

**Molecular structures of  $M(\text{Bu}^t)_3$  ( $M = \text{Al, Ga, In}$ ) using gas-phase electron diffraction and *ab initio* calculations: experimental and CASSCF evidence for charge-transfer processes leading to photodissociation**

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**Supplementary Material**

**Table S1** Nozzle-to-plate distances (mm), sample and nozzle temperatures (K), weighting functions ( $\text{\AA}^{-1}$ ), correlation parameters, scale factors and electron wavelengths (pm) used in the electron diffraction study of  $\text{Al}(\text{Bu}^t)_3$ , **1**, and  $\text{Ga}(\text{Bu}^t)_3$ , **2**.

|                                      | <b>1</b>  |          | <b>2</b>  |          |
|--------------------------------------|-----------|----------|-----------|----------|
| Nozzle-to-film distance <sup>a</sup> | 93.9      | 256.9    | 89.6      | 256.9    |
| $T_{\text{sample}}$                  | 419       | 363      | 389       | 348      |
| $T_{\text{nozzle}}$                  | 442       | 383      | 398       | 382      |
| $\Delta s$                           | 0.4       | 0.2      | 0.4       | 0.2      |
| $s_{\text{min}}$                     | 10.0      | 2.0      | 12.0      | 2.0      |
| $s_{\text{w1}}$                      | 12.0      | 4.0      | 14.0      | 4.0      |
| $s_{\text{w2}}$                      | 25.6      | 12.8     | 27.6      | 12.8     |
| $s_{\text{max}}$                     | 30.0      | 15.0     | 32.0      | 15.0     |
| Correlation parameter                | 0.312     | 0.025    | 0.332     | 0.014    |
| Scale factor <sup>b</sup>            | 0.681(10) | 0.796(4) | 0.657(17) | 0.723(6) |
| Electron wavelength                  | 6.02      | 6.02     | 6.02      | 6.02     |

<sup>a</sup> Determined by reference to the scattering pattern of benzene vapour. <sup>b</sup> Values in parentheses are the estimated standard deviations.

**Table S2** Coordinates (in Å) from the *ab initio* calculated [MP2(FC)/6-311+G\*] structure of Al(Bu<sup>f</sup>)<sub>3</sub>, **1**.

|       | <i>x</i> | <i>y</i> | <i>z</i> |
|-------|----------|----------|----------|
| Al(1) | 0.0000   | 0.0000   | 0.1766   |
| C(2)  | 0.0000   | 2.0089   | 0.0491   |
| C(3)  | 0.4766   | 2.3351   | -1.3824  |
| C(4)  | -1.3703  | 2.6726   | 0.2444   |
| C(5)  | 0.9742   | 2.6637   | 1.0427   |
| H(6)  | 1.4751   | 1.9382   | -1.5990  |
| H(7)  | -0.2103  | 1.9536   | -2.1489  |
| H(8)  | 0.5302   | 3.4270   | -1.5186  |
| H(9)  | -1.7546  | 2.5375   | 1.2608   |
| H(10) | -1.2832  | 3.7570   | 0.0724   |
| H(11) | -2.1259  | 2.2973   | -0.4529  |
| H(12) | 0.9841   | 3.7544   | 0.8888   |
| H(13) | 0.6778   | 2.4916   | 2.0846   |
| H(14) | 2.0014   | 2.3114   | 0.9240   |
| C(15) | 1.7397   | -1.0044  | 0.0491   |
| C(16) | 2.9997   | -0.1496  | 0.2444   |
| C(17) | 1.8198   | -2.1755  | 1.0427   |
| C(18) | 1.7839   | -1.5803  | -1.3824  |
| H(19) | 3.0525   | 0.6924   | -0.4529  |
| H(20) | 3.0748   | 0.2508   | 1.2608   |
| H(21) | 3.8952   | -0.7672  | 0.0724   |
| H(22) | 1.0010   | -2.8890  | 0.9240   |
| H(23) | 2.7594   | -2.7294  | 0.8888   |
| H(24) | 1.8188   | -1.8328  | 2.0846   |
| H(25) | 2.7027   | -2.1727  | -1.5186  |
| H(26) | 0.9410   | -2.2465  | -1.5990  |
| H(27) | 1.7970   | -0.7947  | -2.1489  |
| C(28) | -1.7397  | -1.0044  | 0.0491   |
| C(29) | -1.6294  | -2.5230  | 0.2444   |
| C(30) | -2.7939  | -0.4882  | 1.0427   |
| C(31) | -2.2605  | -0.7548  | -1.3824  |
| H(32) | -0.9266  | -2.9897  | -0.4529  |
| H(33) | -1.3202  | -2.7882  | 1.2608   |
| H(34) | -2.6120  | -2.9897  | 0.0724   |
| H(35) | -3.0024  | 0.5776   | 0.9240   |
| H(36) | -3.7434  | -1.0250  | 0.8888   |
| H(37) | -2.4967  | -0.6588  | 2.0846   |
| H(38) | -3.2329  | -1.2543  | -1.5186  |
| H(39) | -2.4160  | 0.3084   | -1.5990  |
| H(40) | -1.5867  | -1.1589  | -2.1489  |

Energy = -713.5177 Hartrees (not corrected for zero-point energy)

**Table S3** Coordinates (in Å) from the *ab initio* calculated [MP2(full)/6-311+G\*] structure of Ga(Bu<sup>t</sup>)<sub>3</sub>, **2**.

|       | <i>x</i> | <i>y</i> | <i>z</i> |
|-------|----------|----------|----------|
| Ga(1) | 0.0000   | 0.0000   | 0.1456   |
| C(2)  | 0.0000   | 2.0133   | 0.0194   |
| C(3)  | -1.3722  | 2.6603   | 0.2189   |
| C(4)  | 0.9672   | 2.6482   | 1.0247   |
| C(5)  | 0.4796   | 2.3447   | -1.4036  |
| H(6)  | -2.1216  | 2.2850   | -0.4840  |
| H(7)  | -1.7551  | 2.5104   | 1.2330   |
| H(8)  | -1.2937  | 3.7467   | 0.0589   |
| H(9)  | 1.9947   | 2.3028   | 0.8960   |
| H(10) | 0.9705   | 3.7416   | 0.8948   |
| H(11) | 0.6717   | 2.4504   | 2.0616   |
| H(12) | 0.5346   | 3.4368   | -1.5328  |
| H(13) | 1.4771   | 1.9459   | -1.6171  |
| H(14) | -0.2058  | 1.9670   | -2.1721  |
| C(15) | 1.7436   | -1.0066  | 0.0194   |
| C(16) | 1.8098   | -2.1617  | 1.0247   |
| C(17) | 1.7907   | -1.5877  | -1.4036  |
| C(18) | 2.9900   | -0.1418  | 0.2189   |
| H(19) | 1.7863   | -1.8069  | 2.0616   |
| H(20) | 0.9969   | -2.8788  | 0.8960   |
| H(21) | 2.7550   | -2.7113  | 0.8948   |
| H(22) | 1.8064   | -0.8053  | -2.1721  |
| H(23) | 2.7091   | -2.1814  | -1.5328  |
| H(24) | 0.9467   | -2.2521  | -1.6171  |
| H(25) | 3.8916   | -0.7530  | 0.0589   |
| H(26) | 3.0396   | 0.6949   | -0.4840  |
| H(27) | 3.0516   | 0.2648   | 1.2330   |
| C(28) | -1.7436  | -1.0066  | 0.0194   |
| C(29) | -2.7770  | -0.4865  | 1.0247   |
| C(30) | -2.2704  | -0.7570  | -1.4036  |
| C(31) | -1.6178  | -2.5185  | 0.2189   |
| H(32) | -2.4580  | -0.6435  | 2.0616   |
| H(33) | -2.9916  | 0.5760   | 0.8960   |
| H(34) | -3.7255  | -1.0303  | 0.8948   |
| H(35) | -1.6006  | -1.1618  | -2.1721  |
| H(36) | -3.2437  | -1.2554  | -1.5328  |
| H(37) | -2.4238  | 0.3062   | -1.6171  |
| H(38) | -2.5979  | -2.9938  | 0.0589   |
| H(39) | -0.9180  | -2.9799  | -0.4840  |
| H(40) | -1.2965  | -2.7751  | 1.2330   |

Energy = -2395.4412 Hartrees (not corrected for zero-point energy)

**Table S4** Coordinates (in Å) from the *ab initio* calculated [MP2(full)/6-311+G\*/Huzinaga] structure of In(Bu<sup>t</sup>)<sub>3</sub>, **3**.

