.853057000
H	2.791371000	-0.138620000	-2.592085000
H	1.179443000	0.599125000	-2.447487000
H	2.630324000	1.627578000	-2.435513000
H	2.130280000	0.817632000	-3.936850000
S	0.132881000	-0.027940000	4.506887000
C	-1.565370000	-0.204642000	5.061300000
H	-2.025085000	-1.109873000	4.665431000
H	-1.512402000	-0.284320000	6.146080000
H	-2.165386000	0.667543000	4.802926000

### 3A<sup>TS</sup>

C	-0.024300000	0.080714000	0.001834000
C	-0.104327000	0.338885000	2.750956000
C	0.955650000	0.817366000	0.634370000
C	0.914402000	0.946085000	2.012931000
C	-1.080221000	-0.398541000	2.088252000
C	-1.037959000	-0.527312000	0.702852000
H	1.749742000	1.291913000	0.070086000
H	1.677140000	1.521706000	2.524704000
H	-1.879851000	-0.878940000	2.634976000
H	-1.801597000	-1.103304000	0.193272000
C	0.045174000	-0.172517000	-2.651277000
H	0.014138000	-0.048715000	-1.366377000
H	-0.849808000	-0.731676000	-2.911091000
H	0.039917000	0.839939000	-3.045736000
H	0.961071000	-0.712792000	-2.874585000
S	-0.047995000	0.575706000	4.497332000
C	-1.480987000	-0.328314000	5.091275000
H	-1.478842000	-0.203386000	6.173089000

H	-2.408373000	0.082158000	4.692648000
H	-1.409410000	-1.390946000	4.860790000

### **3A<sup>P</sup>**

C	-0.003056000	-0.000154000	0.010877000
C	-0.001898000	0.000538000	2.804214000
C	1.195995000	-0.000210000	0.711665000
C	1.199833000	0.000138000	2.093647000
C	-1.201809000	0.000587000	2.101243000
C	-1.195528000	0.000247000	0.712746000
H	2.137730000	-0.000518000	0.177215000
H	2.140300000	0.000109000	2.631794000
H	-2.149278000	0.000885000	2.621495000
H	-2.138623000	0.000296000	0.180415000
S	0.127243000	0.000928000	4.561485000
C	-1.582554000	0.001688000	5.109421000
H	-1.541992000	0.002095000	6.197665000
H	-2.110042000	0.895601000	4.777732000
H	-2.110638000	-0.892133000	4.778431000
H	-0.004451000	-0.000420000	-1.071221000

### **4**

C	0.000000000	-0.000001000	0.019272000
C	0.000000000	0.000001000	2.734559000
C	1.216443000	0.060591000	0.642205000
C	1.204807000	0.055973000	2.033053000
C	-1.204807000	-0.055972000	2.033053000
C	-1.216443000	-0.060592000	0.642204000
H	2.147628000	0.117281000	0.093506000
H	2.143088000	0.125304000	2.570950000
H	-2.143088000	-0.125302000	2.570949000
H	-2.147627000	-0.117282000	0.093506000
C	-0.000001000	0.000002000	4.213677000
C	0.936165000	-0.748419000	4.929213000
C	-0.936166000	0.748424000	4.929212000
C	0.945518000	-0.751820000	6.311550000
H	1.662678000	-1.346810000	4.395749000
C	-0.945520000	0.751826000	6.311549000
H	-1.662679000	1.346815000	4.395747000
C	-0.000001000	0.000004000	6.987070000
H	1.689141000	-1.323577000	6.852770000
H	-1.689143000	1.323584000	6.852768000
C	0.100795000	1.166287000	9.099776000
C	-0.100798000	-1.166277000	9.099777000
C	0.095058000	1.193195000	10.473567000
H	0.199922000	2.051538000	8.488790000
C	-0.095062000	-1.193184000	10.473568000
H	-0.199924000	-2.051529000	8.488792000
C	-0.000002000	0.000006000	11.173760000
H	0.177835000	2.142575000	10.982518000

H	-0.177840000	-2.142563000	10.982520000
H	-0.000002000	0.000007000	12.255700000
N	-0.000001000	0.000004000	8.435575000

**4<sup>RC</sup>**

C	-0.038809000	0.037348000	0.017450000
C	-0.025424000	0.023595000	2.732090000
C	1.181500000	0.079522000	0.634091000
C	1.176572000	0.068098000	2.024989000
C	-1.234294000	-0.013862000	2.036180000
C	-1.253001000	-0.011170000	0.645614000
H	2.110712000	0.127358000	0.081225000
H	2.118315000	0.123287000	2.558464000
H	-2.170751000	-0.074414000	2.578345000
H	-2.185225000	-0.053184000	0.097503000
C	-0.018216000	0.016448000	4.210991000
C	0.913137000	-0.745424000	4.918635000
C	-0.942653000	0.771631000	4.934702000
C	0.929311000	-0.755204000	6.300825000
H	1.630363000	-1.349349000	4.378909000
C	-0.945214000	0.768799000	6.317002000
H	-1.665151000	1.380378000	4.407574000
C	-0.004575000	0.003769000	6.984412000
H	1.669247000	-1.337495000	6.835825000
H	-1.679792000	1.346179000	6.864561000
C	0.118354000	1.159940000	9.101428000
C	-0.105889000	-1.170520000	9.092737000
C	0.119854000	1.181072000	10.475311000
H	0.223028000	2.046692000	8.493578000
C	-0.093236000	-1.203235000	10.466341000
H	-0.216840000	-2.052115000	8.478528000
C	0.016918000	-0.014038000	11.171042000
H	0.214381000	2.127473000	10.987752000
H	-0.182509000	-2.153935000	10.971721000
H	0.022498000	-0.018613000	12.252946000
N	0.002807000	-0.002482000	8.432873000
C	-2.425998000	-0.049978000	-2.780974000
H	-2.869637000	-0.958740000	-2.375598000
H	-2.532148000	-0.051519000	-3.864182000
H	-1.368294000	-0.012327000	-2.520986000
H	-2.933899000	0.822740000	-2.371838000

**4<sup>TS</sup>**

C	-0.001041000	0.003993000	0.016541000
C	-0.000546000	0.001388000	2.774877000
C	1.178056000	0.257855000	0.682495000
C	1.176363000	0.252017000	2.069819000
C	-1.177757000	-0.247928000	2.069754000
C	-1.179943000	-0.251158000	0.682483000
H	2.091901000	0.465353000	0.139257000

H	2.092096000	0.472545000	2.605932000
H	-2.093289000	-0.469456000	2.605805000
H	-2.093934000	-0.457608000	0.139050000
C	-0.000272000	0.000042000	4.253104000
C	1.052794000	-0.572955000	4.968633000
C	-1.053061000	0.571783000	4.970044000
C	1.062904000	-0.576027000	6.350800000
H	1.872971000	-1.033713000	4.434434000
C	-1.062579000	0.572537000	6.352217000
H	-1.873470000	1.033435000	4.436974000
C	0.000316000	-0.002295000	7.027161000
H	1.895507000	-1.008695000	6.891567000
H	-1.894945000	1.004305000	6.894068000
C	-0.110696000	1.161265000	9.140774000
C	0.112373000	-1.169085000	9.138972000
C	-0.121156000	1.185628000	10.514595000
H	-0.172834000	2.050233000	8.530355000
C	0.123530000	-1.195500000	10.512751000
H	0.174209000	-2.057137000	8.527191000
C	0.001365000	-0.005460000	11.213968000
H	-0.211296000	2.133988000	11.024184000
H	0.213932000	-2.144621000	11.020875000
H	0.001641000	-0.006271000	12.295885000
N	0.000669000	-0.003412000	8.475546000
C	-0.002161000	0.006043000	-2.653247000
H	-0.321268000	-0.989884000	-2.947543000
H	1.021940000	0.225884000	-2.942354000
H	-0.002450000	0.004988000	-1.371535000
H	-0.701658000	0.783979000	-2.946208000

#### 4P

C	0.0000000000	0.000002000	0.020696000
C	0.0000000000	0.000000000	2.807706000
C	1.198124000	0.063440000	0.715705000
C	1.199133000	0.059610000	2.100122000
C	-1.199133000	-0.059609000	2.100121000
C	-1.198123000	-0.063437000	0.715705000
H	2.135350000	0.121993000	0.177994000
H	2.139239000	0.132044000	2.633438000
H	-2.139240000	-0.132044000	2.633437000
H	-2.135350000	-0.121990000	0.177994000
C	0.0000000000	-0.000001000	4.286146000
C	0.948178000	-0.733200000	5.001748000
C	-0.948178000	0.733198000	5.001748000
C	0.957305000	-0.736970000	6.384002000
H	1.684608000	-1.318882000	4.467850000
C	-0.957306000	0.736966000	6.384002000
H	-1.684608000	1.318880000	4.467851000
C	-0.000001000	-0.000002000	7.059399000
H	1.709817000	-1.296722000	6.925498000

H	-1.709818000	1.296718000	6.925499000
C	0.081571000	1.167732000	9.172143000
C	-0.081573000	-1.167738000	9.172142000
C	0.075298000	1.194549000	10.545932000
H	0.166110000	2.054358000	8.560978000
C	-0.075300000	-1.194556000	10.545931000
H	-0.166112000	-2.054364000	8.560976000
C	-0.000001000	-0.000004000	11.246157000
H	0.142412000	2.145177000	11.054866000
H	-0.142414000	-2.145185000	11.054864000
H	-0.000001000	-0.000005000	12.328084000
N	-0.000001000	-0.000003000	8.507905000
H	0.000000000	0.000002000	-1.061391000

#### 4A

C	0.000000000	0.000000000	0.020030000
C	0.000000000	0.000000000	2.749085000
C	1.214999000	0.032797000	0.648151000
C	1.201389000	0.033844000	2.040469000
C	-1.201389000	-0.033843000	2.040469000
C	-1.214999000	-0.032796000	0.648151000
H	2.149803000	0.067042000	0.102918000
H	2.139422000	0.083405000	2.580919000
H	-2.139422000	-0.083405000	2.580918000
H	-2.149802000	-0.067042000	0.102917000
C	-0.000001000	0.000000000	4.230551000
C	0.905119000	-0.773712000	4.952517000
C	-0.905120000	0.773712000	4.952517000
C	0.916687000	-0.769895000	6.335058000
H	1.616784000	-1.395876000	4.423540000
C	-0.916689000	0.769895000	6.335058000
H	-1.616785000	1.395876000	4.423540000
C	-0.000001000	0.000000000	7.049197000
H	1.656873000	-1.356554000	6.862769000
H	-1.656875000	1.356553000	6.862768000
C	-0.269246000	1.156379000	9.181316000
C	0.269243000	-1.156380000	9.181316000
C	-0.275319000	1.199091000	10.510226000
H	-0.434477000	2.043748000	8.587722000
C	0.275315000	-1.199093000	10.510226000
H	0.434474000	-2.043749000	8.587721000
C	-0.000002000	-0.000001000	11.373757000
H	-0.468045000	2.151275000	10.986312000
H	0.468041000	-2.151277000	10.986312000
H	-0.848072000	-0.198971000	12.041318000
N	-0.000001000	0.000000000	8.452837000
H	0.848069000	0.198970000	12.041318000

#### 4A<sup>RC</sup>

C	-0.322261000	0.793754000	0.177164000
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C	-0.201910000	0.510362000	2.887797000
C	0.916750000	0.646754000	0.738062000
C	0.964586000	0.504442000	2.122364000
C	-1.430882000	0.663510000	2.245243000
C	-1.505910000	0.810445000	0.862834000
H	1.825360000	0.649369000	0.149279000
H	1.925852000	0.409249000	2.613594000
H	-2.344466000	0.646359000	2.827908000
H	-2.460970000	0.921209000	0.365124000
C	-0.136633000	0.356232000	4.359710000
C	0.717206000	-0.571107000	4.951368000
C	-0.927007000	1.133208000	5.202734000
C	0.789811000	-0.712479000	6.324761000
H	1.338866000	-1.199803000	4.325581000
C	-0.878139000	0.986500000	6.576617000
H	-1.595204000	1.872038000	4.777335000
C	-0.012822000	0.062603000	7.160146000
H	1.489715000	-1.418865000	6.750977000
H	-1.531729000	1.582873000	7.199255000
C	-0.069610000	1.011162000	9.407904000
C	0.231004000	-1.330166000	9.149209000
C	-0.013546000	0.915548000	10.732885000
H	-0.169433000	1.967167000	8.914791000
C	0.290461000	-1.511508000	10.465045000
H	0.279890000	-2.162361000	8.462101000
C	0.175366000	-0.388031000	11.456883000
H	-0.087494000	1.827038000	11.310929000
H	0.406662000	-2.522140000	10.833192000
H	-0.659206000	-0.572689000	12.145301000
N	0.048702000	-0.083645000	8.554835000
C	-2.738622000	1.188418000	-2.573810000
H	-3.291127000	0.298377000	-2.275163000
H	-2.766965000	1.284732000	-3.658061000
H	-1.704631000	1.101236000	-2.241103000
H	-3.191724000	2.069303000	-2.120590000
H	1.066993000	-0.342631000	12.095187000

#### 4A<sup>TS</sup>

C	-0.001859000	0.028091000	-0.010415000
C	-0.001289000	0.018623000	2.756997000
C	1.201196000	-0.041972000	0.656301000
C	1.196279000	-0.045180000	2.044802000
C	-1.199186000	0.087349000	2.045713000
C	-1.204685000	0.093683000	0.657278000
H	2.138243000	-0.084598000	0.113715000
H	2.136015000	-0.075898000	2.583590000
H	-2.138692000	0.114357000	2.585104000
H	-2.141914000	0.140259000	0.115317000
C	-0.001015000	0.013549000	4.237990000
C	0.844417000	-0.827427000	4.957250000

C	-0.846183000	0.849642000	4.963234000
C	0.856337000	-0.829325000	6.339797000
H	1.507964000	-1.498620000	4.425786000
C	-0.857574000	0.842229000	6.345762000
H	-1.509934000	1.524404000	4.436566000
C	-0.000472000	0.004053000	7.056640000
H	1.550732000	-1.471215000	6.865534000
H	-1.551755000	1.480564000	6.876091000
C	-0.177336000	1.170773000	9.192946000
C	0.177410000	-1.176926000	9.185024000
C	-0.179758000	1.209548000	10.522065000
H	-0.272756000	2.070040000	8.601914000
C	0.180566000	-1.224569000	10.513850000
H	0.272541000	-2.072222000	8.587944000
C	0.000628000	-0.010390000	11.381480000
H	-0.297099000	2.172311000	11.001387000
H	0.298199000	-2.190505000	10.986673000
H	0.861904000	0.118990000	12.049351000
N	-0.000178000	-0.000653000	8.460740000
C	-0.001032000	0.036275000	-2.676821000
H	-0.760250000	-0.682625000	-2.972645000
H	-0.002704000	0.033700000	-1.382831000
H	-0.239596000	1.054636000	-2.970991000
H	-0.860296000	-0.144226000	12.048927000
H	1.002054000	-0.265336000	-2.966412000