|       | <i>x</i> | <i>y</i> | <i>z</i> |
|-------|----------|----------|----------|
| In(1) | 0.0000   | 0.0000   | 0.1184   |
| C(2)  | 0.0000   | 2.2441   | -0.0039  |
| C(3)  | -1.3914  | 2.8410   | 0.2021   |
| C(4)  | 0.9608   | 2.8578   | 1.0160   |
| C(5)  | 0.4856   | 2.6042   | -1.4129  |
| H(6)  | -2.1249  | 2.4485   | -0.5099  |
| H(7)  | -1.7770  | 2.6569   | 1.2103   |
| H(8)  | -1.3579  | 3.9342   | 0.0631   |
| H(9)  | 1.9864   | 2.4976   | 0.8916   |
| H(10) | 0.9845   | 3.9539   | 0.8997   |
| H(11) | 0.6567   | 2.6544   | 2.0491   |
| H(12) | 0.5310   | 3.6996   | -1.5290  |
| H(13) | 1.4905   | 2.2200   | -1.6213  |
| H(14) | -0.1869  | 2.2323   | -2.1956  |
| C(15) | -1.9435  | -1.1221  | -0.0039  |
| C(16) | -2.9553  | -0.5969  | 1.0160   |
| C(17) | -2.4981  | -0.8816  | -1.4129  |
| C(18) | -1.7647  | -2.6255  | 0.2021   |
| H(19) | -2.6271  | -0.7585  | 2.0491   |
| H(20) | -3.1562  | 0.4715   | 0.8916   |
| H(21) | -3.9165  | -1.1243  | 0.8997   |
| H(22) | -1.8398  | -1.2780  | -2.1956  |
| H(23) | -3.4695  | -1.3900  | -1.5290  |
| H(24) | -2.6678  | 0.1808   | -1.6213  |
| H(25) | -2.7282  | -3.1431  | 0.0631   |
| H(26) | -1.0580  | -3.0645  | -0.5099  |
| H(27) | -1.4125  | -2.8674  | 1.2103   |
| C(28) | 1.9435   | -1.1221  | -0.0039  |
| C(29) | 1.9946   | -2.2610  | 1.0160   |
| C(30) | 2.0125   | -1.7226  | -1.4129  |
| C(31) | 3.1561   | -0.2155  | 0.2021   |
| H(32) | 1.9704   | -1.8959  | 2.0491   |
| H(33) | 1.1698   | -2.9691  | 0.8916   |
| H(34) | 2.9319   | -2.8296  | 0.8997   |
| H(35) | 2.0267   | -0.9543  | -2.1956  |
| H(36) | 2.9385   | -2.3097  | -1.5290  |
| H(37) | 1.1773   | -2.4008  | -1.6213  |
| H(38) | 4.0861   | -0.7911  | 0.0631   |
| H(39) | 3.1829   | 0.6160   | -0.5099  |
| H(40) | 3.1894   | 0.2105   | 1.2103   |

Energy = -6212.7569 Hartrees (not corrected for zero-point energy)

**Table S5** Interatomic distances ( $r_a$ ), vibrational amplitudes ( $u_{h1}$ ) and curvilinear corrections ( $k_{h1}$ ) [in Å] for the GED structure of Al(Bu<sup>t</sup>)<sub>3</sub>, **1**, along with amplitudes of vibration calculated at the MP2/6-311+G\* level.

|          | Atom pair     | $r_a$     | $u_{h1}$                 | $k_{h1}$ | $u_{calc}$ |
|----------|---------------|-----------|--------------------------|----------|------------|
| $u_3$    | C(4)–H(9)     | 1.108(1)  | 0.079(tied to $u_1$ )    | 0.004    | 0.076      |
| $u_8$    | C(5)–H(12)    | 1.108(1)  | 0.080(tied to $u_1$ )    | 0.004    | 0.077      |
| $u_9$    | C(3)–H(8)     | 1.109(1)  | 0.080(tied to $u_1$ )    | 0.004    | 0.077      |
| $u_4$    | C(3)–H(6)     | 1.109(1)  | 0.079(tied to $u_1$ )    | 0.004    | 0.077      |
| $u_7$    | C(4)–H(10)    | 1.109(1)  | 0.080(tied to $u_1$ )    | 0.004    | 0.077      |
| $u_1$    | C(5)–H(14)    | 1.109(1)  | 0.078(1)                 | 0.004    | 0.076      |
| $u_{10}$ | C(2)–C(4)     | 1.541(1)  | 0.045(1)                 | 0.001    | 0.052      |
| $u_{11}$ | C(2)–C(5)     | 1.545(1)  | 0.045(tied to $u_{10}$ ) | 0.001    | 0.053      |
| $u_{12}$ | C(2)–C(3)     | 1.550(1)  | 0.045(tied to $u_{10}$ ) | 0.000    | 0.053      |
| $u_{19}$ | H(13)...H(14) | 1.753(5)  | 0.125(fixed)             | –0.017   | 0.125      |
| $u_{15}$ | H(10)...H(11) | 1.769(4)  | 0.125(fixed)             | –0.018   | 0.125      |
| $u_{21}$ | H(6)...H(7)   | 1.770(5)  | 0.123(fixed)             | –0.001   | 0.123      |
| $u_{20}$ | H(9)...H(11)  | 1.770(5)  | 0.123(fixed)             | 0.000    | 0.123      |
| $u_{16}$ | H(12)...H(13) | 1.788(4)  | 0.124(fixed)             | 0.000    | 0.124      |
| $u_{13}$ | H(6)...H(8)   | 1.788(4)  | 0.124(fixed)             | 0.000    | 0.124      |
| $u_{22}$ | Al(1)–C(2)    | 2.007(2)  | 0.067(3)                 | 0.001    | 0.063      |
| $u_{32}$ | H(6)...H(19)  | 2.017(35) | 0.407(fixed)             | 0.200    | 0.407      |
| $u_{23}$ | C(2)...H(10)  | 2.174(6)  | 0.131(6)                 | 0.000    | 0.108      |
| $u_{25}$ | C(2)...H(8)   | 2.182(6)  | 0.131(tied to $u_{23}$ ) | 0.001    | 0.108      |
| $u_{24}$ | C(2)...H(12)  | 2.188(6)  | 0.131(tied to $u_{23}$ ) | 0.012    | 0.109      |
| $u_{27}$ | C(2)...H(13)  | 2.212(4)  | 0.132(tied to $u_{23}$ ) | 0.002    | 0.109      |
| $u_{26}$ | C(2)...H(9)   | 2.220(4)  | 0.131(tied to $u_{23}$ ) | 0.012    | 0.108      |
| $u_{31}$ | C(2)...H(6)   | 2.228(4)  | 0.132(tied to $u_{23}$ ) | 0.012    | 0.109      |
| $u_{35}$ | H(10)...H(12) | 2.301(28) | 0.254(fixed)             | 0.044    | 0.254      |
| $u_{33}$ | H(9)...H(35)  | 2.364(29) | 0.363(fixed)             | 0.063    | 0.363      |
| $u_{38}$ | C(4)...C(5)   | 2.426(12) | 0.067(tied to $u_{23}$ ) | –0.013   | 0.078      |
| $u_{36}$ | H(8)...H(10)  | 2.491(22) | 0.257(fixed)             | 0.010    | 0.257      |
| $u_{39}$ | C(3)...C(4)   | 2.510(11) | 0.067(7)                 | –0.004   | 0.078      |
| $u_{40}$ | C(3)...C(5)   | 2.541(13) | 0.068(tied to $u_{39}$ ) | –0.001   | 0.079      |
| $u_{41}$ | H(9)...H(13)  | 2.593(33) | 0.271(fixed)             | 0.035    | 0.271      |
| $u_{44}$ | C(4)...H(12)  | 2.593(16) | 0.166(21)                | 0.000    | 0.177      |
| $u_{37}$ | H(8)...H(12)  | 2.603(30) | 0.267(fixed)             | 0.057    | 0.267      |
| $u_{42}$ | H(7)...H(11)  | 2.606(33) | 0.266(fixed)             | 0.016    | 0.266      |
| $u_{45}$ | C(5)...H(10)  | 2.610(18) | 0.160(tied to $u_{44}$ ) | 0.004    | 0.170      |
| $u_{43}$ | H(6)...H(14)  | 2.682(34) | 0.275(fixed)             | 0.071    | 0.275      |
| $u_{47}$ | C(4)...H(8)   | 2.706(14) | 0.166(tied to $u_{44}$ ) | –0.002   | 0.177      |
| $u_{50}$ | C(5)...H(9)   | 2.721(19) | 0.193(tied to $u_{58}$ ) | –0.005   | 0.175      |
| $u_{53}$ | C(4)...H(13)  | 2.740(21) | 0.209(tied to $u_{58}$ ) | 0.002    | 0.190      |
| $u_{46}$ | C(3)...H(10)  | 2.747(12) | 0.163(tied to $u_{44}$ ) | –0.016   | 0.173      |
| $u_{54}$ | C(3)...H(11)  | 2.759(20) | 0.164(tied to $u_{44}$ ) | 0.002    | 0.174      |
| $u_{48}$ | C(5)...H(8)   | 2.763(19) | 0.169(tied to $u_{44}$ ) | 0.006    | 0.179      |
| $u_{55}$ | C(3)...H(14)  | 2.797(22) | 0.176(tied to $u_{44}$ ) | 0.011    | 0.186      |
| $u_{52}$ | C(4)...H(7)   | 2.801(19) | 0.174(tied to $u_{44}$ ) | –0.012   | 0.185      |
| $u_{70}$ | C(4)...H(39)  | 2.815(38) | 0.387(tied to $u_{58}$ ) | 0.090    | 0.351      |
| $u_{49}$ | C(3)...H(12)  | 2.819(17) | 0.170(tied to $u_{44}$ ) | 0.021    | 0.181      |
| $u_{58}$ | Al(1)...C(3)  | 2.835(11) | 0.151(5)                 | 0.014    | 0.137      |