#### 4A<sup>P</sup>

C	0.0000000000	0.0000000000	0.021112000
C	0.0000000000	0.0000000000	2.819923000
C	1.197145000	0.035282000	0.719822000
C	1.196353000	0.036242000	2.105073000
C	-1.196353000	-0.036241000	2.105073000
C	-1.197145000	-0.035281000	0.719821000
H	2.137354000	0.070933000	0.183824000
H	2.136009000	0.087683000	2.641542000
H	-2.136009000	-0.087683000	2.641541000
H	-2.137354000	-0.070933000	0.183824000
C	0.0000000000	0.0000000000	4.300542000
C	0.921003000	-0.754745000	5.022731000
C	-0.921004000	0.754745000	5.022731000
C	0.932083000	-0.751245000	6.405239000
H	1.645583000	-1.361603000	4.493636000
C	-0.932084000	0.751244000	6.405239000
H	-1.645583000	1.361603000	4.493636000
C	0.0000000000	0.0000000000	7.119088000
H	1.683706000	-1.322857000	6.933354000
H	-1.683707000	1.322857000	6.933354000
C	-0.288482000	1.151630000	9.251388000
C	0.288480000	-1.151631000	9.251388000
C	-0.295319000	1.194356000	10.580352000

H	-0.468821000	2.035864000	8.657490000
C	0.295317000	-1.194357000	10.580352000
H	0.468819000	-2.035865000	8.657489000
C	-0.000001000	-0.000001000	11.443906000
H	-0.504066000	2.143164000	11.056432000
H	0.504063000	-2.143166000	11.056431000
H	0.844641000	0.213074000	12.111532000
N	-0.000001000	0.000000000	8.523102000
H	0.000000000	0.000000000	-1.061412000
H	-0.844643000	-0.213075000	12.111533000

### 5

C	-0.000498000	0.000058000	0.006851000
C	-0.000478000	-0.000084000	2.664714000
C	1.224165000	0.000082000	0.613285000
C	1.224595000	0.000017000	2.005167000
C	-1.229031000	-0.000104000	2.006810000
C	-1.228109000	-0.000023000	0.620322000
H	2.152625000	0.000158000	0.057484000
H	2.159433000	0.000058000	2.552183000
H	-2.165011000	-0.000183000	2.551957000
H	-2.156286000	-0.000025000	0.063809000
H	-0.750566000	0.988468000	4.773355000
H	-0.749859000	-0.989512000	4.773226000
S	0.102258000	-0.000192000	4.431552000

### 5<sup>RC</sup>

C	0.114521000	0.081637000	0.004067000
C	0.016136000	-0.015558000	2.658901000
C	1.312026000	-0.040113000	0.651526000
C	1.260948000	-0.091023000	2.041154000
C	-1.183457000	0.108405000	1.959697000
C	-1.131205000	0.159009000	0.575304000
H	2.254520000	-0.094767000	0.122685000
H	2.171815000	-0.187009000	2.619435000
H	-2.135918000	0.164549000	2.472535000
H	-2.035148000	0.254819000	-0.011993000
C	2.346532000	0.033992000	-2.730892000
H	3.332340000	-0.073672000	-2.278999000
H	1.723313000	-0.820829000	-2.468207000
H	1.879695000	0.956571000	-2.386008000
H	2.455563000	0.074399000	-3.812640000
S	0.053434000	-0.088525000	4.425129000
H	-0.887201000	-1.016855000	4.699973000
H	-0.729327000	0.953037000	4.778047000

### 5<sup>TS</sup>

C	-0.002198000	-0.000508000	0.004760000
C	-0.000562000	-0.000727000	2.711566000
C	1.209685000	-0.001565000	0.659155000

C	1.220916000	-0.001684000	2.047774000
C	-1.226476000	0.000343000	2.050674000
C	-1.216546000	0.000448000	0.667548000
H	2.143743000	-0.002295000	0.111795000
H	2.157005000	-0.002501000	2.592621000
H	-2.163041000	0.001075000	2.594892000
H	-2.150910000	0.001269000	0.120311000
C	-0.014317000	-0.000282000	-2.675335000
H	-0.008288000	-0.000388000	-1.414212000
H	1.031966000	-0.001914000	-2.968213000
H	-0.538430000	-0.907169000	-2.963599000
H	-0.535570000	0.908293000	-2.963465000
H	-0.748568000	0.987608000	4.821042000
H	-0.750075000	-0.988286000	4.820874000
S	0.103206000	-0.000960000	4.475949000

### **5<sup>P</sup>**

C	-0.000524000	0.000014000	0.008087000
C	-0.000265000	-0.000032000	2.739908000
C	1.205622000	0.000026000	0.689486000
C	1.218714000	0.000006000	2.075825000
C	-1.222863000	-0.000043000	2.077604000
C	-1.209628000	-0.000018000	0.696533000
H	2.141133000	0.000054000	0.147163000
H	2.155943000	0.000025000	2.617409000
H	-2.161186000	-0.000072000	2.617465000
H	-2.145162000	-0.000023000	0.153923000
H	-0.752965000	0.988116000	4.847386000
H	-0.752688000	-0.988506000	4.847343000
S	0.101620000	-0.000067000	4.509030000
H	-0.003758000	0.000033000	-1.073901000

### **5A**

C	0.000504000	-0.000010000	0.005101000
C	-0.000054000	0.000022000	2.723570000
C	1.213917000	0.000000000	0.635649000
C	1.205938000	0.000047000	2.028580000
C	-1.206175000	-0.000012000	2.026366000
C	-1.214250000	-0.000005000	0.634474000
H	2.150872000	-0.000004000	0.093050000
H	2.147276000	0.000115000	2.564769000
H	-2.145425000	-0.000066000	2.566876000
H	-2.150566000	-0.000027000	0.090960000
H	1.235697000	-0.001037000	4.717441000
S	-0.082588000	0.000157000	4.490773000

### **5A<sup>RC</sup>**

C	0.047010000	0.013296000	-0.001125000
C	0.004167000	-0.004138000	2.716373000
C	1.250758000	0.015828000	0.647645000

C	1.220888000	0.006579000	2.040052000
C	-1.191062000	-0.005964000	2.000361000
C	-1.177664000	0.002680000	0.608561000
H	2.194184000	0.024365000	0.116588000
H	2.153771000	0.007645000	2.590852000
H	-2.138579000	-0.013932000	2.526223000
H	-2.105347000	0.001223000	0.050484000
C	2.398555000	0.033211000	-2.830119000
H	2.907650000	-0.857878000	-2.464794000
H	1.367258000	0.031200000	-2.478158000
H	2.906158000	0.922853000	-2.459223000
H	2.412916000	0.036649000	-3.918862000
S	-0.106187000	-0.017091000	4.481406000
H	1.208603000	0.000743000	4.727810000

### 5A<sup>TS</sup>

C	-0.008691000	-0.016209000	-0.053324000
C	0.005443000	-0.026016000	2.703069000
C	1.182426000	0.173672000	0.610349000
C	1.190094000	0.168964000	1.999338000
C	-1.186870000	-0.216141000	2.008674000
C	-1.193953000	-0.211129000	0.620662000
H	2.107176000	0.325650000	0.066286000
H	2.122574000	0.317875000	2.530350000
H	-2.111557000	-0.368492000	2.552783000
H	-2.123785000	-0.359496000	0.084505000
C	-0.019261000	-0.005415000	-2.719389000
H	-0.015340000	-0.012144000	-1.429118000
H	-0.154680000	-1.040484000	-3.020732000
H	-0.848592000	0.634886000	-3.007432000
H	0.946593000	0.398373000	-3.011189000
H	1.237724000	0.160191000	4.688224000
S	-0.066145000	-0.044755000	4.469212000

### 5A<sup>P</sup>

C	0.000424000	0.000005000	0.006110000
C	-0.000309000	-0.000009000	2.793016000
C	1.196360000	0.000001000	0.706636000
C	1.201093000	0.000013000	2.092282000
C	-1.201836000	-0.000020000	2.090220000
C	-1.196872000	0.000004000	0.705440000
H	2.138623000	0.000002000	0.173166000
H	2.143687000	0.000051000	2.625412000
H	-2.142488000	-0.000065000	2.627290000
H	-2.138425000	-0.000002000	0.170860000
H	1.237082000	-0.000756000	4.784026000
S	-0.081512000	0.000069000	4.558229000
H	0.001292000	0.000007000	-1.075923000

C	0.001991000	0.000003000	0.013311000
C	-0.001814000	-0.000002000	2.709781000
C	1.221422000	0.000008000	0.630933000
C	1.212322000	0.000005000	2.022288000
C	-1.215890000	-0.000007000	2.015033000
C	-1.222529000	-0.000005000	0.627009000
H	2.152998000	0.000014000	0.080185000
H	2.156710000	0.000010000	2.551613000
H	-2.162746000	-0.000013000	2.544090000
H	-2.151699000	-0.000008000	0.072279000
P	-0.050085000	-0.000008000	4.492531000
C	1.605908000	0.000034000	5.175534000
H	1.533788000	0.000025000	6.263633000
H	2.146758000	-0.890858000	4.857203000
H	2.146707000	0.890959000	4.857213000
C	-0.914341000	1.457057000	5.081930000
H	-1.926903000	1.474784000	4.679040000
H	-0.963190000	1.443768000	6.171223000
H	-0.386572000	2.351142000	4.750249000
C	-0.914266000	-1.457121000	5.081923000
H	-0.386418000	-2.351177000	4.750288000
H	-0.963169000	-1.443811000	6.171214000
H	-1.926806000	-1.474929000	4.678983000

#### 6<sup>RC</sup>

C	0.113313000	0.077005000	-0.156699000
C	0.039346000	0.027572000	2.538130000
C	1.318994000	0.024222000	0.491163000
C	1.272349000	-0.000907000	1.877939000
C	-1.153888000	0.081342000	1.817103000
C	-1.122717000	0.107087000	0.426291000
H	2.260617000	0.002941000	-0.041687000
H	2.202953000	-0.042693000	2.433556000
H	-2.112538000	0.103637000	2.319607000
H	-2.037639000	0.148742000	-0.150190000
P	0.036877000	-0.006205000	4.320700000
C	2.413783000	0.045916000	-2.900226000
H	3.403087000	-0.000569000	-2.445597000
H	1.832874000	-0.829864000	-2.611835000
H	1.901294000	0.952291000	-2.578560000
H	2.521122000	0.062050000	-3.982891000
C	0.837846000	-1.500365000	4.906356000
H	1.861280000	-1.541523000	4.533751000
H	0.853670000	-1.510053000	5.996669000
H	0.293613000	-2.370974000	4.540568000
C	-1.636702000	0.034205000	4.957740000
H	-2.140173000	0.947421000	4.641359000
H	-2.195948000	-0.833079000	4.607578000
H	-1.595514000	0.012313000	6.047223000
C	0.929294000	1.411462000	4.961670000

H	0.441182000	2.327735000	4.629793000
H	0.944480000	1.378836000	6.051547000
H	1.953688000	1.402392000	4.589513000

**6<sup>TS</sup>**

C	-0.005582000	0.000213000	-0.159818000
C	0.001043000	-0.000064000	2.583495000
C	1.206936000	0.004528000	0.499548000
C	1.211488000	0.004495000	1.884158000
C	-1.210803000	-0.004727000	1.893766000
C	-1.211443000	-0.004690000	0.505858000
H	2.140849000	0.007786000	-0.048560000
H	2.159763000	0.008004000	2.410793000
H	-2.155508000	-0.008419000	2.422565000
H	-2.148799000	-0.008568000	-0.036370000
C	-0.014031000	-0.004240000	-2.835424000
H	-0.009595000	-0.001736000	-1.565777000
H	0.832546000	0.609889000	-3.129598000
H	0.090434000	-1.045794000	-3.125834000
H	-0.969655000	0.425965000	-3.122045000
P	0.051411000	0.000307000	4.363737000
C	-1.602985000	-0.006268000	5.050778000
H	-2.140600000	-0.898950000	4.732111000
H	-1.530017000	-0.005920000	6.138747000
H	-2.147715000	0.882060000	4.732027000
C	0.910887000	1.459944000	4.954455000
H	1.922901000	1.480397000	4.550311000
H	0.380315000	2.352042000	4.621987000
H	0.960427000	1.447698000	6.043685000
C	0.922570000	-1.452263000	4.954756000
H	1.934706000	-1.464722000	4.550595000
H	0.972045000	-1.439356000	6.043982000
H	0.399138000	-2.348658000	4.622529000

**6<sup>P</sup>**

C	0.001467000	0.000005000	0.014106000
C	-0.001977000	-0.000002000	2.784078000
C	1.202522000	0.000002000	0.705345000
C	1.206269000	-0.000001000	2.090704000
C	-1.210518000	0.000001000	2.084109000
C	-1.204759000	0.000004000	0.702033000
H	2.140567000	0.000003000	0.166852000
H	2.152664000	-0.000002000	2.615401000
H	-2.159233000	0.000001000	2.608666000
H	-2.140725000	0.000006000	0.159927000
P	-0.049151000	0.000005000	4.566305000
C	1.607220000	-0.000071000	5.248421000
H	1.537443000	-0.000106000	6.336617000
H	2.147409000	-0.890680000	4.928230000
H	2.147466000	0.890526000	4.928291000

C	-0.913912000	1.456863000	5.155836000
H	-1.925506000	1.474465000	4.750540000
H	-0.964751000	1.443395000	6.245002000
H	-0.385561000	2.350918000	4.825085000
C	-0.914048000	-1.456768000	5.155846000
H	-0.385780000	-2.350875000	4.825102000
H	-0.964884000	-1.443286000	6.245012000
H	-1.925644000	-1.474280000	4.750552000
H	0.003063000	0.000007000	-1.067958000