|                         |               |           |  |        |       |
|-------------------------|---------------|-----------|--|--------|-------|
| <i>u</i> <sub>56</sub>  | C(5)...H(6)   | 2.858(20) | 0.173(tied to <i>u</i> <sub>44</sub> ) | 0.030  | 0.184 |
| <i>u</i> <sub>59</sub>  | Al(1)...C(5)  | 2.947(11) | 0.129(tied to <i>u</i> <sub>58</sub> ) | -0.021 | 0.117 |
| <i>u</i> <sub>62</sub>  | H(9)...H(12)  | 2.954(19) | 0.284(fixed)                           | -0.022 | 0.284 |
| <i>u</i> <sub>34</sub>  | H(11)...H(35) | 2.964(61) | 0.399(fixed)                           | 0.157  | 0.399 |
| <i>u</i> <sub>72</sub>  | C(3)...H(19)  | 2.984(26) | 0.368(tied to <i>u</i> <sub>58</sub> ) | 0.117  | 0.333 |
| <i>u</i> <sub>66</sub>  | H(8)...H(11)  | 3.002(20) | 0.279(fixed)                           | -0.012 | 0.279 |
| <i>u</i> <sub>61</sub>  | Al(1)...H(6)  | 3.005(14) | 0.247(tied to <i>u</i> <sub>58</sub> ) | 0.030  | 0.224 |
| <i>u</i> <sub>60</sub>  | Al(1)...C(4)  | 3.009(8)  | 0.113(tied to <i>u</i> <sub>58</sub> ) | 0.002  | 0.102 |
| <i>u</i> <sub>63</sub>  | Al(1)...H(7)  | 3.020(14) | 0.269(tied to <i>u</i> <sub>58</sub> ) | 0.049  | 0.244 |
| <i>u</i> <sub>67</sub>  | H(10)...H(13) | 3.033(23) | 0.287(fixed)                           | 0.018  | 0.287 |
| <i>u</i> <sub>51</sub>  | C(4)...H(35)  | 3.059(37) | 0.244(tied to <i>u</i> <sub>44</sub> ) | 0.077  | 0.260 |
| <i>u</i> <sub>65</sub>  | H(8)...H(14)  | 3.074(25) | 0.298(fixed)                           | 0.003  | 0.298 |
| <i>u</i> <sub>57</sub>  | H(6)...H(27)  | 3.085(41) | 0.538(fixed)                           | 0.289  | 0.538 |
| <i>u</i> <sub>74</sub>  | Al(1)...H(13) | 3.128(15) | 0.251(tied to <i>u</i> <sub>58</sub> ) | -0.036 | 0.227 |
| <i>u</i> <sub>64</sub>  | H(7)...H(10)  | 3.133(17) | 0.286(fixed)                           | -0.052 | 0.286 |
| <i>u</i> <sub>92</sub>  | H(6)...H(20)  | 3.143(52) | 0.416(fixed)                           | 0.060  | 0.416 |
| <i>u</i> <sub>69</sub>  | Al(1)...H(14) | 3.154(15) | 0.229(tied to <i>u</i> <sub>58</sub> ) | -0.014 | 0.208 |
| <i>u</i> <sub>80</sub>  | H(7)...H(27)  | 3.203(47) | 0.608(fixed)                           | 0.289  | 0.608 |
| <i>u</i> <sub>78</sub>  | C(2)...H(39)  | 3.214(27) | 0.310(fixed)                           | 0.065  | 0.310 |
| <i>u</i> <sub>68</sub>  | H(6)...H(12)  | 3.232(20) | 0.292(fixed)                           | 0.031  | 0.292 |
| <i>u</i> <sub>76</sub>  | Al(1)...H(9)  | 3.238(13) | 0.218(tied to <i>u</i> <sub>58</sub> ) | 0.018  | 0.198 |
| <i>u</i> <sub>71</sub>  | Al(1)...H(11) | 3.246(13) | 0.211(tied to <i>u</i> <sub>58</sub> ) | 0.025  | 0.191 |
| <i>u</i> <sub>73</sub>  | C(5)...H(20)  | 3.261(29) | 0.361(tied to <i>u</i> <sub>58</sub> ) | 0.033  | 0.327 |
| <i>u</i> <sub>82</sub>  | C(4)...H(14)  | 3.416(10) | 0.105(tied to <i>u</i> <sub>88</sub> ) | -0.025 | 0.105 |
| <i>u</i> <sub>83</sub>  | C(5)...H(11)  | 3.421(10) | 0.104(tied to <i>u</i> <sub>88</sub> ) | -0.022 | 0.105 |
| <i>u</i> <sub>88</sub>  | C(2)...C(15)  | 3.456(4)  | 0.100(3)                               | 0.001  | 0.100 |
| <i>u</i> <sub>77</sub>  | C(2)...H(19)  | 3.461(18) | 0.272(tied to <i>u</i> <sub>88</sub> ) | 0.085  | 0.272 |
| <i>u</i> <sub>112</sub> | H(7)...H(19)  | 3.489(44) | 0.412(fixed)                           | 0.101  | 0.412 |
| <i>u</i> <sub>85</sub>  | C(4)...H(6)   | 3.491(9)  | 0.105(tied to <i>u</i> <sub>88</sub> ) | -0.011 | 0.105 |
| <i>u</i> <sub>84</sub>  | C(3)...H(9)   | 3.493(9)  | 0.105(tied to <i>u</i> <sub>88</sub> ) | -0.010 | 0.105 |
| <i>u</i> <sub>87</sub>  | C(5)...H(7)   | 3.506(11) | 0.106(tied to <i>u</i> <sub>88</sub> ) | -0.017 | 0.106 |
| <i>u</i> <sub>86</sub>  | C(3)...H(13)  | 3.509(11) | 0.106(tied to <i>u</i> <sub>88</sub> ) | -0.015 | 0.106 |
| <i>u</i> <sub>89</sub>  | C(3)...H(27)  | 3.550(34) | 0.489(tied to <i>u</i> <sub>88</sub> ) | 0.232  | 0.490 |
| <i>u</i> <sub>79</sub>  | H(13)...H(20) | 3.568(51) | 0.499(fixed)                           | 0.010  | 0.499 |
| <i>u</i> <sub>81</sub>  | C(2)...H(35)  | 3.603(23) | 0.259(tied to <i>u</i> <sub>88</sub> ) | 0.022  | 0.260 |
| <i>u</i> <sub>94</sub>  | H(10)...H(14) | 3.605(17) | 0.187(fixed)                           | -0.017 | 0.187 |
| <i>u</i> <sub>93</sub>  | H(11)...H(12) | 3.607(16) | 0.187(fixed)                           | -0.014 | 0.187 |
| <i>u</i> <sub>101</sub> | C(2)...H(20)  | 3.624(20) | 0.282(tied to <i>u</i> <sub>88</sub> ) | 0.024  | 0.282 |
| <i>u</i> <sub>90</sub>  | C(3)...H(39)  | 3.626(28) | 0.433(tied to <i>u</i> <sub>88</sub> ) | 0.160  | 0.434 |
| <i>u</i> <sub>113</sub> | C(3)...C(16)  | 3.649(26) | 0.251(tied to <i>u</i> <sub>88</sub> ) | 0.048  | 0.251 |
| <i>u</i> <sub>75</sub>  | C(5)...H(19)  | 3.653(43) | 0.334(tied to <i>u</i> <sub>88</sub> ) | 0.095  | 0.334 |
| <i>u</i> <sub>95</sub>  | C(2)...C(16)  | 3.695(10) | 0.156(tied to <i>u</i> <sub>88</sub> ) | 0.023  | 0.157 |
| <i>u</i> <sub>108</sub> | C(2)...C(31)  | 3.708(23) | 0.206(tied to <i>u</i> <sub>88</sub> ) | 0.041  | 0.206 |
| <i>u</i> <sub>110</sub> | H(8)...H(19)  | 3.714(24) | 0.378(fixed)                           | 0.111  | 0.378 |
| <i>u</i> <sub>97</sub>  | H(8)...H(9)   | 3.737(12) | 0.189(fixed)                           | -0.020 | 0.189 |
| <i>u</i> <sub>96</sub>  | H(6)...H(10)  | 3.741(12) | 0.188(fixed)                           | -0.026 | 0.188 |
| <i>u</i> <sub>91</sub>  | C(4)...C(30)  | 3.755(28) | 0.205(tied to <i>u</i> <sub>88</sub> ) | 0.000  | 0.205 |
| <i>u</i> <sub>120</sub> | H(6)...H(21)  | 3.762(33) | 0.391(fixed)                           | 0.133  | 0.391 |
| <i>u</i> <sub>102</sub> | H(9)...H(14)  | 3.764(20) | 0.185(fixed)                           | -0.023 | 0.185 |
| <i>u</i> <sub>103</sub> | H(11)...H(13) | 3.778(20) | 0.195(fixed)                           | -0.015 | 0.195 |