### 6A

C	0.026755000	0.066231000	0.023717000
C	-0.158592000	-0.157206000	2.734976000
C	1.053544000	-0.567893000	0.672183000
C	0.945077000	-0.674364000	2.055492000
C	-1.163680000	0.474801000	2.006396000
C	-1.082902000	0.596842000	0.618220000
H	1.911164000	-0.970174000	0.147540000
H	1.739431000	-1.170495000	2.602432000
H	-2.024182000	0.879112000	2.527936000
H	-1.866527000	1.088895000	0.055978000
P	-0.366213000	-0.263845000	4.558924000
C	1.254950000	0.394195000	5.134115000
H	1.312350000	0.287247000	6.218760000
H	2.107688000	-0.120478000	4.686699000
H	1.319194000	1.456158000	4.895629000
C	-0.079703000	-2.061599000	4.838455000
H	-0.069976000	-2.252547000	5.912987000
H	-0.900755000	-2.630721000	4.401721000
H	0.861252000	-2.415378000	4.412241000

### 6A<sup>RC</sup>

C	0.192195000	-0.416514000	0.020420000
C	0.243404000	-0.344304000	2.744747000
C	1.319749000	0.081998000	0.608669000
C	1.331024000	0.112575000	2.004006000
C	-0.873268000	-0.839749000	2.070400000
C	-0.914126000	-0.882900000	0.680025000
H	2.165606000	0.437249000	0.033788000
H	2.202113000	0.498753000	2.521708000
H	-1.731305000	-1.200785000	2.626866000
H	-1.781903000	-1.267958000	0.159236000
P	0.363531000	-0.258195000	4.577793000
C	2.241492000	0.412335000	-2.924602000
H	3.078554000	-0.188545000	-2.571202000
H	1.312816000	0.016187000	-2.514634000
H	2.369384000	1.444230000	-2.599852000
H	2.205157000	0.377474000	-4.012316000
C	-1.211869000	0.602118000	4.990875000
H	-1.324069000	0.626800000	6.076229000

H	-1.166748000	1.630832000	4.632485000
H	-2.089478000	0.116042000	4.559863000
C	-0.101397000	-1.979477000	5.039879000
H	-1.052032000	-2.296174000	4.606033000
H	0.681002000	-2.665287000	4.713905000
H	-0.175296000	-2.043031000	6.126930000

### 6A<sup>TS</sup>

C	-0.003004000	0.006049000	0.007075000
C	-0.002675000	0.015373000	2.772415000
C	1.201621000	0.046716000	0.669659000
C	1.194206000	0.051112000	2.061393000
C	-1.202377000	-0.025160000	2.061392000
C	-1.209915000	-0.030057000	0.673793000
H	2.138569000	0.074867000	0.125956000
H	2.132210000	0.082727000	2.604463000
H	-2.148250000	-0.053524000	2.591189000
C	-0.006328000	-0.004532000	-2.659757000
H	-0.005551000	0.002488000	-1.364089000
H	0.943453000	-0.446788000	-2.948108000
H	-0.860147000	-0.611979000	-2.947543000
H	-0.101241000	1.035039000	-2.960919000
P	0.089909000	0.024508000	4.608598000
C	-1.072614000	1.396159000	5.009682000
H	-0.643288000	2.342118000	4.678588000
H	-2.053801000	1.272541000	4.546884000
H	-1.200252000	1.443235000	6.092611000
C	-0.986838000	-1.412657000	5.019574000
H	-0.500753000	-2.332936000	4.694629000
H	-1.111167000	-1.460056000	6.102871000
H	-1.973845000	-1.352182000	4.556599000
H	-2.146734000	-0.061560000	0.129749000

### 6A<sup>P</sup>

C	-0.003819000	0.004382000	0.015191000
C	-0.016086000	0.003050000	2.815594000
C	1.186831000	0.069148000	0.719402000
C	1.180492000	0.072184000	2.107729000
C	-1.206640000	-0.081142000	2.091470000
C	-1.204470000	-0.069184000	0.707365000
H	2.129192000	0.120441000	0.188066000
H	2.125178000	0.128825000	2.632905000
H	-2.149704000	-0.163954000	2.621409000
H	-2.140791000	-0.128788000	0.166602000
P	-0.148112000	-0.025128000	4.644931000
H	0.002148000	0.004472000	-1.067431000
C	1.602758000	0.137047000	5.176841000
H	2.107281000	0.999626000	4.736214000
H	1.613317000	0.246288000	6.262313000
H	2.156725000	-0.769541000	4.930695000

C	-0.708238000	1.708973000	4.931335000
H	-1.712012000	1.837912000	4.525868000
H	-0.752827000	1.896832000	6.005548000
H	-0.042319000	2.437417000	4.464848000

**7**

C	0.000001000	0.000042000	0.013472000
C	-0.000004000	-0.000043000	2.756856000
C	1.203183000	0.028790000	0.703022000
C	1.211709000	0.030229000	2.088275000
C	-1.211715000	-0.030273000	2.088268000
C	-1.203184000	-0.028750000	0.703016000
H	2.140033000	0.059670000	0.163550000
H	2.144904000	0.076280000	2.635566000
H	-2.144912000	-0.076358000	2.635553000
H	-2.140032000	-0.059597000	0.163538000
N	-0.000007000	-0.000086000	4.207284000
C	0.648171000	-0.975382000	4.870458000
C	-0.648187000	0.975172000	4.870512000
C	0.668202000	-0.993661000	6.244229000
H	1.123968000	-1.728382000	4.259228000
C	-0.668222000	0.993371000	6.244285000
H	-1.123983000	1.728207000	4.259324000
C	-0.000011000	-0.000165000	6.944076000
H	1.194367000	-1.788061000	6.753445000
H	-1.194389000	1.787742000	6.753546000
H	-0.000012000	-0.000196000	8.026061000
H	0.000003000	0.000075000	-1.068241000

**7<sup>RC</sup>**

C	0.030793000	-0.027019000	-0.001059000
C	0.013592000	-0.009976000	2.668929000
C	1.246758000	0.045869000	0.622587000
C	1.234077000	0.053086000	2.013372000
C	-1.198388000	-0.081492000	1.998893000
C	-1.193039000	-0.092084000	0.607786000
H	2.177046000	0.085428000	0.071317000
H	2.161384000	0.086334000	2.572587000
H	-2.132812000	-0.107765000	2.546474000
H	-2.118992000	-0.139335000	0.049848000
C	2.278080000	-0.051537000	-2.785513000
H	1.671488000	0.811475000	-2.511748000
H	3.274442000	0.045426000	-2.354931000
H	1.806463000	-0.964933000	-2.423784000
H	2.362720000	-0.098640000	-3.869296000
N	0.004384000	-0.000908000	4.119336000
C	-0.537587000	-1.037232000	4.785602000
C	0.538173000	1.043642000	4.779336000
C	-0.564275000	-1.048753000	6.159290000
H	-0.924750000	-1.841317000	4.176833000

C	0.547759000	1.072256000	6.153001000
H	0.933049000	1.840051000	4.165446000
C	-0.012612000	0.016110000	6.855818000
H	-1.004132000	-1.892436000	6.671125000
H	0.981328000	1.922256000	6.659724000
H	-0.019327000	0.022839000	7.937764000

### 7<sup>TS</sup>

C	0.002552000	-0.002855000	0.010016000
C	0.001184000	-0.000830000	2.726466000
C	1.204769000	0.123512000	0.672844000
C	1.209692000	0.126406000	2.060816000
C	-1.206689000	-0.128833000	2.059789000
C	-1.200383000	-0.127804000	0.671834000
H	2.134830000	0.229445000	0.128622000
H	2.134369000	0.247517000	2.612223000
H	-2.131928000	-0.249062000	2.610446000
H	-2.129965000	-0.233794000	0.126790000
C	0.002147000	-0.000174000	-2.665491000
H	0.988976000	-0.349489000	-2.956428000
H	-0.189910000	1.028533000	-2.957000000
H	0.002593000	-0.001841000	-1.398061000
H	-0.791233000	-0.682935000	-2.956733000
N	0.000482000	0.000038000	4.176884000
C	0.721376000	-0.921886000	4.841202000
C	-0.721060000	0.922754000	4.839397000
C	0.742504000	-0.937440000	6.215032000
H	1.253611000	-1.636418000	4.230420000
C	-0.743535000	0.939953000	6.213186000
H	-1.252704000	1.636551000	4.227244000
C	-0.000855000	0.001676000	6.914019000
H	1.328337000	-1.688458000	6.724909000
H	-1.329864000	1.691581000	6.721591000
H	-0.001381000	0.002324000	7.995978000

### 7<sup>P</sup>

C	0.000001000	0.000042000	0.013472000
C	-0.000004000	-0.000043000	2.756856000
C	1.203183000	0.028790000	0.703022000
C	1.211709000	0.030229000	2.088275000
C	-1.211715000	-0.030273000	2.088268000
C	-1.203184000	-0.028750000	0.703016000
H	2.140033000	0.059670000	0.163550000
H	2.144904000	0.076280000	2.635566000
H	-2.144912000	-0.076358000	2.635553000
H	-2.140032000	-0.059597000	0.163538000
N	-0.000007000	-0.000086000	4.207284000
C	0.648171000	-0.975382000	4.870458000
C	-0.648187000	0.975172000	4.870512000
C	0.668202000	-0.993661000	6.244229000

H	1.123968000	-1.728382000	4.259228000
C	-0.668222000	0.993371000	6.244285000
H	-1.123983000	1.728207000	4.259324000
C	-0.000011000	-0.000165000	6.944076000
H	1.194367000	-1.788061000	6.753445000
H	-1.194389000	1.787742000	6.753546000
H	-0.000012000	-0.000196000	8.026061000
H	0.000003000	0.000075000	-1.068241000

### 7A

C	-0.000032000	-0.000006000	0.012087000
C	0.000034000	0.000015000	2.738258000
C	1.213194000	0.004496000	0.644128000
C	1.205663000	0.017837000	2.035509000
C	-1.205629000	-0.017820000	2.035568000
C	-1.213226000	-0.004498000	0.644187000
H	2.149765000	0.019140000	0.101102000
H	2.142978000	0.068243000	2.574690000
H	-2.142918000	-0.068221000	2.574793000
H	-2.149824000	-0.019150000	0.101206000
N	0.000070000	0.000016000	4.144604000
C	0.924213000	-0.745491000	4.872220000
C	-0.923972000	0.745600000	4.872271000
C	0.955916000	-0.775123000	6.201141000
H	1.600915000	-1.341295000	4.276641000
C	-0.955470000	0.775393000	6.201193000
H	-1.600790000	1.341305000	4.276727000
C	0.000305000	0.000206000	7.064510000
H	1.694834000	-1.405684000	6.677408000
H	-1.694345000	1.405976000	6.677498000
H	-0.545276000	-0.678734000	7.732279000
H	0.546009000	0.679255000	7.732068000

### 7A<sup>RC</sup>

C	-0.857076000	0.689165000	-0.044775000
C	-0.364687000	0.315243000	2.608798000
C	0.441379000	0.783326000	0.375688000
C	0.686895000	0.578034000	1.729717000
C	-1.670083000	0.245442000	2.120202000
C	-1.927443000	0.421909000	0.764129000
H	1.256133000	0.986380000	-0.307743000
H	1.704656000	0.598247000	2.098196000
H	-2.492644000	0.076947000	2.803564000
H	-2.940781000	0.367855000	0.386695000
C	0.840710000	1.276099000	-3.241821000
H	-0.077021000	1.097607000	-2.681888000
H	1.304867000	2.197527000	-2.892228000
H	1.524738000	0.441838000	-3.090979000
H	0.610093000	1.367300000	-4.302090000
N	-0.110674000	0.121640000	3.978397000

C	-0.786811000	-0.848754000	4.713271000
C	0.828003000	0.891669000	4.660134000
C	-0.574626000	-1.065284000	6.007979000
H	-1.479425000	-1.452662000	4.144618000
C	1.094846000	0.742866000	5.954311000
H	1.306544000	1.658753000	4.068199000
C	0.415366000	-0.279627000	6.822310000
H	-1.129956000	-1.860334000	6.487484000
H	1.822413000	1.406521000	6.402215000
H	1.153397000	-0.953011000	7.276612000
H	-0.082514000	0.210629000	7.668662000

#### 7A<sup>TS</sup>

C	-2.917007000	0.001054000	0.000147000
C	-0.153168000	0.000376000	0.000048000
C	-2.246070000	1.139534000	0.387609000
C	-0.858368000	1.135839000	0.399704000
C	-0.858907000	-1.134688000	-0.399552000
C	-2.246680000	-1.137690000	-0.387326000
H	-2.785708000	2.025744000	0.700162000
H	-0.320461000	2.009518000	0.744858000
H	-0.321480000	-2.008648000	-0.744732000
H	-2.786698000	-2.023674000	-0.699831000
C	-5.583042000	-0.001076000	-0.000133000
H	-4.292998000	0.002023000	0.000483000
H	-5.879905000	0.210850000	1.023415000
H	-5.880664000	0.774969000	-0.700017000
H	-5.871384000	-0.997005000	-0.325921000
N	1.252970000	0.000053000	0.000064000
C	1.980836000	1.119389000	-0.394557000
C	1.980317000	-1.119656000	0.394580000
C	3.309960000	1.158954000	-0.412372000
H	1.385784000	1.956557000	-0.730076000
C	3.309422000	-1.159894000	0.412233000
H	1.384874000	-1.956519000	0.730169000
C	4.173398000	-0.000690000	-0.000124000
H	3.786206000	2.065760000	-0.760702000
H	3.785251000	-2.066937000	0.760516000
H	4.841002000	-0.288971000	-0.822251000
H	4.841249000	0.287253000	0.821921000

#### 7A<sup>P</sup>

C	-0.000030000	-0.000060000	0.013232000
C	0.000049000	0.000073000	2.810154000
C	1.194895000	0.004387000	0.715780000
C	1.200429000	0.015085000	2.100170000
C	-1.200371000	-0.015008000	2.100239000
C	-1.194917000	-0.004442000	0.715849000
H	2.137388000	0.018968000	0.182815000
H	2.140952000	0.063643000	2.632674000

H	-2.140866000	-0.063520000	2.632798000
H	-2.137439000	-0.019076000	0.182939000
N	0.000089000	0.000123000	4.214872000
C	0.952902000	-0.707763000	4.943532000
C	-0.952556000	0.708225000	4.943545000
C	0.985355000	-0.736367000	6.272417000
H	1.652083000	-1.278095000	4.349548000
C	-0.984632000	0.737307000	6.272429000
H	-1.651976000	1.278260000	4.349559000
C	0.000528000	0.000686000	7.135873000
H	1.747928000	-1.338261000	6.748551000
H	-1.747153000	1.339268000	6.748562000
H	-0.517808000	-0.699126000	7.803863000
H	0.519120000	0.700831000	7.803318000
H	-0.000061000	-0.000113000	-1.068697000

## 8

C	-0.000063000	0.000185000	0.006627000
C	0.000209000	-0.000252000	2.682487000
C	1.225946000	-0.000003000	0.616521000
C	1.223794000	-0.000563000	2.004662000
C	-1.223534000	0.001471000	2.004917000
C	-1.225960000	0.002048000	0.616812000
H	2.154040000	0.005445000	0.060028000
H	2.165523000	0.005407000	2.541459000
H	-2.165110000	0.008986000	2.541957000
H	-2.154131000	0.009048000	0.060464000
P	0.000557000	-0.049192000	4.445614000
H	1.125495000	0.585750000	4.978677000
H	-1.122778000	0.588009000	4.979379000
H	-0.000608000	-1.338928000	4.991489000

## 8<sup>RC</sup>

C	0.038207000	0.057011000	-0.001361000
C	0.002259000	0.003167000	2.673823000
C	1.252170000	-0.051714000	0.623176000
C	1.231306000	-0.079097000	2.010492000
C	-1.208660000	0.111634000	1.981921000
C	-1.192245000	0.139348000	0.594240000
H	2.181334000	-0.118739000	0.072524000
H	2.162164000	-0.170225000	2.558533000
H	-2.155015000	0.167290000	2.507668000
H	-2.110480000	0.216643000	0.026853000
P	-0.017147000	0.016871000	4.436809000
H	-1.194904000	-0.538419000	4.944524000
H	1.045764000	-0.717099000	4.970441000
C	2.225787000	-0.089587000	-2.786555000
H	3.223222000	-0.174206000	-2.355773000
H	1.617236000	-0.940847000	-2.481548000
H	1.758623000	0.839159000	-2.459177000

H	2.308025000	-0.082440000	-3.871412000
H	0.077914000	1.291249000	5.010175000

**8<sup>TS</sup>**

C	0.000785000	0.004259000	0.000005000
C	-0.001215000	0.000062000	2.724843000
C	1.209257000	0.101256000	0.659851000
C	1.215868000	0.099712000	2.044498000
C	-1.217336000	-0.097032000	2.042406000
C	-1.208697000	-0.094250000	0.657776000
H	2.139984000	0.182804000	0.112662000
H	2.154290000	0.181880000	2.580863000
H	-2.157685000	-0.166762000	2.577156000
H	-2.139504000	-0.163206000	0.108995000
C	0.003345000	0.003594000	-2.678947000
H	0.001916000	0.006134000	-1.415079000
H	0.857375000	0.609857000	-2.967852000
H	0.099916000	-1.039121000	-2.967910000
H	-0.946828000	0.443084000	-2.969495000
P	0.001503000	-0.052281000	4.485339000
H	1.070006000	0.669850000	5.024033000
H	-1.169529000	0.489769000	5.022215000
H	0.104368000	-1.337456000	5.032978000

**8<sup>P</sup>**

C	-0.000001000	-0.001175000	0.007382000
C	0.000014000	0.002188000	2.758541000
C	1.207385000	-0.000146000	0.692861000
C	1.217586000	0.001825000	2.075224000
C	-1.217576000	-0.000830000	2.075242000
C	-1.207391000	-0.002773000	0.692898000
H	2.142557000	-0.005482000	0.149808000
H	2.161401000	-0.003275000	2.607037000
H	-2.161377000	-0.007980000	2.607064000
H	-2.142554000	-0.010132000	0.149855000
P	0.000040000	0.054670000	4.521597000
H	-0.004566000	1.345564000	5.064692000
H	-1.121443000	-0.583319000	5.058406000
H	1.126424000	-0.575211000	5.057672000
H	-0.000011000	-0.005908000	-1.074732000

**8<sup>A</sup>**

C	0.001946000	0.044569000	0.007545000
C	-0.011176000	-0.069302000	2.727810000
C	1.216347000	-0.037108000	0.636922000
C	1.195914000	-0.094229000	2.026768000
C	-1.207755000	0.013336000	2.020072000
C	-1.215647000	0.073324000	0.625377000
H	2.152278000	-0.056932000	0.092888000
H	2.132774000	-0.158858000	2.568024000

H	-2.149357000	0.031033000	2.557258000
H	-2.146776000	0.137933000	0.076838000
P	-0.107767000	-0.140925000	4.560673000
H	0.834194000	0.877126000	4.847446000
H	0.832025000	-1.180050000	4.766247000

#### **8A<sup>RC</sup>**

C	0.030458000	0.034035000	0.002830000
C	0.016681000	0.068274000	2.724334000
C	1.243117000	0.015844000	0.630537000
C	1.221228000	0.033967000	2.026049000
C	-1.184391000	0.085274000	2.012974000
C	-1.191312000	0.068153000	0.621817000
H	2.178271000	-0.010856000	0.085895000
H	2.158086000	0.021356000	2.571604000
H	-2.127306000	0.112121000	2.546855000
H	-2.122614000	0.081491000	0.069751000
P	0.095429000	0.089167000	4.559400000
H	-0.855148000	-0.930738000	4.808760000
H	-0.840455000	1.127996000	4.784540000
C	2.390224000	-0.044972000	-2.850788000
H	1.359002000	-0.021220000	-2.499558000
H	2.915876000	0.838857000	-2.491362000
H	2.881048000	-0.941241000	-2.473366000
H	2.404916000	-0.056276000	-3.939464000

#### **8A<sup>TS</sup>**

C	-0.104316000	-0.026644000	0.048334000
C	0.005390000	-0.030034000	2.807672000
C	1.119670000	-0.152927000	0.661992000
C	1.169055000	-0.152263000	2.053064000
C	-1.218024000	0.096215000	2.147822000
C	-1.278347000	0.099184000	0.761921000
H	2.029712000	-0.249271000	0.081842000
H	2.125245000	-0.246978000	2.555173000
H	-2.131555000	0.192968000	2.723029000
C	-0.212030000	-0.021618000	-2.616353000
H	-0.161505000	-0.024618000	-1.322813000
H	-0.775428000	0.867554000	-2.885695000
H	0.822774000	0.016685000	-2.945903000
H	-0.712148000	-0.945404000	-2.893768000
P	0.165274000	-0.042686000	4.637079000
H	-2.231078000	0.198329000	0.255170000
H	-0.744356000	1.005113000	4.920485000
H	-0.789410000	-1.052702000	4.911792000

#### **8A<sup>P</sup>**

C	0.000788000	-0.015470000	0.007607000
C	0.018596000	0.037870000	2.799829000
C	1.203006000	-0.036716000	0.694199000

C	1.210044000	-0.015933000	2.082167000
C	-1.185204000	0.057598000	2.096195000
C	-1.194826000	0.028950000	0.712008000
H	2.139085000	-0.075852000	0.151562000
H	2.154178000	-0.045260000	2.613548000
H	-2.123141000	0.096605000	2.636899000
H	-2.137784000	0.042625000	0.179871000
P	0.118959000	0.072606000	4.632867000
H	-1.100953000	-0.592201000	4.904669000
H	-0.007796000	-0.036828000	-1.074851000
H	-0.442879000	1.357761000	4.835862000

### 9

C	-0.437004000	0.080306000	0.052969000
C	-0.154415000	0.086756000	2.746867000
C	0.536597000	-0.726573000	0.575421000
C	0.675060000	-0.711048000	1.959287000
C	-1.110665000	0.902516000	2.142772000
C	-1.268522000	0.904541000	0.760892000
H	1.179980000	-1.337200000	-0.044581000
H	1.449031000	-1.314311000	2.421440000
H	-1.728756000	1.556913000	2.747959000
H	-2.003102000	1.539210000	0.282518000
N	-0.830234000	-0.917669000	4.997482000
C	-0.537556000	-0.757333000	6.451562000
H	-1.128428000	-1.476595000	7.013921000
H	0.521611000	-0.935161000	6.622782000
H	-0.797423000	0.253543000	6.757151000
C	-2.283744000	-0.683267000	4.763492000
H	-2.502284000	-0.820600000	3.708423000
H	-2.850859000	-1.395721000	5.358202000
H	-2.531883000	0.331673000	5.066228000
C	-0.484749000	-2.306519000	4.580353000
H	0.576490000	-2.473754000	4.751082000
H	-1.069568000	-3.003851000	5.175844000
H	-0.716027000	-2.430845000	3.526368000
C	0.014565000	0.104647000	4.234304000
H	-0.262219000	1.072468000	4.651246000
H	1.045094000	-0.107983000	4.516954000

### 9RC

C	-0.514970000	0.065781000	0.051584000
C	-0.180448000	0.021163000	2.739047000
C	0.771792000	0.091623000	0.515931000
C	0.930634000	0.063525000	1.897171000
C	-1.463140000	-0.026862000	2.193992000
C	-1.648027000	0.000089000	0.815677000
H	1.625021000	0.117459000	-0.149276000
H	1.931284000	0.057255000	2.315842000
H	-2.328326000	-0.103463000	2.843743000

H	-2.639168000	-0.043697000	0.383250000
C	1.387638000	-0.006162000	-3.006259000
H	0.807099000	0.845423000	-2.652250000
H	2.429219000	0.106400000	-2.706363000
H	0.981284000	-0.927249000	-2.589568000
H	1.332859000	-0.049925000	-4.092168000
C	0.005131000	-0.021581000	4.223831000
H	-0.805535000	-0.565572000	4.707616000
H	0.946503000	-0.501059000	4.490446000
N	0.040437000	1.343608000	4.914276000
C	1.172087000	2.167031000	4.400861000
H	1.193249000	3.107496000	4.946730000
H	2.102979000	1.626729000	4.558500000
H	1.025613000	2.353973000	3.340958000
C	0.229044000	1.111402000	6.375753000
H	1.165453000	0.581290000	6.533605000
H	0.257144000	2.070896000	6.886947000
H	-0.600688000	0.517032000	6.751337000
C	-1.238051000	2.078996000	4.697815000
H	-1.366787000	2.266106000	3.635636000
H	-2.061633000	1.474772000	5.071944000
H	-1.193686000	3.020494000	5.240497000

### 9TS

C	-0.011571000	-0.013820000	-0.020763000
C	-0.003924000	-0.005877000	2.733559000
C	1.197798000	-0.012078000	0.640675000
C	1.197981000	-0.012858000	2.028157000
C	-1.209526000	-0.030568000	2.034899000
C	-1.217111000	-0.029852000	0.647435000
H	2.132688000	-0.024308000	0.094040000
H	2.141381000	-0.036688000	2.563213000
H	-2.149462000	-0.068245000	2.575228000
H	-2.154762000	-0.055863000	0.106033000
C	-0.019135000	-0.065993000	-2.693575000
H	-0.015447000	-0.035163000	-1.420313000
H	0.885039000	0.452937000	-2.999686000
H	-0.018499000	-1.118989000	-2.960415000
H	-0.926470000	0.450529000	-2.994353000
C	0.000357000	-0.018415000	4.229787000
H	-0.878576000	-0.528075000	4.623588000
H	0.888851000	-0.515125000	4.618651000
N	-0.007914000	1.362589000	4.890169000
C	1.200174000	2.142632000	4.498080000
H	1.182795000	3.096433000	5.020500000
H	2.089399000	1.582598000	4.779042000
H	1.187329000	2.303911000	3.424031000
C	-0.002409000	1.162971000	6.368082000
H	0.892658000	0.612843000	6.649151000
H	-0.008140000	2.133990000	6.857880000

H	-0.887810000	0.599870000	6.654031000
C	-1.229381000	2.124904000	4.504721000
H	-1.224761000	2.286282000	3.430618000
H	-2.108788000	1.551969000	4.790528000
H	-1.223058000	3.078885000	5.027060000

### 9P

C	0.000227000	-0.001200000	-0.065197000
C	-0.000050000	0.000585000	2.716503000
C	1.201820000	-0.001641000	0.627465000
C	1.201195000	0.004315000	2.012219000
C	-1.200935000	0.023173000	2.011968000
C	-1.201367000	0.017254000	0.627212000
H	2.139892000	0.006888000	0.088626000
H	2.144222000	0.029246000	2.546633000
H	-2.143564000	0.062888000	2.546183000
H	-2.139078000	0.040533000	0.088185000
N	-0.010454000	-1.357108000	4.879623000
C	-0.009647000	-1.150300000	6.356849000
H	-0.016792000	-2.119081000	6.851004000
H	0.884496000	-0.598765000	6.638062000
H	-0.896082000	-0.586051000	6.637246000
C	-1.230900000	-2.121596000	4.494439000
H	-1.222746000	-2.289657000	3.421395000
H	-1.226333000	-3.072441000	5.022451000
H	-2.111200000	-1.546980000	4.774051000
C	1.199084000	-2.139315000	4.495612000
H	2.087396000	-1.577580000	4.776053000
H	1.180155000	-3.089977000	5.023629000
H	1.189494000	-2.307297000	3.422570000
C	-0.000105000	0.019880000	4.213382000
H	-0.880113000	0.532191000	4.601237000
H	0.887281000	0.519071000	4.601539000
H	0.000357000	0.000914000	-1.147146000

### 9A

C	0.000854000	0.051817000	-0.033122000
C	0.000252000	0.028633000	2.694678000
C	1.216710000	0.040456000	0.593934000
C	1.199758000	0.029515000	1.987367000
C	-1.198871000	0.048151000	1.987001000
C	-1.215222000	0.059370000	0.593558000
H	2.151896000	0.044865000	0.048206000
H	2.139026000	0.027527000	2.530092000
H	-2.138226000	0.060753000	2.529433000
H	-2.150059000	0.078330000	0.047547000
N	-0.010367000	-1.372268000	4.789937000
C	-1.214476000	-2.121724000	4.508877000
H	-1.316633000	-2.411772000	3.450445000
H	-1.219475000	-3.034099000	5.108321000

H	-2.090636000	-1.531325000	4.785343000
C	1.182643000	-2.139360000	4.509141000
H	2.067331000	-1.561885000	4.785752000
H	1.174127000	-3.051697000	5.108605000
H	1.280723000	-2.430896000	3.450731000
C	-0.000471000	-0.036164000	4.209741000
H	-0.875672000	0.494813000	4.592790000
H	0.882314000	0.481890000	4.593083000