|                         |               |           |   |        |       |
|-------------------------|---------------|-----------|---|--------|-------|
| <i>u</i> <sub>99</sub>  | H(8)...H(13)  | 3.790(18) | 0.192(fixed)                            | -0.011 | 0.192 |
| <i>u</i> <sub>105</sub> | H(6)...H(11)  | 3.794(20) | 0.185(fixed)                            | -0.015 | 0.185 |
| <i>u</i> <sub>100</sub> | H(7)...H(12)  | 3.801(17) | 0.194(fixed)                            | -0.009 | 0.194 |
| <i>u</i> <sub>104</sub> | H(7)...H(9)   | 3.807(20) | 0.189(fixed)                            | -0.020 | 0.189 |
| <i>u</i> <sub>106</sub> | H(7)...H(14)  | 3.826(21) | 0.191(fixed)                            | -0.004 | 0.191 |
| <i>u</i> <sub>109</sub> | Al(1)...H(8)  | 3.836(9)  | 0.140(tied to <i>u</i> <sub>88</sub> )  | -0.010 | 0.140 |
| <i>u</i> <sub>127</sub> | C(3)...H(20)  | 3.840(35) | 0.327(tied to <i>u</i> <sub>88</sub> )  | 0.007  | 0.328 |
| <i>u</i> <sub>107</sub> | H(6)...H(13)  | 3.845(21) | 0.191(fixed)                            | 0.004  | 0.191 |
| <i>u</i> <sub>124</sub> | C(2)...H(40)  | 3.914(32) | 0.326(tied to <i>u</i> <sub>88</sub> )  | 0.051  | 0.327 |
| <i>u</i> <sub>116</sub> | Al(1)...H(12) | 3.926(8)  | 0.125(tied to <i>u</i> <sub>88</sub> )  | -0.029 | 0.125 |
| <i>u</i> <sub>111</sub> | C(2)...C(30)  | 3.958(17) | 0.164(tied to <i>u</i> <sub>88</sub> )  | -0.029 | 0.164 |
| <i>u</i> <sub>123</sub> | C(3)...H(40)  | 3.962(40) | 0.494(tied to <i>u</i> <sub>88</sub> )  | 0.180  | 0.495 |
| <i>u</i> <sub>118</sub> | Al(1)...H(10) | 3.967(7)  | 0.117(tied to <i>u</i> <sub>88</sub> )  | -0.015 | 0.118 |
| <i>u</i> <sub>130</sub> | H(13)...H(35) | 4.014(39) | 0.481(fixed)                            | -0.071 | 0.481 |
| <i>u</i> <sub>98</sub>  | H(10)...H(35) | 4.015(39) | 0.284(fixed)                            | 0.053  | 0.284 |
| <i>u</i> <sub>119</sub> | C(2)...H(27)  | 4.030(21) | 0.377(tied to <i>u</i> <sub>88</sub> )  | 0.101  | 0.378 |
| <i>u</i> <sub>121</sub> | H(9)...H(36)  | 4.056(25) | 0.341(fixed)                            | -0.047 | 0.341 |
| <i>u</i> <sub>140</sub> | C(4)...H(40)  | 4.121(39) | 0.340(tied to <i>u</i> <sub>88</sub> )  | 0.024  | 0.341 |
| <i>u</i> <sub>122</sub> | C(3)...C(18)  | 4.164(28) | 0.237(19)                               | 0.145  | 0.362 |
| <i>u</i> <sub>138</sub> | H(13)...H(24) | 4.211(30) | 0.567(fixed)                            | -0.144 | 0.567 |
| <i>u</i> <sub>117</sub> | C(4)...H(37)  | 4.227(43) | 0.253(tied to <i>u</i> <sub>122</sub> ) | -0.034 | 0.387 |
| <i>u</i> <sub>125</sub> | C(2)...H(37)  | 4.263(24) | 0.208(tied to <i>u</i> <sub>122</sub> ) | -0.052 | 0.319 |
| <i>u</i> <sub>128</sub> | C(2)...C(18)  | 4.286(14) | 0.150(tied to <i>u</i> <sub>122</sub> ) | 0.043  | 0.230 |
| <i>u</i> <sub>131</sub> | H(11)...H(14) | 4.326(9)  | 0.137(fixed)                            | -0.029 | 0.137 |
| <i>u</i> <sub>129</sub> | H(6)...H(25)  | 4.329(29) | 0.480(fixed)                            | 0.196  | 0.480 |
| <i>u</i> <sub>115</sub> | H(11)...H(36) | 4.333(38) | 0.364(fixed)                            | 0.097  | 0.364 |
| <i>u</i> <sub>114</sub> | H(11)...H(37) | 4.340(52) | 0.438(fixed)                            | 0.034  | 0.438 |
| <i>u</i> <sub>135</sub> | H(6)...H(40)  | 4.356(36) | 0.569(fixed)                            | 0.180  | 0.569 |
| <i>u</i> <sub>133</sub> | H(7)...H(13)  | 4.375(9)  | 0.138(fixed)                            | -0.027 | 0.138 |
| <i>u</i> <sub>132</sub> | H(6)...H(9)   | 4.384(8)  | 0.137(fixed)                            | -0.007 | 0.137 |
| <i>u</i> <sub>126</sub> | H(6)...H(26)  | 4.404(31) | 0.490(fixed)                            | 0.143  | 0.490 |
| <i>u</i> <sub>139</sub> | C(5)...H(35)  | 4.407(22) | 0.224(tied to <i>u</i> <sub>122</sub> ) | -0.053 | 0.343 |
| <i>u</i> <sub>146</sub> | C(4)...H(38)  | 4.458(24) | 0.197(tied to <i>u</i> <sub>122</sub> ) | 0.009  | 0.301 |
| <i>u</i> <sub>147</sub> | C(5)...H(24)  | 4.478(28) | 0.268(tied to <i>u</i> <sub>122</sub> ) | -0.108 | 0.411 |
| <i>u</i> <sub>159</sub> | H(8)...H(20)  | 4.513(36) | 0.393(fixed)                            | -0.020 | 0.393 |
| <i>u</i> <sub>137</sub> | H(7)...H(38)  | 4.545(38) | 0.523(fixed)                            | 0.221  | 0.523 |
| <i>u</i> <sub>148</sub> | C(2)...H(24)  | 4.557(17) | 0.230(tied to <i>u</i> <sub>145</sub> ) | -0.057 | 0.297 |
| <i>u</i> <sub>163</sub> | H(7)...H(20)  | 4.572(39) | 0.355(fixed)                            | 0.009  | 0.355 |
| <i>u</i> <sub>145</sub> | C(2)...C(17)  | 4.581(10) | 0.119(13)                               | -0.048 | 0.153 |
| <i>u</i> <sub>136</sub> | C(4)...H(36)  | 4.617(23) | 0.180(tied to <i>u</i> <sub>145</sub> ) | -0.009 | 0.232 |
| <i>u</i> <sub>152</sub> | C(3)...H(21)  | 4.647(25) | 0.231(tied to <i>u</i> <sub>145</sub> ) | 0.052  | 0.298 |
| <i>u</i> <sub>156</sub> | C(5)...H(39)  | 4.659(31) | 0.264(tied to <i>u</i> <sub>157</sub> ) | 0.019  | 0.306 |
| <i>u</i> <sub>144</sub> | C(2)...H(26)  | 4.666(15) | 0.255(tied to <i>u</i> <sub>157</sub> ) | 0.015  | 0.295 |
| <i>u</i> <sub>143</sub> | C(3)...H(26)  | 4.700(28) | 0.371(tied to <i>u</i> <sub>157</sub> ) | 0.115  | 0.430 |
| <i>u</i> <sub>153</sub> | C(2)...H(38)  | 4.720(21) | 0.196(tied to <i>u</i> <sub>157</sub> ) | 0.005  | 0.227 |
| <i>u</i> <sub>158</sub> | C(5)...H(37)  | 4.782(24) | 0.380(tied to <i>u</i> <sub>157</sub> ) | -0.135 | 0.439 |
| <i>u</i> <sub>150</sub> | C(2)...H(21)  | 4.783(10) | 0.154(tied to <i>u</i> <sub>157</sub> ) | 0.006  | 0.179 |
| <i>u</i> <sub>151</sub> | C(2)...C(29)  | 4.806(4)  | 0.094(tied to <i>u</i> <sub>157</sub> ) | -0.003 | 0.109 |
| <i>u</i> <sub>157</sub> | C(5)...C(17)  | 4.807(19) | 0.226(14)                               | -0.100 | 0.262 |
| <i>u</i> <sub>134</sub> | H(7)...H(35)  | 4.816(45) | 0.416(fixed)                            | 0.098  | 0.416 |