### **9A<sup>RC</sup>**

C	-0.531320000	-0.032093000	0.048836000
C	-0.156247000	-0.029563000	2.749743000
C	0.759510000	-0.034842000	0.501687000
C	0.934479000	-0.034399000	1.884087000
C	-1.441573000	-0.034604000	2.214134000
C	-1.649937000	-0.035200000	0.836150000
H	1.608359000	-0.042018000	-0.170346000
H	1.939484000	-0.043717000	2.292292000
H	-2.297343000	-0.044037000	2.880697000
H	-2.651132000	-0.042938000	0.423961000
C	1.344469000	0.022384000	-3.122388000
H	0.389546000	0.005641000	-2.597740000
H	1.904445000	0.908579000	-2.826200000
H	1.913013000	-0.871284000	-2.867885000
H	1.171054000	0.046649000	-4.197117000
C	0.052220000	0.024106000	4.250878000
H	-0.766550000	-0.502762000	4.747524000
H	0.974827000	-0.503639000	4.505639000
N	0.134055000	1.355886000	4.835220000
C	1.283838000	2.115731000	4.398054000
H	1.366212000	3.023128000	4.999435000
H	2.192936000	1.528954000	4.546023000
H	1.237890000	2.415349000	3.338339000
C	-1.090480000	2.117025000	4.727387000
H	-1.334401000	2.416688000	3.695112000
H	-1.925600000	1.531225000	5.117363000
H	-1.005085000	3.024464000	5.328281000

### **9A<sup>TS</sup>**

C	-0.082454000	0.017951000	0.005278000
C	-0.228834000	0.043476000	2.766973000
C	1.038756000	-0.310572000	0.734447000
C	0.956874000	-0.296425000	2.121600000
C	-1.341762000	0.362031000	1.993641000
C	-1.275991000	0.352497000	0.605665000
H	1.965771000	-0.579759000	0.241934000
H	1.827515000	-0.559461000	2.712826000
H	-2.275271000	0.615765000	2.484488000
H	-2.149078000	0.598956000	0.012883000
C	0.057864000	-0.013980000	-2.657255000

H	-0.011648000	0.002638000	-1.363894000
H	1.060481000	-0.363273000	-2.889201000
H	-0.716412000	-0.702288000	-2.984911000
H	-0.118245000	1.009932000	-2.975345000
C	-0.294660000	0.107442000	4.279968000
H	-1.303830000	-0.154190000	4.608532000
H	0.384467000	-0.637667000	4.702382000
N	0.040317000	1.393267000	4.878061000
C	1.414422000	1.792711000	4.671185000
H	1.630574000	2.670811000	5.282902000
H	2.084281000	0.989240000	4.984837000
H	1.647976000	2.043937000	3.623742000
C	-0.886364000	2.451506000	4.543556000
H	-0.843503000	2.757479000	3.485567000
H	-1.907325000	2.132113000	4.763276000
H	-0.667812000	3.328844000	5.155517000

### **9A<sup>P</sup>**

C	0.000815000	0.042936000	-0.093554000
C	0.000114000	0.025750000	2.703314000
C	1.199161000	0.032381000	0.604068000
C	1.195026000	0.025042000	1.990362000
C	-1.194365000	0.043945000	1.989886000
C	-1.197825000	0.051380000	0.603586000
H	2.139576000	0.034528000	0.067100000
H	2.135451000	0.024334000	2.530197000
H	-2.134904000	0.058100000	2.529339000
H	-2.137872000	0.068437000	0.066243000
N	-0.010320000	-1.372640000	4.798508000
C	-1.214190000	-2.122458000	4.517232000
H	-1.315871000	-2.412877000	3.458927000
H	-1.219257000	-3.034381000	5.117507000
H	-2.090468000	-1.531731000	4.792551000
C	1.182461000	-2.139882000	4.516998000
H	2.067284000	-1.561912000	4.792064000
H	1.174446000	-3.051753000	5.117320000
H	1.279654000	-2.431801000	3.458681000
C	-0.000662000	-0.036359000	4.217411000
H	-0.876522000	0.494212000	4.599834000
H	0.882555000	0.481592000	4.600207000
H	0.001099000	0.051360000	-1.176192000

### **10**

C	0.000061000	0.000039000	0.005769000
C	-0.000107000	-0.000029000	2.740361000
C	1.216182000	-0.000001000	0.638064000
C	1.198026000	-0.000060000	2.034383000
C	-1.198150000	0.000040000	2.034237000
C	-1.216134000	0.000047000	0.637911000
H	2.153178000	-0.000025000	0.092119000

H	2.116006000	-0.000135000	2.610828000
H	-2.116206000	0.000083000	2.610561000
H	-2.153066000	0.000093000	0.091856000
C	-0.000196000	-0.000070000	4.292597000
O	-1.126416000	-0.000242000	4.822446000
O	1.125958000	0.000460000	4.822586000

**10<sup>RC</sup>**

C	0.052682000	0.032297000	-0.002980000
C	0.008016000	-0.000738000	2.728795000
C	1.258937000	0.032307000	0.647489000
C	1.217666000	0.015291000	2.043113000
C	-1.178559000	0.000262000	2.003470000
C	-1.174205000	0.017062000	0.607193000
H	2.203429000	0.044764000	0.114773000
H	2.125853000	0.014097000	2.634866000
H	-2.105873000	-0.012488000	2.564539000
H	-2.101659000	0.017747000	0.045420000
C	2.071546000	0.090821000	-3.065673000
H	1.227490000	0.081980000	-2.375725000
H	2.686716000	0.968076000	-2.868729000
H	2.665980000	-0.809905000	-2.916832000
H	1.709639000	0.122888000	-4.093208000
C	-0.017320000	-0.019487000	4.281200000
O	-1.151964000	-0.032956000	4.792139000
O	1.100160000	-0.018799000	4.828803000

**10<sup>TS</sup>**

C	-0.001437000	0.000650000	0.000317000
C	-0.000295000	-0.001073000	2.764637000
C	1.206836000	0.008559000	0.664305000
C	1.196429000	0.007601000	2.056067000
C	-1.197638000	-0.008848000	2.056915000
C	-1.209283000	-0.008036000	0.665238000
H	2.143594000	0.015354000	0.116384000
H	2.114404000	0.013565000	2.632002000
H	-2.115125000	-0.015508000	2.633624000
H	-2.146501000	-0.014110000	0.118125000
C	0.008574000	0.003315000	-2.667385000
H	-0.001379000	0.001600000	-1.348141000
H	-0.483079000	-0.917779000	-2.969719000
H	-0.535823000	0.895074000	-2.967312000
H	1.058390000	0.034337000	-2.948348000
C	0.000247000	-0.002037000	4.317003000
O	-1.125780000	-0.010187000	4.847059000
O	1.126627000	0.005456000	4.846301000

**10<sup>P</sup>**

C	0.0000000000	-0.000014000	0.006345000
C	0.000006000	-0.000012000	2.807111000

C	1.199280000	-0.000011000	0.707209000
C	1.194575000	-0.000011000	2.095236000
C	-1.194566000	-0.000017000	2.095240000
C	-1.199276000	-0.000019000	0.707213000
H	2.140453000	-0.000009000	0.166852000
H	2.113217000	-0.000009000	2.669536000
H	-2.113206000	-0.000020000	2.669543000
H	-2.140451000	-0.000023000	0.166861000
C	0.000009000	-0.000010000	4.358774000
O	-1.126077000	0.000066000	4.889409000
O	1.126097000	0.000112000	4.889404000
H	-0.000002000	-0.000014000	-1.078439000

### 10A

C	0.000256000	-0.000018000	0.005945000
C	0.000284000	0.000023000	2.707166000
C	1.220336000	-0.000003000	0.626288000
C	1.210853000	0.000019000	2.017762000
C	-1.209099000	0.000006000	2.015923000
C	-1.220879000	-0.000015000	0.626092000
H	2.152101000	-0.000006000	0.075587000
H	2.142867000	0.000032000	2.566611000
H	-2.133526000	0.000010000	2.579219000
H	-2.152713000	-0.000027000	0.075583000
C	-0.053056000	0.000047000	4.191899000
O	-1.064710000	0.000017000	4.841493000
O	1.163474000	0.000026000	4.764793000
H	1.018208000	0.000014000	5.718089000

### 10A<sup>RC</sup>

C	0.006477000	0.001559000	0.003369000
C	0.002660000	0.000171000	2.703834000
C	1.225800000	0.001495000	0.624947000
C	1.214280000	0.000771000	2.016256000
C	-1.205741000	0.000266000	2.010916000
C	-1.215786000	0.000979000	0.621016000
H	2.155791000	0.002022000	0.071623000
H	2.145665000	0.000691000	2.566104000
H	-2.130942000	-0.000215000	2.572909000
H	-2.146872000	0.001062000	0.069283000
C	2.420531000	0.032574000	-2.846226000
H	1.378460000	0.029172000	-2.527942000
H	2.916962000	0.919339000	-2.454033000
H	2.917548000	-0.861265000	-2.471200000
H	2.469001000	0.043049000	-3.933864000
C	-0.053285000	-0.000576000	4.188526000
O	-1.066166000	-0.001418000	4.836212000
O	1.162108000	-0.001032000	4.763694000
H	1.015082000	-0.001793000	5.716714000

**10A<sup>TS</sup>**

C	0.000576000	-0.000206000	0.002373000
C	0.000552000	0.000068000	2.743948000
C	1.209599000	-0.001019000	0.663643000
C	1.208639000	-0.000835000	2.051499000
C	-1.206308000	0.000708000	2.049741000
C	-1.209495000	0.000532000	0.663438000
H	2.144593000	-0.001877000	0.116721000
H	2.141470000	-0.001372000	2.598648000
H	-2.131416000	0.001357000	2.611576000
H	-2.144500000	0.000864000	0.116626000
C	0.001140000	-0.000365000	-2.665039000
H	0.001512000	-0.001625000	-1.372036000
H	0.107636000	-1.040410000	-2.960471000
H	-0.954086000	0.429517000	-2.953937000
H	0.847816000	0.615532000	-2.955678000
C	-0.052730000	0.000396000	4.228446000
O	-1.063959000	0.001158000	4.879269000
O	1.163586000	-0.000261000	4.802683000
H	1.016155000	0.000011000	5.755670000

**10A<sup>P</sup>**

C	0.000214000	-0.000031000	0.006968000
C	0.000274000	0.000062000	2.778900000
C	1.202423000	0.000007000	0.698959000
C	1.205680000	0.000053000	2.083896000
C	-1.203976000	0.000024000	2.082389000
C	-1.202964000	-0.000023000	0.698962000
H	2.139944000	0.000000000	0.158106000
H	2.139334000	0.000083000	2.628864000
H	-2.130068000	0.000031000	2.641769000
H	-2.140498000	-0.000052000	0.158201000
C	-0.052511000	0.000111000	4.264030000
O	-1.063662000	0.000125000	4.914638000
O	1.164102000	0.000149000	4.837063000
H	1.018110000	0.000182000	5.790280000
H	0.000672000	-0.000068000	-1.075865000

**11**

C	0.000015000	-0.000115000	0.004310000
C	-0.000042000	-0.002418000	2.766341000
C	1.212667000	-0.000056000	0.640316000
C	1.190362000	-0.001746000	2.038642000
C	-1.190386000	-0.006475000	2.038620000
C	-1.212628000	-0.004882000	0.640257000
H	2.152469000	-0.001542000	0.098547000
H	2.131940000	-0.011260000	2.578531000
H	-2.131893000	-0.019694000	2.578534000
H	-2.152396000	-0.010110000	0.098450000
B	0.000149000	0.037868000	4.405090000

F	0.003262000	1.381997000	4.855673000
F	1.153141000	-0.609337000	4.912931000
F	-1.155555000	-0.604232000	4.913203000

### **11<sup>RC</sup>**

C	-0.665240000	-0.007099000	-0.121177000
C	-0.063510000	0.009610000	2.572569000
C	0.655243000	0.063407000	0.233664000
C	0.937948000	0.070952000	1.603279000
C	-1.382442000	-0.055891000	2.121961000
C	-1.709438000	-0.065851000	0.762327000
H	1.451213000	0.113966000	-0.501622000
H	1.972494000	0.135342000	1.925188000
H	-2.182866000	-0.091728000	2.854164000
H	-2.743253000	-0.115493000	0.437914000
C	0.568746000	0.137054000	-3.576954000
H	-0.071741000	0.088665000	-2.695991000
H	1.155546000	1.054372000	-3.544162000
H	1.238584000	-0.722116000	-3.581270000
H	-0.041784000	0.127319000	-4.479781000
B	0.294828000	-0.022617000	4.172543000
F	0.449506000	-1.363382000	4.605011000
F	-0.748121000	0.574753000	4.921377000
F	1.503165000	0.673073000	4.419611000

### **11<sup>TS</sup>**

C	-0.006461000	0.003868000	-0.000820000
C	0.001491000	0.004385000	2.790247000
C	1.190745000	-0.149438000	0.663347000
C	1.179508000	-0.146672000	2.056572000
C	-1.180119000	0.160062000	2.063066000
C	-1.199520000	0.161284000	0.670052000
H	2.120969000	-0.267127000	0.116245000
H	2.115351000	-0.257034000	2.594801000
H	-2.110092000	0.292302000	2.606543000
H	-2.131948000	0.285728000	0.128260000
C	-0.002363000	0.004201000	-2.669070000
H	-0.009441000	0.005546000	-1.346852000
H	-0.681205000	-0.790214000	-2.968644000
H	-0.342872000	0.991670000	-2.970043000
H	1.028909000	-0.192113000	-2.952031000
B	0.000213000	-0.037288000	4.428880000
F	-0.178720000	-1.370349000	4.876577000
F	1.231516000	0.446382000	4.934371000
F	-1.056195000	0.755273000	4.940246000

### **11<sup>P</sup>**

C	0.000002000	-0.000085000	0.004567000
C	0.000009000	-0.002506000	2.831686000
C	1.196526000	-0.000135000	0.708486000

C	1.187570000	-0.001955000	2.097322000
C	-1.187525000	-0.006879000	2.097348000
C	-1.196486000	-0.005107000	0.708484000
H	2.139474000	-0.000954000	0.170493000
H	2.128609000	-0.011286000	2.637213000
H	-2.128484000	-0.020081000	2.637284000
H	-2.139427000	-0.009841000	0.170500000
B	0.000191000	0.038302000	4.468844000
F	0.001833000	1.383392000	4.918944000
F	1.153791000	-0.607150000	4.978723000
F	-1.154703000	-0.604547000	4.979036000
H	0.000002000	-0.000126000	-1.080276000