|           |               |           |                           |        |       |
|-----------|---------------|-----------|---------------------------|--------|-------|
| $u_{142}$ | C(5)...H(21)  | 4.824(30) | 0.204(tied to $u_{157}$ ) | 0.002  | 0.236 |
| $u_{141}$ | C(3)...H(35)  | 4.848(33) | 0.256(tied to $u_{157}$ ) | 0.046  | 0.296 |
| $u_{165}$ | H(7)...H(25)  | 4.859(46) | 0.542(fixed)              | 0.179  | 0.542 |
| $u_{154}$ | C(2)...H(36)  | 4.956(14) | 0.162(tied to $u_{157}$ ) | -0.041 | 0.187 |
| $u_{176}$ | H(6)...H(24)  | 4.960(40) | 0.343(fixed)              | 0.027  | 0.343 |
| $u_{155}$ | C(4)...H(19)  | 4.966(15) | 0.237(tied to $u_{157}$ ) | 0.064  | 0.274 |
| $u_{162}$ | C(3)...H(25)  | 4.981(30) | 0.351(tied to $u_{157}$ ) | 0.126  | 0.406 |
| $u_{166}$ | H(12)...H(35) | 5.029(17) | 0.347(fixed)              | -0.050 | 0.347 |
| $u_{164}$ | C(2)...H(22)  | 5.033(12) | 0.246(tied to $u_{177}$ ) | -0.039 | 0.221 |
| $u_{149}$ | C(5)...H(27)  | 5.035(31) | 0.410(tied to $u_{177}$ ) | 0.076  | 0.367 |
| $u_{182}$ | H(7)...H(21)  | 5.065(42) | 0.402(fixed)              | 0.065  | 0.402 |
| $u_{167}$ | C(2)...H(32)  | 5.098(10) | 0.213(tied to $u_{177}$ ) | 0.036  | 0.191 |
| $u_{170}$ | C(4)...H(20)  | 5.103(22) | 0.335(tied to $u_{177}$ ) | 0.004  | 0.300 |
| $u_{168}$ | C(2)...H(33)  | 5.125(14) | 0.227(tied to $u_{177}$ ) | -0.009 | 0.203 |
| $u_{160}$ | C(3)...C(30)  | 5.125(23) | 0.253(tied to $u_{177}$ ) | 0.010  | 0.227 |
| $u_{177}$ | C(3)...C(17)  | 5.127(24) | 0.219(10)                 | 0.007  | 0.196 |
| $u_{171}$ | C(3)...H(38)  | 5.166(30) | 0.432(tied to $u_{177}$ ) | 0.108  | 0.387 |
| $u_{175}$ | H(7)...H(32)  | 5.171(35) | 0.472(fixed)              | 0.224  | 0.472 |
| $u_{178}$ | H(14)...H(22) | 5.173(26) | 0.370(fixed)              | -0.087 | 0.370 |
| $u_{174}$ | C(4)...H(27)  | 5.174(25) | 0.454(tied to $u_{177}$ ) | 0.093  | 0.406 |
| $u_{172}$ | C(4)...C(16)  | 5.201(12) | 0.182(tied to $u_{177}$ ) | 0.002  | 0.163 |
| $u_{161}$ | H(10)...H(37) | 5.202(45) | 0.424(fixed)              | -0.071 | 0.424 |
| $u_{173}$ | C(2)...H(25)  | 5.215(13) | 0.273(tied to $u_{177}$ ) | 0.024  | 0.245 |
| $u_{186}$ | H(6)...H(23)  | 5.216(34) | 0.346(fixed)              | 0.087  | 0.346 |
| $u_{190}$ | H(13)...H(22) | 5.275(26) | 0.479(fixed)              | -0.178 | 0.479 |
| $u_{198}$ | C(3)...H(24)  | 5.314(28) | 0.336(tied to $u_{192}$ ) | -0.031 | 0.270 |
| $u_{199}$ | C(5)...H(40)  | 5.363(30) | 0.394(tied to $u_{192}$ ) | 0.010  | 0.317 |
| $u_{183}$ | H(11)...H(19) | 5.368(22) | 0.302(fixed)              | 0.062  | 0.302 |
| $u_{188}$ | H(6)...H(22)  | 5.400(26) | 0.333(fixed)              | 0.076  | 0.333 |
| $u_{180}$ | H(10)...H(19) | 5.404(17) | 0.305(fixed)              | 0.070  | 0.305 |
| $u_{201}$ | H(8)...H(21)  | 5.420(24) | 0.353(fixed)              | 0.033  | 0.353 |
| $u_{194}$ | C(5)...H(22)  | 5.421(22) | 0.386(tied to $u_{192}$ ) | -0.112 | 0.310 |
| $u_{193}$ | C(2)...H(23)  | 5.435(8)  | 0.198(tied to $u_{192}$ ) | -0.060 | 0.160 |
| $u_{181}$ | H(9)...H(20)  | 5.452(37) | 0.375(fixed)              | 0.029  | 0.375 |
| $u_{169}$ | H(8)...H(35)  | 5.466(35) | 0.330(fixed)              | 0.029  | 0.330 |
| $u_{212}$ | H(12)...H(24) | 5.495(30) | 0.430(fixed)              | -0.157 | 0.430 |
| $u_{192}$ | C(3)...C(29)  | 5.519(16) | 0.300(13)                 | 0.070  | 0.241 |
| $u_{197}$ | C(3)...H(32)  | 5.534(23) | 0.397(tied to $u_{192}$ ) | 0.130  | 0.319 |
| $u_{206}$ | H(9)...H(34)  | 5.544(20) | 0.327(fixed)              | -0.057 | 0.327 |
| $u_{187}$ | C(3)...H(37)  | 5.551(24) | 0.373(tied to $u_{192}$ ) | -0.036 | 0.300 |
| $u_{179}$ | H(6)...H(35)  | 5.557(28) | 0.310(fixed)              | 0.020  | 0.310 |
| $u_{203}$ | C(5)...H(23)  | 5.577(15) | 0.340(tied to $u_{192}$ ) | -0.112 | 0.273 |
| $u_{184}$ | H(9)...H(19)  | 5.602(26) | 0.312(fixed)              | 0.058  | 0.312 |
| $u_{200}$ | H(6)...H(32)  | 5.604(23) | 0.402(fixed)              | 0.153  | 0.402 |
| $u_{202}$ | C(2)...H(34)  | 5.606(7)  | 0.173(tied to $u_{192}$ ) | -0.019 | 0.139 |
| $u_{211}$ | H(12)...H(37) | 5.613(26) | 0.464(fixed)              | -0.165 | 0.464 |
| $u_{185}$ | H(10)...H(36) | 5.617(26) | 0.270(fixed)              | -0.030 | 0.270 |
| $u_{195}$ | C(4)...H(33)  | 5.632(25) | 0.301(tied to $u_{192}$ ) | -0.015 | 0.242 |
| $u_{196}$ | C(5)...H(26)  | 5.649(19) | 0.325(tied to $u_{192}$ ) | -0.036 | 0.261 |
| $u_{209}$ | C(4)...H(26)  | 5.655(17) | 0.400(tied to $u_{192}$ ) | 0.015  | 0.322 |



|                         |               |           |   |        |       |
|-------------------------|---------------|-----------|---|--------|-------|
| <i>u</i> <sub>189</sub> | H(7)...H(37)  | 5.656(29) | 0.374(fixed)                            | 0.026  | 0.374 |
| <i>u</i> <sub>207</sub> | C(4)...H(32)  | 5.668(16) | 0.258(tied to <i>u</i> <sub>192</sub> ) | 0.021  | 0.207 |
| <i>u</i> <sub>205</sub> | H(9)...H(24)  | 5.677(28) | 0.458(fixed)                            | -0.066 | 0.458 |
| <i>u</i> <sub>208</sub> | C(3)...H(22)  | 5.684(21) | 0.303(tied to <i>u</i> <sub>192</sub> ) | 0.029  | 0.243 |
| <i>u</i> <sub>214</sub> | C(4)...H(24)  | 5.721(16) | 0.435(tied to <i>u</i> <sub>192</sub> ) | -0.081 | 0.349 |
| <i>u</i> <sub>215</sub> | H(9)...H(32)  | 5.732(22) | 0.303(fixed)                            | -0.020 | 0.303 |
| <i>u</i> <sub>204</sub> | H(6)...H(38)  | 5.756(30) | 0.453(fixed)                            | 0.086  | 0.453 |
| <i>u</i> <sub>213</sub> | C(4)...H(34)  | 5.761(10) | 0.242(tied to <i>u</i> <sub>192</sub> ) | -0.014 | 0.195 |
| <i>u</i> <sub>226</sub> | H(7)...H(24)  | 5.790(29) | 0.321(fixed)                            | 0.012  | 0.321 |
| <i>u</i> <sub>223</sub> | C(3)...H(23)  | 5.795(26) | 0.294(tied to <i>u</i> <sub>192</sub> ) | 0.012  | 0.237 |
| <i>u</i> <sub>217</sub> | C(4)...C(17)  | 5.808(10) | 0.229(tied to <i>u</i> <sub>192</sub> ) | -0.070 | 0.184 |
| <i>u</i> <sub>191</sub> | H(7)...H(36)  | 5.832(30) | 0.439(fixed)                            | 0.112  | 0.439 |
| <i>u</i> <sub>222</sub> | C(5)...H(36)  | 5.841(19) | 0.336(tied to <i>u</i> <sub>192</sub> ) | -0.137 | 0.270 |
| <i>u</i> <sub>218</sub> | H(7)...H(22)  | 5.844(30) | 0.373(fixed)                            | 0.105  | 0.373 |
| <i>u</i> <sub>219</sub> | C(5)...H(33)  | 5.868(20) | 0.384(tied to <i>u</i> <sub>192</sub> ) | -0.087 | 0.308 |
| <i>u</i> <sub>221</sub> | H(7)...H(33)  | 5.882(20) | 0.382(fixed)                            | 0.120  | 0.382 |
| <i>u</i> <sub>210</sub> | C(5)...H(25)  | 5.913(24) | 0.317(tied to <i>u</i> <sub>192</sub> ) | -0.002 | 0.255 |
| <i>u</i> <sub>224</sub> | H(8)...H(25)  | 5.957(32) | 0.444(fixed)                            | 0.108  | 0.444 |
| <i>u</i> <sub>227</sub> | C(3)...H(33)  | 5.981(11) | 0.307(tied to <i>u</i> <sub>192</sub> ) | 0.041  | 0.247 |
| <i>u</i> <sub>220</sub> | H(7)...H(34)  | 5.982(29) | 0.456(fixed)                            | 0.173  | 0.456 |
| <i>u</i> <sub>225</sub> | H(6)...H(37)  | 6.018(20) | 0.318(fixed)                            | -0.036 | 0.318 |
| <i>u</i> <sub>216</sub> | C(3)...H(36)  | 6.030(22) | 0.352(tied to <i>u</i> <sub>192</sub> ) | 0.020  | 0.283 |
| <i>u</i> <sub>229</sub> | H(9)...H(22)  | 6.052(21) | 0.383(fixed)                            | -0.068 | 0.383 |
| <i>u</i> <sub>236</sub> | C(5)...H(38)  | 6.078(22) | 0.273(tied to <i>u</i> <sub>192</sub> ) | -0.059 | 0.219 |
| <i>u</i> <sub>228</sub> | C(4)...H(22)  | 6.080(13) | 0.325(tied to <i>u</i> <sub>192</sub> ) | -0.054 | 0.261 |
| <i>u</i> <sub>237</sub> | H(7)...H(23)  | 6.096(35) | 0.365(fixed)                            | 0.069  | 0.365 |
| <i>u</i> <sub>231</sub> | H(6)...H(33)  | 6.096(16) | 0.326(fixed)                            | 0.060  | 0.326 |
| <i>u</i> <sub>230</sub> | C(5)...H(32)  | 6.164(12) | 0.280(tied to <i>u</i> <sub>192</sub> ) | -0.031 | 0.225 |
| <i>u</i> <sub>240</sub> | H(8)...H(24)  | 6.208(28) | 0.315(fixed)                            | -0.080 | 0.315 |
| <i>u</i> <sub>234</sub> | H(11)...H(24) | 6.254(17) | 0.357(fixed)                            | -0.046 | 0.357 |
| <i>u</i> <sub>235</sub> | C(4)...H(21)  | 6.279(11) | 0.223(tied to <i>u</i> <sub>192</sub> ) | -0.020 | 0.179 |
| <i>u</i> <sub>232</sub> | H(11)...H(22) | 6.327(20) | 0.299(fixed)                            | 0.006  | 0.299 |
| <i>u</i> <sub>233</sub> | H(8)...H(37)  | 6.334(26) | 0.340(fixed)                            | -0.077 | 0.340 |
| <i>u</i> <sub>238</sub> | C(3)...H(34)  | 6.339(19) | 0.356(tied to <i>u</i> <sub>192</sub> ) | 0.067  | 0.286 |
| <i>u</i> <sub>241</sub> | C(4)...H(25)  | 6.492(15) | 0.308(tied to <i>u</i> <sub>192</sub> ) | 0.004  | 0.247 |
| <i>u</i> <sub>244</sub> | H(12)...H(22) | 6.504(21) | 0.308(fixed)                            | -0.139 | 0.308 |
| <i>u</i> <sub>247</sub> | H(10)...H(24) | 6.534(17) | 0.367(fixed)                            | -0.110 | 0.367 |
| <i>u</i> <sub>246</sub> | H(8)...H(32)  | 6.582(24) | 0.328(fixed)                            | 0.090  | 0.328 |
| <i>u</i> <sub>248</sub> | H(12)...H(23) | 6.594(14) | 0.288(fixed)                            | -0.141 | 0.288 |
| <i>u</i> <sub>239</sub> | H(6)...H(36)  | 6.622(18) | 0.310(fixed)                            | 0.000  | 0.310 |
| <i>u</i> <sub>242</sub> | H(6)...H(34)  | 6.649(18) | 0.359(fixed)                            | 0.068  | 0.359 |
| <i>u</i> <sub>249</sub> | C(5)...H(34)  | 6.650(9)  | 0.247(tied to <i>u</i> <sub>192</sub> ) | -0.105 | 0.198 |
| <i>u</i> <sub>251</sub> | H(8)...H(22)  | 6.710(19) | 0.248(fixed)                            | -0.021 | 0.248 |
| <i>u</i> <sub>250</sub> | H(10)...H(32) | 6.720(15) | 0.227(fixed)                            | 0.004  | 0.227 |
| <i>u</i> <sub>245</sub> | H(9)...H(21)  | 6.727(24) | 0.253(fixed)                            | -0.027 | 0.253 |
| <i>u</i> <sub>255</sub> | H(8)...H(23)  | 6.748(26) | 0.265(fixed)                            | -0.031 | 0.265 |
| <i>u</i> <sub>252</sub> | C(4)...H(23)  | 6.749(8)  | 0.224(tied to <i>u</i> <sub>192</sub> ) | -0.089 | 0.180 |
| <i>u</i> <sub>243</sub> | H(8)...H(36)  | 6.797(23) | 0.319(fixed)                            | -0.010 | 0.319 |
| <i>u</i> <sub>253</sub> | H(10)...H(21) | 6.850(10) | 0.220(fixed)                            | -0.023 | 0.220 |
| <i>u</i> <sub>254</sub> | H(9)...H(23)  | 6.893(19) | 0.306(fixed)                            | -0.104 | 0.306 |

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|                         |               |           |              |        |       |
|-------------------------|---------------|-----------|--------------|--------|-------|
| <i>u</i> <sub>256</sub> | H(8)...H(33)  | 6.990(9)  | 0.244(fixed) | -0.006 | 0.244 |
| <i>u</i> <sub>257</sub> | H(10)...H(22) | 7.038(11) | 0.264(fixed) | -0.081 | 0.264 |
| <i>u</i> <sub>258</sub> | H(11)...H(23) | 7.113(11) | 0.222(fixed) | -0.046 | 0.222 |
| <i>u</i> <sub>259</sub> | H(8)...H(34)  | 7.297(20) | 0.304(fixed) | 0.028  | 0.304 |
| <i>u</i> <sub>260</sub> | H(10)...H(23) | 7.557(11) | 0.199(fixed) | -0.108 | 0.199 |

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**Table S6** Interatomic distances ( $r_a$ ), vibrational amplitudes ( $u_{h1}$ ) and curvilinear corrections ( $k_{h1}$ ) [in Å] for the GED structure of Ga(Bu')<sub>3</sub>, **2**, along with amplitudes of vibration calculated at the MP2/6-311+G\* level.

|          | Atom pair     | $r_a$      | $u_{h1}$                 | $k_{h1}$ | $u_{calc}$ |
|----------|---------------|------------|--------------------------|----------|------------|
| $u_1$    | C(4)–H(9)     | 1.104(1)   | 0.086(2)                 | 0.004    | 0.076      |
| $u_9$    | C(5)–H(12)    | 1.104(1)   | 0.088(tied to $u_1$ )    | 0.004    | 0.077      |
| $u_2$    | C(3)–H(6)     | 1.104(1)   | 0.087(tied to $u_1$ )    | 0.004    | 0.076      |
| $u_7$    | C(3)–H(8)     | 1.104(1)   | 0.088(tied to $u_1$ )    | 0.004    | 0.077      |
| $u_8$    | C(4)–H(10)    | 1.104(1)   | 0.088(tied to $u_1$ )    | 0.004    | 0.077      |
| $u_4$    | C(5)–H(13)    | 1.105(1)   | 0.087(tied to $u_1$ )    | 0.004    | 0.077      |
| $u_{10}$ | C(2)–C(3)     | 1.535(1)   | 0.050(2)                 | 0.000    | 0.052      |
| $u_{11}$ | C(2)–C(4)     | 1.539(1)   | 0.050(tied to $u_{10}$ ) | 0.001    | 0.052      |
| $u_{12}$ | C(2)–C(5)     | 1.544(1)   | 0.051(tied to $u_{10}$ ) | 0.001    | 0.053      |
| $u_{21}$ | H(13)...H(14) | 1.709(8)   | 0.125(fixed)             | –0.018   | 0.125      |
| $u_{20}$ | H(6)...H(7)   | 1.727(8)   | 0.123(fixed)             | 0.000    | 0.123      |
| $u_{19}$ | H(9)...H(11)  | 1.727(8)   | 0.123(fixed)             | 0.000    | 0.123      |
| $u_{17}$ | H(9)...H(10)  | 1.746(7)   | 0.123(fixed)             | –0.001   | 0.123      |
| $u_{13}$ | H(6)...H(8)   | 1.747(7)   | 0.124(fixed)             | 0.000    | 0.124      |
| $u_{16}$ | H(12)...H(13) | 1.747(7)   | 0.124(fixed)             | 0.000    | 0.124      |
| $u_{22}$ | Ga(1)–C(2)    | 2.031(2)   | 0.072(3)                 | 0.001    | 0.061      |
| $u_{32}$ | H(6)...H(37)  | 2.113(108) | 0.402(fixed)             | 0.189    | 0.402      |
| $u_{23}$ | C(2)...H(8)   | 2.200(7)   | 0.127(8)                 | –0.001   | 0.108      |
| $u_{24}$ | C(2)...H(10)  | 2.203(7)   | 0.128(tied to $u_{23}$ ) | 0.000    | 0.108      |
| $u_{25}$ | C(2)...H(12)  | 2.221(7)   | 0.128(tied to $u_{23}$ ) | 0.013    | 0.108      |
| $u_{31}$ | C(2)...H(13)  | 2.244(6)   | 0.128(tied to $u_{23}$ ) | 0.001    | 0.109      |
| $u_{28}$ | C(2)...H(6)   | 2.248(6)   | 0.128(tied to $u_{23}$ ) | 0.013    | 0.108      |
| $u_{29}$ | C(2)...H(9)   | 2.251(6)   | 0.127(tied to $u_{23}$ ) | 0.013    | 0.108      |
| $u_{33}$ | H(7)...H(33)  | 2.273(35)  | 0.350(fixed)             | 0.114    | 0.350      |
| $u_{37}$ | C(3)...C(4)   | 2.490(13)  | 0.065(4)                 | –0.004   | 0.076      |
| $u_{35}$ | H(8)...H(10)  | 2.496(26)  | 0.250(fixed)             | 0.010    | 0.250      |
| $u_{38}$ | C(3)...C(5)   | 2.505(15)  | 0.066(tied to $u_{37}$ ) | –0.002   | 0.077      |
| $u_{40}$ | C(4)...C(5)   | 2.539(17)  | 0.069(tied to $u_{37}$ ) | –0.013   | 0.080      |
| $u_{36}$ | H(8)...H(12)  | 2.660(27)  | 0.255(fixed)             | 0.048    | 0.255      |
| $u_{42}$ | H(6)...H(14)  | 2.696(41)  | 0.264(fixed)             | 0.065    | 0.264      |
| $u_{44}$ | C(3)...H(10)  | 2.707(16)  | 0.196(tied to $u_{58}$ ) | –0.011   | 0.174      |
| $u_{46}$ | C(4)...H(8)   | 2.723(16)  | 0.189(tied to $u_{58}$ ) | –0.006   | 0.167      |
| $u_{41}$ | H(7)...H(11)  | 2.728(40)  | 0.268(fixed)             | 0.015    | 0.268      |
| $u_{39}$ | H(10)...H(12) | 2.737(29)  | 0.266(fixed)             | 0.042    | 0.266      |
| $u_{43}$ | H(9)...H(13)  | 2.743(46)  | 0.273(fixed)             | 0.042    | 0.273      |
| $u_{47}$ | C(3)...H(12)  | 2.782(18)  | 0.198(tied to $u_{58}$ ) | 0.019    | 0.175      |
| $u_{54}$ | C(5)...H(6)   | 2.798(25)  | 0.194(tied to $u_{58}$ ) | 0.026    | 0.172      |
| $u_{45}$ | C(5)...H(8)   | 2.810(17)  | 0.194(tied to $u_{58}$ ) | 0.002    | 0.172      |
| $u_{50}$ | C(4)...H(7)   | 2.811(24)  | 0.194(tied to $u_{58}$ ) | –0.010   | 0.172      |
| $u_{52}$ | C(3)...H(14)  | 2.827(24)  | 0.206(tied to $u_{58}$ ) | 0.010    | 0.183      |
| $u_{55}$ | C(3)...H(11)  | 2.828(23)  | 0.210(tied to $u_{58}$ ) | –0.002   | 0.187      |
| $u_{58}$ | Ga(1)...C(5)  | 2.829(9)   | 0.137(4)                 | 0.002    | 0.121      |
| $u_{48}$ | C(4)...H(12)  | 2.832(20)  | 0.201(tied to $u_{58}$ ) | 0.003    | 0.178      |
| $u_{53}$ | C(5)...H(9)   | 2.834(29)  | 0.208(tied to $u_{58}$ ) | 0.002    | 0.184      |
| $u_{34}$ | H(6)...H(33)  | 2.857(141) | 0.393(fixed)             | 0.134    | 0.393      |
| $u_{51}$ | C(5)...H(10)  | 2.859(19)  | 0.203(tied to $u_{58}$ ) | –0.001   | 0.180      |