### 11A

C	0.000017000	0.000037000	0.002940000
C	-0.000024000	-0.000042000	2.720965000
C	1.220877000	-0.000010000	0.622129000
C	1.206359000	-0.000041000	2.013485000
C	-1.206384000	-0.000003000	2.013450000
C	-1.220861000	0.000049000	0.622091000
H	2.152420000	-0.000010000	0.070745000
H	2.145330000	-0.000076000	2.554844000
H	-2.145373000	-0.000001000	2.554778000
H	-2.152389000	0.000080000	0.070682000
B	-0.000047000	-0.000083000	4.268942000
F	-1.126478000	-0.000157000	4.967158000
F	1.126365000	-0.000196000	4.967190000

### 11A<sup>RC</sup>

C	0.039845000	0.013668000	-0.000950000
C	0.006562000	-0.000347000	2.716057000
C	1.253250000	0.014354000	0.632434000
C	1.221535000	0.007134000	2.023407000
C	-1.191125000	-0.000528000	1.993973000
C	-1.188728000	0.006603000	0.602481000
H	2.189603000	0.020156000	0.089483000
H	2.153804000	0.007322000	2.576217000
H	-2.136655000	-0.006303000	2.523724000
H	-2.113458000	0.006490000	0.039792000
C	2.387602000	0.031913000	-2.848298000
H	1.348980000	0.026646000	-2.518729000
H	2.884697000	0.922829000	-2.466457000
H	2.891637000	-0.857919000	-2.473088000
H	2.424748000	0.036111000	-3.936437000
B	-0.012442000	-0.008338000	4.263895000
F	-1.147321000	-0.015512000	4.948176000
F	1.105274000	-0.008373000	4.975878000

### 11A<sup>TS</sup>

C	1.915696000	0.000259000	-0.0000008000
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C	-0.843230000	0.000036000	-0.000023000
C	1.255328000	-1.209685000	-0.000042000
C	-0.132273000	-1.203847000	-0.000039000
C	-0.132439000	1.204083000	-0.000033000
C	1.255097000	1.210153000	-0.000043000
H	1.803343000	-2.144231000	-0.000096000
H	-0.672519000	-2.143350000	-0.000044000
H	-0.672870000	2.143482000	-0.000033000
H	1.803074000	2.144738000	-0.000093000
C	4.583275000	0.000160000	-0.000042000
H	3.288282000	0.001350000	-0.000370000
H	4.870624000	-1.043544000	0.094239000
H	4.876937000	0.437972000	-0.950014000
H	4.875847000	0.600215000	0.857148000
B	-2.390918000	-0.000107000	0.000015000
F	-3.090278000	-1.126277000	0.000038000
F	-3.090485000	1.125938000	0.000026000

### 11A<sup>P</sup>

C	0.000001000	0.000084000	0.003930000
C	0.000120000	-0.000151000	2.793393000
C	1.203168000	0.000011000	0.695307000
C	1.201508000	-0.000107000	2.079873000
C	-1.201321000	-0.000079000	2.079978000
C	-1.203102000	0.000039000	0.695406000
H	2.140164000	0.000048000	0.153181000
H	2.141689000	-0.000164000	2.618023000
H	-2.141460000	-0.000112000	2.618204000
H	-2.140149000	0.000094000	0.153369000
B	0.000201000	-0.000282000	4.341796000
F	-1.125964000	-0.000289000	5.040919000
F	1.126460000	-0.000286000	5.040779000
H	-0.000041000	0.000175000	-1.079106000

### 12

C	0.000023000	0.000007000	-0.010004000
C	-0.000028000	-0.000052000	2.821798000
C	1.209130000	0.000046000	0.648943000
C	1.209369000	0.000149000	2.037933000
C	-1.209395000	-0.000131000	2.037891000
C	-1.209106000	-0.000021000	0.648900000
H	2.151372000	0.000161000	0.106752000
H	2.149943000	0.000307000	2.581463000
H	-2.149992000	-0.000237000	2.581383000
H	-2.151329000	-0.000116000	0.106676000
O	-0.000049000	0.000025000	4.081892000

### 12<sup>RC</sup>

C	0.0000000000	0.0000000000	0.0000000000
C	0.0000000000	0.0000000000	2.829164000

C	1.209998000	0.000000000	0.657521000
C	1.210086000	0.001729000	2.046060000
C	-1.209973000	-0.001908000	2.045373000
C	-1.210176000	-0.003860000	0.656842000
H	2.151124000	0.000522000	0.113243000
H	2.150433000	0.002265000	2.589628000
H	-2.150313000	-0.003700000	2.588992000
H	-2.151809000	-0.004468000	0.113901000
C	1.655162000	-0.684273000	-3.130953000
H	1.007092000	-0.593519000	-2.257270000
H	2.245235000	-1.597127000	-3.051543000
H	1.050467000	-0.719781000	-4.037498000
H	2.322363000	0.176267000	-3.173682000
O	-0.000680000	0.000299000	4.088747000

### **12<sup>TS</sup>**

C	0.010599000	-0.076786000	0.000084000
C	-0.008836000	0.010922000	2.852950000
C	1.142680000	0.339341000	0.680560000
C	1.139046000	0.383861000	2.063276000
C	-1.146004000	-0.410269000	2.072355000
C	-1.130621000	-0.450701000	0.689519000
H	2.035767000	0.631699000	0.132649000
H	2.023256000	0.709174000	2.603535000
H	-2.037652000	-0.702135000	2.619429000
H	-2.016213000	-0.776507000	0.148265000
C	0.004999000	-0.166653000	-2.665481000
H	0.017585000	-0.119088000	-1.350445000
H	0.204767000	0.845087000	-3.011199000
H	0.781506000	-0.871146000	-2.954890000
H	-0.991074000	-0.510229000	-2.936544000
O	-0.017158000	0.049659000	4.110343000

### **12<sup>P</sup>**

C	0.000000000	0.000005000	-0.048439000
C	0.000000000	0.000092000	2.845336000
C	1.192928000	0.000073000	0.676158000
C	1.205925000	0.000112000	2.056106000
C	-1.205925000	0.000010000	2.056106000
C	-1.192927000	-0.000027000	0.676159000
H	2.140136000	0.000096000	0.140208000
H	2.147110000	0.000162000	2.598119000
H	-2.147109000	-0.000019000	2.598119000
H	-2.140135000	-0.000084000	0.140208000
O	0.000001000	0.000106000	4.103557000
H	0.000000000	-0.000026000	-1.132183000

### **12A**

C	0.005153000	0.000008000	0.041351000
C	0.004356000	0.000074000	2.754957000

C	1.218381000	0.000069000	0.671246000
C	1.211823000	0.000115000	2.065281000
C	-1.204408000	0.000006000	2.066271000
C	-1.209209000	-0.000020000	0.675683000
H	2.154592000	0.000096000	0.127459000
H	2.150198000	0.000176000	2.610399000
H	-2.129690000	-0.000020000	2.627866000
H	-2.145270000	-0.000074000	0.131549000
O	-0.055744000	0.000126000	4.113332000
H	0.831209000	0.000123000	4.476985000

### **12A<sup>RC</sup>**

C	0.050131000	0.028295000	-0.003572000
C	0.003507000	-0.007389000	2.708380000
C	1.252880000	0.024687000	0.645959000
C	1.222657000	0.006322000	2.039328000
C	-1.193678000	-0.003005000	1.999504000
C	-1.175172000	0.015263000	0.609332000
H	2.196373000	0.035472000	0.115060000
H	2.151571000	0.002769000	2.600456000
H	-2.128131000	-0.013963000	2.545673000
H	-2.101812000	0.018802000	0.049324000
C	2.380495000	0.077296000	-2.842390000
H	1.360114000	0.076823000	-2.459818000
H	2.362886000	0.092219000	-3.931035000
H	2.903663000	0.960264000	-2.477187000
H	2.895272000	-0.820171000	-2.501429000
O	-0.079791000	-0.025471000	4.065303000
H	0.800948000	-0.026791000	4.443738000

### **12A<sup>TS</sup>**

C	-0.005156000	0.019635000	0.000773000
C	-0.033051000	0.079168000	2.750127000
C	0.871084000	0.852582000	0.664493000
C	0.859167000	0.884626000	2.050887000
C	-0.909971000	-0.755079000	2.066237000
C	-0.894460000	-0.783868000	0.676426000
H	1.565231000	1.479085000	0.116783000
H	1.532357000	1.525962000	2.605045000
H	-1.604275000	-1.381665000	2.616908000
H	-1.577560000	-1.433795000	0.142365000
C	0.021440000	-0.038267000	-2.664024000
H	0.010481000	-0.008905000	-1.375057000
H	1.008948000	-0.394517000	-2.944413000
H	-0.771287000	-0.725891000	-2.946933000
H	-0.170722000	0.981805000	-2.985385000
O	-0.004077000	0.148212000	4.107271000
H	-0.659120000	-0.447707000	4.474488000

### **12A<sup>P</sup>**

C	0.004552000	-0.000060000	-0.016660000
C	0.003313000	0.000137000	2.764608000
C	1.200510000	0.000093000	0.682600000
C	1.206260000	0.000199000	2.069380000
C	-1.200604000	0.000059000	2.070596000
C	-1.192436000	-0.000041000	0.686784000
H	2.142413000	0.000123000	0.148537000
H	2.146365000	0.000345000	2.610859000
H	-2.127913000	0.000069000	2.628025000
H	-2.133941000	-0.000130000	0.151849000
O	-0.054537000	0.000434000	4.121490000
H	0.003717000	-0.000150000	-1.098494000
H	0.833692000	0.000486000	4.482440000

### 5m

C	-0.001912000	-0.036752000	0.031191000
C	0.058618000	0.044719000	2.351258000
C	1.359569000	-0.048914000	-0.080098000
C	2.096426000	-0.011532000	1.106467000
C	-0.719354000	0.008573000	1.194080000
C	1.449874000	0.035551000	2.329141000
H	1.857266000	-0.085917000	-1.040989000
H	3.177965000	-0.019359000	1.072123000
H	2.026461000	0.064299000	3.244637000
H	-1.802488000	0.015671000	1.215051000
S	-0.850007000	0.103970000	3.876183000
H	-0.250055000	-0.861987000	4.603175000
H	-0.241871000	1.115205000	4.531282000

### 5m<sup>RC</sup>

C	0.085786000	0.051272000	-0.040345000
C	0.014820000	0.060051000	2.280917000
C	1.445512000	-0.077205000	-0.073769000
C	2.110804000	-0.138972000	1.153094000
C	-0.693060000	0.125963000	1.080761000
C	1.398945000	-0.070718000	2.337940000
H	1.989571000	-0.129300000	-1.008424000
H	3.187788000	-0.240621000	1.180336000
H	1.919950000	-0.119119000	3.285369000
H	-1.770881000	0.227935000	1.040709000
C	0.599313000	0.014773000	-3.517953000
H	0.200779000	-0.844446000	-2.978339000
H	0.133333000	0.064746000	-4.499837000
H	0.380429000	0.933233000	-2.973131000
H	1.676512000	-0.093770000	-3.641255000
S	-0.974386000	0.155011000	3.752764000
H	-0.509758000	-0.884644000	4.477407000
H	-0.317987000	1.084479000	4.478721000

### 5m<sup>TS</sup>

C	-0.019576000	0.003498000	-0.034005000
C	-0.014083000	-0.042000000	2.322740000
C	1.353742000	0.102005000	-0.045875000
C	2.054688000	0.128912000	1.158957000
C	-0.741003000	-0.071125000	1.136896000
C	1.373026000	0.056793000	2.359407000
H	1.892506000	0.158616000	-0.984001000
H	3.133952000	0.206200000	1.161300000
H	1.913822000	0.077412000	3.296828000
H	-1.822307000	-0.148762000	1.131610000
C	-1.324366000	-0.048320000	-2.373282000
H	-0.720286000	-0.024129000	-1.271114000
H	-0.572821000	0.201865000	-3.116936000
H	-1.704758000	-1.060617000	-2.477033000
H	-2.107840000	0.700321000	-2.294945000
S	-0.978276000	-0.140151000	3.809018000
H	-0.335883000	-1.098141000	4.509757000
H	-0.478027000	0.872479000	4.547783000

### **5m<sup>P</sup>**

C	-0.000524000	0.000014000	0.008087000
C	-0.000265000	-0.000032000	2.739908000
C	1.205622000	0.000026000	0.689486000
C	1.218714000	0.000006000	2.075825000
C	-1.222863000	-0.000043000	2.077604000
C	-1.209628000	-0.000018000	0.696533000
H	2.141133000	0.000054000	0.147163000
H	2.155943000	0.000025000	2.617409000
H	-2.161186000	-0.000072000	2.617465000
H	-2.145162000	-0.000023000	0.153923000
H	-0.752965000	0.988116000	4.847386000
H	-0.752688000	-0.988506000	4.847343000
S	0.101620000	-0.000067000	4.509030000
H	-0.003758000	0.000033000	-1.073901000

### **5Am**

C	-0.005052000	0.000176000	0.037317000
C	-0.000948000	-0.000449000	2.390981000
C	1.358301000	0.000191000	-0.072152000
C	2.061256000	-0.000133000	1.131380000
C	-0.728552000	-0.000191000	1.195692000
C	1.391599000	-0.000392000	2.345184000
H	1.870964000	0.000441000	-1.024885000
H	3.144610000	-0.000150000	1.120977000
H	1.962136000	-0.000519000	3.265152000
H	-1.811987000	-0.000363000	1.200605000
S	-0.913592000	-0.000596000	3.903150000
H	0.139632000	-0.003042000	4.728286000

### **5Am<sup>RC</sup>**

C	0.010869000	-0.005167000	-0.011317000
C	0.001467000	-0.000440000	2.341510000
C	1.375020000	-0.003916000	-0.113826000
C	2.070758000	-0.000595000	1.093269000
C	-0.719889000	-0.003669000	1.141946000
C	1.393841000	0.001088000	2.303495000
H	1.888190000	-0.005595000	-1.066114000
H	3.154136000	0.000585000	1.089548000
H	1.959155000	0.003566000	3.226631000
H	-1.803301000	-0.004796000	1.141133000
C	0.529527000	-0.118387000	-3.672581000
H	-0.160014000	-0.091805000	-2.829276000
H	1.158621000	-1.004619000	-3.598389000
H	-0.033880000	-0.152192000	-4.603763000
H	1.152770000	0.774997000	-3.659724000
S	-0.920247000	0.001530000	3.847833000
H	0.128289000	0.004401000	4.679057000