|                         |               |            |   |        |       |
|-------------------------|---------------|------------|---|--------|-------|
| <i>u</i> <sub>56</sub>  | C(4)...H(13)  | 2.863(28)  | 0.206(tied to <i>u</i> <sub>58</sub> )  | 0.001  | 0.183 |
| <i>u</i> <sub>70</sub>  | C(3)...H(37)  | 2.923(103) | 0.389(tied to <i>u</i> <sub>58</sub> )  | 0.106  | 0.345 |
| <i>u</i> <sub>59</sub>  | Ga(1)...C(4)  | 2.938(9)   | 0.123(tied to <i>u</i> <sub>58</sub> )  | -0.008 | 0.109 |
| <i>u</i> <sub>49</sub>  | C(3)...H(33)  | 2.965(73)  | 0.286(tied to <i>u</i> <sub>58</sub> )  | 0.094  | 0.253 |
| <i>u</i> <sub>73</sub>  | C(5)...H(26)  | 2.985(78)  | 0.370(tied to <i>u</i> <sub>58</sub> )  | 0.061  | 0.328 |
| <i>u</i> <sub>60</sub>  | Ga(1)...C(3)  | 2.988(9)   | 0.108(tied to <i>u</i> <sub>58</sub> )  | 0.005  | 0.096 |
| <i>u</i> <sub>62</sub>  | Ga(1)...H(13) | 3.010(12)  | 0.238(tied to <i>u</i> <sub>58</sub> )  | -0.003 | 0.211 |
| <i>u</i> <sub>63</sub>  | Ga(1)...H(14) | 3.019(12)  | 0.256(tied to <i>u</i> <sub>58</sub> )  | 0.008  | 0.227 |
| <i>u</i> <sub>61</sub>  | H(7)...H(10)  | 3.071(24)  | 0.278(fixed)                            | -0.043 | 0.278 |
| <i>u</i> <sub>71</sub>  | C(4)...H(27)  | 3.075(40)  | 0.355(tied to <i>u</i> <sub>58</sub> )  | -0.013 | 0.315 |
| <i>u</i> <sub>57</sub>  | H(13)...H(22) | 3.076(95)  | 0.527(fixed)                            | 0.211  | 0.527 |
| <i>u</i> <sub>66</sub>  | H(6)...H(12)  | 3.107(26)  | 0.274(fixed)                            | 0.027  | 0.274 |
| <i>u</i> <sub>67</sub>  | H(8)...H(11)  | 3.125(23)  | 0.281(fixed)                            | -0.023 | 0.281 |
| <i>u</i> <sub>64</sub>  | H(9)...H(12)  | 3.155(30)  | 0.293(fixed)                            | -0.009 | 0.293 |
| <i>u</i> <sub>74</sub>  | Ga(1)...H(11) | 3.173(14)  | 0.244(tied to <i>u</i> <sub>58</sub> )  | 0.006  | 0.217 |
| <i>u</i> <sub>69</sub>  | Ga(1)...H(9)  | 3.188(14)  | 0.226(tied to <i>u</i> <sub>58</sub> )  | 0.019  | 0.201 |
| <i>u</i> <sub>92</sub>  | H(7)...H(37)  | 3.204(149) | 0.410(fixed)                            | 0.045  | 0.410 |
| <i>u</i> <sub>65</sub>  | H(8)...H(14)  | 3.224(23)  | 0.282(fixed)                            | 0.004  | 0.282 |
| <i>u</i> <sub>76</sub>  | Ga(1)...H(7)  | 3.244(15)  | 0.210(18)                               | 0.023  | 0.192 |
| <i>u</i> <sub>72</sub>  | Ga(1)...H(6)  | 3.251(15)  | 0.203(tied to <i>u</i> <sub>76</sub> )  | 0.029  | 0.185 |
| <i>u</i> <sub>68</sub>  | H(10)...H(13) | 3.272(26)  | 0.287(fixed)                            | 0.009  | 0.287 |
| <i>u</i> <sub>80</sub>  | H(14)...H(22) | 3.277(52)  | 0.585(fixed)                            | 0.197  | 0.585 |
| <i>u</i> <sub>79</sub>  | C(2)...H(37)  | 3.343(41)  | 0.396(tied to <i>u</i> <sub>88</sub> )  | 0.100  | 0.298 |
| <i>u</i> <sub>77</sub>  | H(7)...H(32)  | 3.382(102) | 0.487(fixed)                            | -0.005 | 0.487 |
| <i>u</i> <sub>78</sub>  | C(2)...H(26)  | 3.392(25)  | 0.349(tied to <i>u</i> <sub>88</sub> )  | 0.028  | 0.263 |
| <i>u</i> <sub>75</sub>  | C(4)...H(26)  | 3.477(96)  | 0.438(tied to <i>u</i> <sub>88</sub> )  | 0.027  | 0.329 |
| <i>u</i> <sub>82</sub>  | C(3)...H(9)   | 3.486(11)  | 0.139(tied to <i>u</i> <sub>88</sub> )  | -0.012 | 0.104 |
| <i>u</i> <sub>83</sub>  | C(4)...H(6)   | 3.490(11)  | 0.138(tied to <i>u</i> <sub>88</sub> )  | -0.008 | 0.104 |
| <i>u</i> <sub>85</sub>  | C(3)...H(13)  | 3.494(12)  | 0.139(tied to <i>u</i> <sub>88</sub> )  | -0.015 | 0.105 |
| <i>u</i> <sub>84</sub>  | C(5)...H(7)   | 3.495(12)  | 0.139(tied to <i>u</i> <sub>88</sub> )  | -0.014 | 0.104 |
| <i>u</i> <sub>88</sub>  | C(2)...C(15)  | 3.508(5)   | 0.133(5)                                | 0.006  | 0.100 |
| <i>u</i> <sub>86</sub>  | C(5)...H(11)  | 3.520(14)  | 0.141(tied to <i>u</i> <sub>88</sub> )  | -0.024 | 0.106 |
| <i>u</i> <sub>87</sub>  | C(4)...H(14)  | 3.520(14)  | 0.141(tied to <i>u</i> <sub>88</sub> )  | -0.024 | 0.106 |
| <i>u</i> <sub>99</sub>  | C(2)...H(27)  | 3.523(32)  | 0.359(tied to <i>u</i> <sub>88</sub> )  | -0.023 | 0.270 |
| <i>u</i> <sub>112</sub> | H(6)...H(35)  | 3.550(126) | 0.406(fixed)                            | 0.081  | 0.406 |
| <i>u</i> <sub>89</sub>  | C(5)...H(22)  | 3.563(56)  | 0.631(tied to <i>u</i> <sub>88</sub> )  | 0.181  | 0.475 |
| <i>u</i> <sub>81</sub>  | C(2)...H(33)  | 3.576(35)  | 0.330(tied to <i>u</i> <sub>88</sub> )  | 0.040  | 0.248 |
| <i>u</i> <sub>90</sub>  | C(3)...C(29)  | 3.649(55)  | 0.268(tied to <i>u</i> <sub>88</sub> )  | 0.013  | 0.201 |
| <i>u</i> <sub>95</sub>  | C(2)...C(18)  | 3.654(14)  | 0.199(tied to <i>u</i> <sub>88</sub> )  | 0.005  | 0.150 |
| <i>u</i> <sub>113</sub> | C(3)...C(30)  | 3.669(74)  | 0.288(12)                               | 0.042  | 0.247 |
| <i>u</i> <sub>91</sub>  | C(5)...H(37)  | 3.670(51)  | 0.564(tied to <i>u</i> <sub>88</sub> )  | 0.183  | 0.424 |
| <i>u</i> <sub>109</sub> | H(6)...H(36)  | 3.734(68)  | 0.373(fixed)                            | 0.097  | 0.373 |
| <i>u</i> <sub>94</sub>  | H(8)...H(9)   | 3.735(15)  | 0.185(fixed)                            | -0.024 | 0.185 |
| <i>u</i> <sub>93</sub>  | H(6)...H(10)  | 3.738(15)  | 0.184(fixed)                            | -0.021 | 0.184 |
| <i>u</i> <sub>108</sub> | C(2)...C(30)  | 3.784(34)  | 0.230(tied to <i>u</i> <sub>113</sub> ) | 0.042  | 0.197 |
| <i>u</i> <sub>126</sub> | C(5)...H(27)  | 3.787(105) | 0.374(tied to <i>u</i> <sub>113</sub> ) | -0.037 | 0.321 |
| <i>u</i> <sub>98</sub>  | H(7)...H(12)  | 3.821(17)  | 0.187(fixed)                            | -0.006 | 0.187 |
| <i>u</i> <sub>119</sub> | H(8)...H(37)  | 3.822(94)  | 0.385(fixed)                            | 0.125  | 0.385 |
| <i>u</i> <sub>97</sub>  | H(8)...H(13)  | 3.827(16)  | 0.187(fixed)                            | -0.014 | 0.187 |
| <i>u</i> <sub>105</sub> | H(6)...H(13)  | 3.833(25)  | 0.184(fixed)                            | 0.003  | 0.184 |