### 5Am<sup>TS</sup>

C	-0.001417000	-0.001150000	0.001092000
C	0.000110000	0.006813000	2.384039000
C	1.374849000	-0.013055000	-0.052899000
C	2.071039000	-0.014939000	1.149459000
C	-0.707150000	0.008799000	1.181220000
C	1.391882000	-0.005117000	2.358042000
H	1.900806000	-0.020751000	-0.999382000
H	3.154309000	-0.024147000	1.149524000
H	1.952208000	-0.006807000	3.284541000
H	-1.791332000	0.018022000	1.180466000
C	-1.381928000	0.003403000	-2.279391000
H	-0.711040000	0.000631000	-1.172293000
H	-0.639469000	0.103853000	-3.066480000
H	-1.905528000	-0.948131000	-2.308047000
H	-2.049848000	0.857937000	-2.214922000
S	-0.932121000	0.019657000	3.884772000
H	0.109222000	0.015047000	4.724899000

### 5Am<sup>P</sup>

C	0.000424000	0.000005000	0.006110000
C	-0.000309000	-0.000009000	2.793016000
C	1.196360000	0.000001000	0.706636000
C	1.201093000	0.000013000	2.092282000
C	-1.201836000	-0.000020000	2.090220000
C	-1.196872000	0.000004000	0.705440000
H	2.138623000	0.000002000	0.173166000
H	2.143687000	0.000051000	2.625412000
H	-2.142488000	-0.000065000	2.627290000
H	-2.138425000	-0.000002000	0.170860000
H	1.237082000	-0.000756000	4.784026000
S	-0.081512000	0.000069000	4.558229000

H 0.001292000 0.000007000 -1.075923000

**5o**

C -0.001035000 0.000060000 0.003153000  
C 0.000763000 0.000278000 1.370864000  
C 1.122910000 -0.000224000 -0.772313000  
C 2.335354000 -0.000377000 -0.086454000  
C 1.219399000 0.000171000 2.056556000  
C 2.379321000 -0.000192000 1.307344000  
H 1.083038000 -0.000397000 -1.853635000  
H 3.259825000 -0.000656000 -0.650045000  
H 3.335337000 -0.000340000 1.812814000  
H 1.258954000 0.000328000 3.139149000  
H -1.433868000 -0.985863000 3.076333000  
H -1.435032000 0.990119000 3.073381000  
S -1.580279000 0.000672000 2.166329000

**5o<sup>RC</sup>**

C 0.000000000 0.000000000 0.000000000  
C 0.000000000 0.000000000 1.367763000  
C 1.125805000 0.000000000 -0.773406000  
C 2.337046000 0.000000000 -0.087169000  
C 1.218561000 0.000000000 2.054882000  
C 2.379239000 0.000000000 1.307453000  
H 1.078613000 0.000004000 -1.854362000  
H 3.262749000 0.000000000 -0.648774000  
H 3.334608000 0.000000000 1.814047000  
H 1.256889000 0.000000000 3.137596000  
C -1.753253000 -0.001810000 -2.895857000  
H -1.643798000 -0.896693000 -2.282365000  
H -2.740609000 -0.001874000 -3.353164000  
H -1.643291000 0.893943000 -2.283727000  
H -0.996595000 -0.002634000 -3.679258000  
S -1.581159000 0.000000000 2.157688000  
H -1.440098000 0.987625000 3.067639000  
H -1.440070000 -0.987570000 3.067691000

**5o<sup>TS</sup>**

C -0.010662000 0.000068000 0.013153000  
C -0.002878000 0.000139000 1.388646000  
C 1.178190000 -0.000261000 -0.684931000  
C 2.369631000 -0.000509000 0.026509000  
C 1.183650000 -0.000108000 2.122151000  
C 2.372133000 -0.000433000 1.420129000  
H 1.181102000 -0.000324000 -1.767478000  
H 3.311340000 -0.000767000 -0.507348000  
H 3.309271000 -0.000629000 1.959816000  
H 1.183790000 -0.000049000 3.205363000  
C -2.256715000 0.000447000 -1.454983000  
H -1.221284000 0.000301000 -0.734757000

H	-2.796678000	-0.909474000	-1.207182000
H	-2.797688000	0.909293000	-1.205438000
H	-1.876421000	0.001648000	-2.472583000
H	-1.462140000	-0.985997000	3.087789000
H	-1.461646000	0.987129000	3.087713000
S	-1.595312000	0.000565000	2.176537000

### **5o<sup>P</sup>**

C	-0.000524000	0.000014000	0.008087000
C	-0.000265000	-0.000032000	2.739908000
C	1.205622000	0.000026000	0.689486000
C	1.218714000	0.000006000	2.075825000
C	-1.222863000	-0.000043000	2.077604000
C	-1.209628000	-0.000018000	0.696533000
H	2.141133000	0.000054000	0.147163000
H	2.155943000	0.000025000	2.617409000
H	-2.161186000	-0.000072000	2.617465000
H	-2.145162000	-0.000023000	0.153923000
H	-0.752965000	0.988116000	4.847386000
H	-0.752688000	-0.988506000	4.847343000
S	0.101620000	-0.000067000	4.509030000
H	-0.003758000	0.000033000	-1.073901000

### **5Ao**

C	0.000607000	-0.000188000	0.001402000
C	0.002503000	-0.000226000	1.373169000
C	1.098893000	0.000024000	-0.809228000
C	2.344248000	0.000199000	-0.181442000
C	1.261986000	-0.000028000	1.979711000
C	2.411779000	0.000163000	1.204094000
H	1.014818000	0.000051000	-1.888770000
H	3.249481000	0.000361000	-0.775115000
H	3.376545000	0.000294000	1.694993000
H	1.340231000	-0.000022000	3.060665000
H	-0.989669000	-0.000854000	3.482380000
S	-1.525918000	-0.000445000	2.256019000

### **5Ao<sup>RC</sup>**

C	0.018220000	0.045847000	-0.037416000
C	-0.000750000	0.022483000	1.334020000
C	1.127421000	0.036046000	-0.832821000
C	2.363086000	-0.001210000	-0.187572000
C	1.249662000	-0.014463000	1.958033000
C	2.410388000	-0.026204000	1.198720000
H	1.054666000	0.055692000	-1.912963000
H	3.276785000	-0.010630000	-0.768081000
H	3.367605000	-0.055266000	1.703270000
H	1.312401000	-0.033946000	3.039849000
C	-1.590199000	0.001655000	-3.288247000
H	-1.719767000	0.044799000	-2.207099000

H	-2.565441000	-0.018587000	-3.772022000
H	-1.038946000	0.879861000	-3.622296000
H	-1.037385000	-0.899628000	-3.550368000
S	-1.542115000	0.041439000	2.192414000
H	-1.025951000	-0.010742000	3.426502000

### 5Ao<sup>TS</sup>

C	-0.007866000	0.000015000	0.010020000
C	0.000169000	0.000007000	1.391483000
C	1.145126000	0.000009000	-0.739635000
C	2.373316000	-0.000005000	-0.088683000
C	1.235339000	-0.000007000	2.037865000
C	2.407655000	-0.000013000	1.297665000
H	1.094116000	0.000016000	-1.822178000
H	3.293635000	-0.000010000	-0.658649000
H	3.358652000	-0.000024000	1.815121000
H	1.283845000	-0.000013000	3.120384000
C	-2.343476000	0.000042000	-1.279245000
H	-1.215160000	0.000029000	-0.654475000
H	-2.851573000	0.906746000	-0.962973000
H	-2.086242000	0.000077000	-2.335164000
H	-2.851562000	-0.906688000	-0.963030000
S	-1.544910000	0.000016000	2.252458000
H	-1.033537000	-0.000005000	3.489042000

### 5Ao<sup>P</sup>

C	0.000424000	0.000005000	0.006110000
C	-0.000309000	-0.000009000	2.793016000
C	1.196360000	0.000001000	0.706636000
C	1.201093000	0.000013000	2.092282000
C	-1.201836000	-0.000020000	2.090220000
C	-1.196872000	0.000004000	0.705440000
H	2.138623000	0.000002000	0.173166000
H	2.143687000	0.000051000	2.625412000
H	-2.142488000	-0.000065000	2.627290000
H	-2.138425000	-0.000002000	0.170860000
H	1.237082000	-0.000756000	4.784026000
S	-0.081512000	0.000069000	4.558229000
H	0.001292000	0.000007000	-1.075923000

### 10m

C	-1.777320000	-1.264275000	-0.000039000
C	0.237211000	-0.026668000	0.000086000
C	-0.532954000	1.132554000	0.000071000
C	-2.577841000	-0.150631000	-0.000065000
C	-1.919804000	1.081726000	0.000000000
C	-0.409706000	-1.266990000	0.000041000
H	-3.660358000	-0.209804000	-0.000131000
H	-2.500620000	1.999255000	-0.000017000
H	0.207907000	-2.157461000	0.000063000

H	-0.001181000	2.075811000	0.000104000
C	1.792367000	0.039742000	0.000134000
O	2.368434000	-1.061895000	-0.000057000
O	2.266883000	1.189326000	-0.000116000

### **10m<sup>RC</sup>**

C	0.036455000	-0.013161000	-0.018804000
C	0.003125000	-0.000702000	2.343356000
C	1.394429000	0.001810000	2.313122000
C	1.405366000	-0.011205000	-0.100503000
C	2.094090000	-0.003257000	1.114660000
C	-0.699113000	-0.008593000	1.133591000
H	1.932717000	-0.015342000	-1.047770000
H	3.179886000	-0.001267000	1.114925000
H	-1.781830000	-0.010258000	1.179880000
C	0.174470000	-0.135383000	-3.681450000
H	-0.189795000	-0.115415000	-2.654000000
H	0.795882000	-1.018625000	-3.825924000
H	-0.668723000	-0.167197000	-4.371069000
H	0.765594000	0.760021000	-3.871156000
H	1.906128000	0.007892000	3.267401000
C	-0.773807000	0.005130000	3.692636000
O	-2.012424000	0.002452000	3.588618000
O	-0.056640000	0.011749000	4.708284000

### **10m<sup>TS</sup>**

C	-0.009312000	-0.021456000	0.004140000
C	0.000356000	0.051617000	2.392511000
C	1.386704000	-0.058210000	2.350898000
C	1.364141000	-0.130870000	-0.057139000
C	2.067463000	-0.148793000	1.144568000
C	-0.703980000	0.069565000	1.189477000
H	1.880846000	-0.200727000	-1.008486000
H	3.149641000	-0.233829000	1.134380000
H	-1.783311000	0.155615000	1.239372000
C	-1.358690000	0.013321000	-2.298558000
H	-0.693328000	-0.003720000	-1.151872000
H	-0.603693000	-0.050692000	-3.078605000
H	-2.013573000	-0.853421000	-2.267970000
H	-1.899785000	0.955762000	-2.306407000
H	1.908449000	-0.069713000	3.299990000
C	-0.753829000	0.152594000	3.747771000
O	-1.990899000	0.246715000	3.658483000
O	-0.027718000	0.126964000	4.757593000

### **10m<sup>P</sup>**

C	0.0000000000	-0.000014000	0.006345000
C	0.000006000	-0.000012000	2.807111000
C	1.199280000	-0.000011000	0.707209000
C	1.194575000	-0.000011000	2.095236000

C	-1.194566000	-0.000017000	2.095240000
C	-1.199276000	-0.000019000	0.707213000
H	2.140453000	-0.000009000	0.166852000
H	2.113217000	-0.000009000	2.669536000
H	-2.113206000	-0.000020000	2.669543000
H	-2.140451000	-0.000023000	0.166861000
C	0.000009000	-0.000010000	4.358774000
O	-1.126077000	0.000066000	4.889409000
O	1.126097000	0.000112000	4.889404000
H	-0.000002000	-0.000014000	-1.078439000

### 10Am

C	-1.791639000	-1.283349000	0.000008000
C	0.180426000	-0.004690000	0.000179000
C	-0.602109000	1.146336000	0.000046000
C	-2.609629000	-0.186066000	-0.000120000
C	-1.984416000	1.060892000	-0.000098000
C	-0.425825000	-1.265597000	0.000151000
H	-3.689215000	-0.269382000	-0.000235000
H	-2.583318000	1.963038000	-0.000195000
H	0.171326000	-2.167292000	0.000252000
H	-0.106948000	2.107954000	0.000074000
C	1.660107000	0.151638000	0.000370000
O	2.312712000	-1.022841000	-0.000247000
O	2.236292000	1.206177000	-0.000074000
H	3.254629000	-0.815990000	-0.000551000

### 10Am<sup>RC</sup>

C	0.004881000	-0.001444000	-0.000324000
C	0.002065000	-0.000009000	2.349341000
C	1.393593000	0.000379000	2.320479000
C	1.370629000	-0.001106000	-0.088672000
C	2.075383000	-0.000152000	1.114906000
C	-0.725105000	-0.000956000	1.154041000
H	1.884704000	-0.001597000	-1.041468000
H	3.158178000	0.000153000	1.104422000
H	-1.806576000	-0.001263000	1.163902000
C	0.604408000	-0.045867000	-3.679203000
H	-0.120988000	-0.028555000	-2.866323000
H	1.223497000	-0.938155000	-3.594320000
H	0.081219000	-0.059139000	-4.633938000
H	1.232714000	0.842331000	-3.624251000
H	1.929811000	0.001106000	3.259836000
C	-0.673586000	0.000624000	3.674937000
O	-2.013940000	-0.000266000	3.581254000
O	-0.103774000	0.001188000	4.732891000
H	-2.354531000	-0.000033000	4.483433000

### 10Am<sup>TS</sup>

C	-0.002049000	0.022105000	0.001884000
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C	0.000148000	-0.019307000	2.381460000
C	1.389978000	0.052657000	2.367569000
C	1.373450000	0.093657000	-0.035331000
C	2.074951000	0.108918000	1.165948000
C	-0.709049000	-0.034975000	1.180436000
H	1.901853000	0.137310000	-0.980471000
H	3.156277000	0.164772000	1.162299000
H	-1.789678000	-0.090897000	1.185906000
C	-1.357770000	-0.007307000	-2.294422000
H	-0.700403000	0.006185000	-1.183370000
H	-1.778715000	-1.005637000	-2.375284000
H	-2.112404000	0.768341000	-2.197305000
H	-0.625475000	0.208879000	-3.067712000
H	1.918857000	0.063530000	3.311191000
C	-0.684321000	-0.077603000	3.699801000
O	-2.023328000	-0.144798000	3.596946000
O	-0.125615000	-0.067415000	4.764310000
H	-2.366443000	-0.178238000	4.497570000

### 10Am<sup>P</sup>

C	0.000214000	-0.000031000	0.006968000
C	0.000274000	0.000062000	2.778900000
C	1.202423000	0.000007000	0.698959000
C	1.205680000	0.000053000	2.083896000
C	-1.203976000	0.000024000	2.082389000
C	-1.202964000	-0.000023000	0.698962000
H	2.139944000	0.000000000	0.158106000
H	2.139334000	0.000083000	2.628864000
H	-2.130068000	0.000031000	2.641769000
H	-2.140498000	-0.000052000	0.158201000
C	-0.052511000	0.000111000	4.264030000
O	-1.063662000	0.000125000	4.914638000
O	1.164102000	0.000149000	4.837063000
H	1.018110000	0.000182000	5.790280000
H	0.000672000	-0.000068000	-1.075865000

### 10o

C	-0.474146000	-1.176211000	0.000043000
C	0.291904000	-0.039582000	0.000036000
C	-0.427680000	1.156854000	-0.000015000
C	-2.532736000	-0.024272000	-0.000013000
C	-1.817236000	1.166998000	-0.000024000
C	-1.844194000	-1.238663000	0.000013000
H	-3.618042000	-0.014120000	-0.000033000
H	-2.349811000	2.111989000	-0.000053000
H	0.155267000	2.071750000	-0.000054000
H	-2.380861000	-2.181546000	0.000014000
C	1.847810000	-0.047047000	0.000080000
O	2.365164000	-1.175612000	-0.000088000
O	2.376226000	1.078544000	0.000015000

**10o<sup>RC</sup>**

C	0.062843000	-0.695445000	-0.018093000
C	-0.051161000	-0.274943000	1.281204000
C	1.107514000	0.283368000	1.824354000
C	2.273596000	0.399121000	1.078029000
C	1.178643000	-0.612522000	-0.810418000
C	2.318029000	-0.045052000	-0.238020000
H	1.187699000	-0.967004000	-1.835498000
H	3.230166000	0.046942000	-0.818791000
C	-2.890083000	0.337511000	-1.633198000
H	-2.752730000	-0.073584000	-0.629539000
H	-2.724667000	-0.444609000	-2.375751000
H	-3.902239000	0.731015000	-1.743250000
H	-2.170194000	1.140476000	-1.795311000
H	3.158005000	0.840046000	1.524941000
H	1.047929000	0.618241000	2.854338000
C	-1.355936000	-0.394405000	2.116148000
O	-2.340242000	-0.832070000	1.493156000
O	-1.257540000	-0.036532000	3.300836000

**10o<sup>TS</sup>**

C	-0.005332000	0.000070000	0.010874000
C	-0.000835000	0.000724000	1.392435000
C	1.252189000	0.000451000	2.006586000
C	2.425568000	-0.000431000	1.265395000
C	1.140782000	-0.000812000	-0.757555000
C	2.378079000	-0.001070000	-0.122885000
H	1.076127000	-0.001297000	-1.841559000
H	3.293722000	-0.001760000	-0.705202000
C	-2.218260000	0.000371000	-1.472218000
H	-1.174389000	0.000261000	-0.708592000
H	-2.170160000	-0.907130000	-2.071282000
H	-3.004902000	0.000768000	-0.725212000
H	-2.169656000	0.907587000	-2.071670000
H	3.384715000	-0.000623000	1.772414000
H	1.260399000	0.000963000	3.090459000
C	-1.287941000	0.001717000	2.273074000
O	-2.364946000	0.001890000	1.652795000
O	-1.078974000	0.002218000	3.498587000

**10o<sup>P</sup>**

C	0.0000000000	-0.000014000	0.006345000
C	0.000006000	-0.000012000	2.807111000
C	1.199280000	-0.000011000	0.707209000
C	1.194575000	-0.000011000	2.095236000
C	-1.194566000	-0.000017000	2.095240000
C	-1.199276000	-0.000019000	0.707213000
H	2.140453000	-0.000009000	0.166852000
H	2.113217000	-0.000009000	2.669536000

H	-2.113206000	-0.000020000	2.669543000
H	-2.140451000	-0.000023000	0.166861000
C	0.000009000	-0.000010000	4.358774000
O	-1.126077000	0.000066000	4.889409000
O	1.126097000	0.000112000	4.889404000
H	-0.000002000	-0.000014000	-1.078439000

### 10Ao

C	-0.474934000	-1.163910000	-0.000159000
C	0.233657000	0.011298000	-0.000202000
C	-0.510854000	1.193338000	-0.000060000
C	-2.556803000	-0.079586000	0.000125000
C	-1.894087000	1.142224000	0.000095000
C	-1.837040000	-1.273704000	-0.000005000
H	-3.639826000	-0.108481000	0.000251000
H	-2.464180000	2.061853000	0.000194000
H	0.020019000	2.137362000	-0.000090000
H	-2.340682000	-2.231911000	0.000019000
C	1.717097000	0.077963000	-0.000417000
O	2.286215000	-1.135441000	0.000208000
O	2.354003000	1.096853000	0.000140000
H	3.240707000	-0.995861000	0.000581000

### 10Ao<sup>RC</sup>

C	-0.106032000	0.067944000	0.068839000
C	-0.034821000	-0.009298000	1.436738000
C	1.243847000	-0.016443000	1.999536000
C	2.360086000	0.052468000	1.183796000
C	0.959154000	0.137999000	-0.783606000
C	2.224257000	0.129231000	-0.197628000
H	0.835505000	0.197368000	-1.857402000
H	3.105112000	0.182750000	-0.826099000
C	-2.414111000	0.183412000	-2.428574000
H	-2.551804000	0.112148000	-1.350323000
H	-1.845104000	-0.677721000	-2.777149000
H	-3.383844000	0.200719000	-2.924286000
H	-1.871676000	1.098611000	-2.663074000
H	3.347579000	0.046516000	1.625972000
H	1.333994000	-0.076624000	3.077109000
C	-1.227789000	-0.083375000	2.316327000
O	-2.377832000	-0.066237000	1.625247000
O	-1.190834000	-0.151626000	3.515275000
H	-3.092109000	-0.117475000	2.271772000

### 10Ao<sup>TS</sup>

C	-0.009030000	0.000082000	0.007129000
C	-0.001462000	-0.000021000	1.391432000
C	1.228667000	-0.000125000	2.049852000
C	2.407963000	-0.000123000	1.326708000
C	1.155380000	0.000085000	-0.727738000

C	2.374573000	-0.000019000	-0.061298000
H	1.120336000	0.000167000	-1.810687000
H	3.299078000	-0.000017000	-0.625907000
C	-2.131786000	0.000288000	-1.597941000
H	-1.161543000	0.000186000	-0.755740000
H	-2.689778000	0.906168000	-1.381036000
H	-1.675811000	0.000333000	-2.584613000
H	-2.689861000	-0.905571000	-1.381156000
H	3.357454000	-0.000204000	1.845926000
H	1.235367000	-0.000205000	3.132318000
C	-1.231701000	-0.000027000	2.226136000
O	-2.365553000	0.000070000	1.506703000
O	-1.238964000	-0.000111000	3.428697000
H	-3.091181000	0.000058000	2.142223000

#### 10Ao<sup>P</sup>

C	0.000214000	-0.000031000	0.006968000
C	0.000274000	0.000062000	2.778900000
C	1.202423000	0.000007000	0.698959000
C	1.205680000	0.000053000	2.083896000
C	-1.203976000	0.000024000	2.082389000
C	-1.202964000	-0.000023000	0.698962000
H	2.139944000	0.000000000	0.158106000
H	2.139334000	0.000083000	2.628864000
H	-2.130068000	0.000031000	2.641769000
H	-2.140498000	-0.000052000	0.158201000
C	-0.052511000	0.000111000	4.264030000
O	-1.063662000	0.000125000	4.914638000
O	1.164102000	0.000149000	4.837063000
H	1.018110000	0.000182000	5.790280000
H	0.000672000	-0.000068000	-1.075865000

#### Nitrobenzene

H	0.000016000	0.004686000	0.013284000
C	0.000019000	-0.003979000	1.095684000
C	1.203547000	-0.003696000	1.786293000
C	-1.203508000	-0.015508000	1.786202000
C	1.211636000	-0.014895000	3.170900000
H	2.141076000	0.005165000	1.246388000
C	-1.211592000	-0.026811000	3.170808000
H	-2.141036000	-0.015832000	1.246225000
C	0.000024000	-0.026303000	3.837986000
H	2.133411000	-0.015004000	3.733641000
H	-2.133364000	-0.036004000	3.733478000
N	0.000027000	-0.038340000	5.311707000
O	1.073776000	-0.037140000	5.873698000
O	-1.073720000	-0.048524000	5.873611000

#### 1TS-NO2

C	0.0000000000	0.0000000000	0.0000000000
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C	0.000000000	0.000000000	2.702190000
C	1.210643000	0.000000000	0.660167000
C	1.217205000	-0.000420000	2.048811000
C	-1.217210000	0.000267000	2.048810000
C	-1.210647000	0.000682000	0.660171000
H	2.145147000	0.003179000	0.113683000
H	2.154162000	-0.000208000	2.594526000
H	-2.154163000	0.001008000	2.594531000
H	-2.145146000	0.004387000	0.113685000
N	-0.000018000	-0.024212000	4.186314000
H	0.823880000	0.449249000	4.560232000
H	-0.822945000	0.450917000	4.560261000
H	-0.000975000	-0.980519000	4.548421000
H	0.000000000	0.003483000	-1.362647000
C	-0.000001000	0.007206000	-2.650528000
C	0.000324000	1.223946000	-3.297509000
C	-0.000328000	-1.205587000	-3.304878000
C	0.000324000	1.228319000	-4.685135000
H	0.000575000	2.156541000	-2.748479000
C	-0.000329000	-1.201517000	-4.692505000
H	-0.000580000	-2.141509000	-2.761540000
C	-0.000002000	0.015407000	-5.350271000
H	0.000570000	2.149481000	-5.249771000
H	-0.000577000	-2.119192000	-5.262798000
N	-0.000003000	0.019846000	-6.828717000
O	0.000286000	1.096566000	-7.379952000
O	-0.000292000	-1.053563000	-7.386379000

### 1A<sup>TS-NO2</sup>

C	-0.000034000	-0.000819000	-0.006187000
C	0.000010000	0.002587000	2.760384000
C	1.203715000	0.000470000	0.664470000
C	1.203401000	0.002793000	2.050889000
C	-1.203404000	0.001957000	2.050928000
C	-1.203762000	-0.000367000	0.664509000
H	2.142323000	-0.000291000	0.123277000
H	2.143119000	0.009102000	2.591637000
H	-2.143109000	0.007613000	2.591707000
H	-2.142386000	-0.001781000	0.123346000
N	0.000013000	0.058323000	4.147803000
H	0.836645000	-0.270974000	4.597689000
H	-0.836375000	-0.271558000	4.597716000
H	-0.000055000	-0.002344000	-1.319043000
C	-0.000082000	-0.002049000	-2.648430000
C	-0.000553000	1.208540000	-3.309931000
C	0.000362000	-1.211724000	-3.311610000
C	-0.000584000	1.213963000	-4.696908000
H	-0.000893000	2.141172000	-2.759950000
C	0.000334000	-1.215295000	-4.698580000
H	0.000725000	-2.145177000	-2.763015000

C	-0.000139000	-0.000211000	-5.362491000
H	-0.000943000	2.134539000	-5.262263000
H	0.000670000	-2.135052000	-5.265263000
N	-0.000170000	0.000712000	-6.835582000
O	0.000227000	-1.072458000	-7.399156000
O	-0.000590000	1.074525000	-7.397837000

### **10<sup>TS-NO2</sup>**

C	-0.000001000	-0.000005000	-0.006847000
C	0.000007000	0.000005000	2.750493000
C	1.210942000	-0.000526000	0.653344000
C	1.198081000	-0.000517000	2.044277000
C	-1.198071000	0.000522000	2.044284000
C	-1.210940000	0.000521000	0.653351000
H	2.145795000	-0.000926000	0.103526000
H	2.114880000	-0.000911000	2.621776000
H	-2.114867000	0.000920000	2.621788000
H	-2.145797000	0.000917000	0.103539000
C	0.000011000	0.000010000	4.304021000
O	-1.126886000	0.000494000	4.830089000
O	1.126911000	-0.000470000	4.830082000
H	-0.000005000	-0.000009000	-1.282408000
C	-0.000011000	-0.000013000	-2.660778000
C	-0.000333000	1.208086000	-3.328553000
C	0.000305000	-1.208117000	-3.328546000
C	-0.000346000	1.214715000	-4.715217000
H	-0.000572000	2.140559000	-2.777524000
C	0.000304000	-1.214755000	-4.715209000
H	0.000548000	-2.140587000	-2.777511000
C	-0.000024000	-0.000022000	-5.382506000
H	-0.000596000	2.135611000	-5.280171000
H	0.000548000	-2.135654000	-5.280158000
N	-0.000032000	-0.000027000	-6.851357000
O	-0.000374000	1.072460000	-7.420370000
O	0.000305000	-1.072517000	-7.420364000

### **10A<sup>TS-NO2</sup>**

C	0.001617000	-0.000070000	-0.005211000
C	-0.000461000	-0.000333000	2.732069000
C	1.212894000	-0.000385000	0.653813000
C	1.207300000	-0.000520000	2.040012000
C	-1.208376000	-0.000012000	2.040004000
C	-1.209554000	0.000120000	0.652206000
H	2.146726000	-0.000518000	0.105712000
H	2.131695000	-0.000768000	2.602758000
H	-2.141376000	0.000132000	2.586544000
H	-2.142496000	0.000361000	0.102506000
C	0.052330000	-0.000486000	4.218360000
O	-1.163888000	-0.000273000	4.789972000
O	1.064531000	-0.000769000	4.866442000

H	0.001234000	0.000062000	-1.320259000
C	-0.001946000	0.000206000	-2.651584000
C	-0.003236000	-1.211032000	-3.310678000
C	-0.004754000	1.211588000	-3.310407000
C	-0.007702000	-1.214341000	-4.697806000
H	-0.000690000	-2.144374000	-2.762124000
C	-0.009233000	1.215202000	-4.697535000
H	-0.003361000	2.144809000	-2.761645000
C	-0.010729000	0.000503000	-5.361665000
H	-0.008830000	-2.134337000	-5.264080000
H	-0.011524000	2.135324000	-5.263599000
N	-0.015861000	0.000662000	-6.835671000
O	-0.017108000	-1.072973000	-7.397381000
O	-0.018657000	1.074417000	-7.397146000
H	-1.020772000	-0.000396000	5.743752000