|           |               |            |                           |        |       |
|-----------|---------------|------------|---------------------------|--------|-------|
| $u_{103}$ | H(7)...H(14)  | 3.842(25)  | 0.188(fixed)              | -0.001 | 0.188 |
| $u_{110}$ | Ga(1)...H(12) | 3.856(8)   | 0.151(tied to $u_{113}$ ) | -0.012 | 0.130 |
| $u_{102}$ | H(7)...H(9)   | 3.858(24)  | 0.183(fixed)              | -0.022 | 0.183 |
| $u_{106}$ | H(9)...H(14)  | 3.864(29)  | 0.190(fixed)              | -0.017 | 0.190 |
| $u_{100}$ | H(11)...H(12) | 3.867(18)  | 0.191(fixed)              | -0.018 | 0.191 |
| $u_{104}$ | H(6)...H(11)  | 3.870(24)  | 0.192(fixed)              | -0.014 | 0.192 |
| $u_{107}$ | H(11)...H(13) | 3.871(29)  | 0.191(fixed)              | -0.017 | 0.191 |
| $u_{101}$ | H(10)...H(14) | 3.874(17)  | 0.193(fixed)              | -0.018 | 0.193 |
| $u_{96}$  | H(8)...H(33)  | 3.878(72)  | 0.277(fixed)              | 0.071  | 0.277 |
| $u_{121}$ | H(7)...H(34)  | 3.920(28)  | 0.329(fixed)              | -0.013 | 0.329 |
| $u_{111}$ | C(2)...C(29)  | 3.926(27)  | 0.182(tied to $u_{113}$ ) | -0.017 | 0.156 |
| $u_{117}$ | Ga(1)...H(10) | 3.935(8)   | 0.140(tied to $u_{113}$ ) | -0.025 | 0.120 |
| $u_{118}$ | Ga(1)...H(8)  | 3.976(8)   | 0.133(tied to $u_{113}$ ) | -0.012 | 0.114 |
| $u_{125}$ | C(2)...H(35)  | 4.027(53)  | 0.366(tied to $u_{113}$ ) | 0.057  | 0.314 |
| $u_{123}$ | C(5)...H(35)  | 4.038(43)  | 0.556(tied to $u_{113}$ ) | 0.158  | 0.476 |
| $u_{116}$ | C(3)...H(32)  | 4.053(94)  | 0.445(tied to $u_{113}$ ) | -0.033 | 0.382 |
| $u_{129}$ | H(9)...H(19)  | 4.096(85)  | 0.468(fixed)              | 0.016  | 0.468 |
| $u_{120}$ | C(2)...H(22)  | 4.102(39)  | 0.420(tied to $u_{113}$ ) | 0.089  | 0.360 |
| $u_{122}$ | C(5)...C(17)  | 4.152(35)  | 0.408(tied to $u_{113}$ ) | 0.095  | 0.350 |
| $u_{140}$ | C(3)...H(35)  | 4.184(103) | 0.334(fixed)              | 0.028  | 0.334 |
| $u_{124}$ | C(2)...H(32)  | 4.187(45)  | 0.362(tied to $u_{113}$ ) | -0.046 | 0.310 |
| $u_{114}$ | H(6)...H(32)  | 4.208(123) | 0.432(fixed)              | 0.007  | 0.432 |
| $u_{135}$ | H(11)...H(19) | 4.222(46)  | 0.549(fixed)              | -0.027 | 0.549 |
| $u_{115}$ | H(6)...H(34)  | 4.228(86)  | 0.357(fixed)              | 0.066  | 0.357 |
| $u_{128}$ | C(2)...C(17)  | 4.311(24)  | 0.208(21)                 | 0.029  | 0.219 |
| $u_{138}$ | C(4)...H(33)  | 4.391(38)  | 0.314(tied to $u_{128}$ ) | -0.005 | 0.330 |
| $u_{127}$ | H(13)...H(24) | 4.393(72)  | 0.478(fixed)              | 0.096  | 0.478 |
| $u_{130}$ | H(12)...H(37) | 4.404(43)  | 0.469(fixed)              | 0.182  | 0.469 |
| $u_{132}$ | H(7)...H(13)  | 4.408(12)  | 0.137(fixed)              | -0.024 | 0.137 |
| $u_{131}$ | H(6)...H(9)   | 4.418(11)  | 0.137(fixed)              | -0.006 | 0.137 |
| $u_{136}$ | H(13)...H(35) | 4.420(50)  | 0.549(fixed)              | 0.150  | 0.549 |
| $u_{133}$ | H(11)...H(14) | 4.421(12)  | 0.138(fixed)              | -0.030 | 0.138 |
| $u_{147}$ | C(3)...H(36)  | 4.474(69)  | 0.283(tied to $u_{128}$ ) | 0.015  | 0.297 |
| $u_{144}$ | C(4)...H(19)  | 4.484(55)  | 0.378(tied to $u_{128}$ ) | -0.035 | 0.398 |
| $u_{159}$ | H(7)...H(36)  | 4.497(106) | 0.384(fixed)              | -0.027 | 0.384 |
| $u_{137}$ | C(3)...H(34)  | 4.500(43)  | 0.272(tied to $u_{145}$ ) | -0.007 | 0.225 |
| $u_{139}$ | H(12)...H(22) | 4.562(61)  | 0.508(fixed)              | 0.153  | 0.508 |
| $u_{162}$ | H(7)...H(35)  | 4.575(116) | 0.347(fixed)              | -0.015 | 0.347 |
| $u_{145}$ | C(2)...C(16)  | 4.602(17)  | 0.177(10)                 | -0.028 | 0.147 |
| $u_{148}$ | C(2)...H(19)  | 4.604(34)  | 0.345(tied to $u_{145}$ ) | -0.020 | 0.286 |
| $u_{152}$ | C(5)...H(25)  | 4.619(71)  | 0.352(tied to $u_{145}$ ) | 0.014  | 0.292 |
| $u_{142}$ | C(4)...H(25)  | 4.641(56)  | 0.279(tied to $u_{145}$ ) | -0.029 | 0.231 |
| $u_{154}$ | C(4)...H(32)  | 4.673(31)  | 0.513(tied to $u_{145}$ ) | -0.098 | 0.425 |
| $u_{143}$ | C(5)...H(24)  | 4.711(51)  | 0.500(tied to $u_{145}$ ) | 0.101  | 0.415 |
| $u_{149}$ | C(2)...H(25)  | 4.736(15)  | 0.207(tied to $u_{145}$ ) | -0.015 | 0.172 |
| $u_{146}$ | C(2)...H(24)  | 4.745(26)  | 0.342(tied to $u_{145}$ ) | 0.040  | 0.284 |
| $u_{156}$ | C(4)...C(16)  | 4.757(27)  | 0.303(tied to $u_{145}$ ) | -0.060 | 0.252 |
| $u_{153}$ | C(2)...H(36)  | 4.785(31)  | 0.264(tied to $u_{145}$ ) | 0.009  | 0.219 |
| $u_{141}$ | C(5)...H(33)  | 4.799(72)  | 0.346(tied to $u_{145}$ ) | 0.051  | 0.287 |
| $u_{158}$ | C(4)...H(37)  | 4.801(56)  | 0.352(tied to $u_{145}$ ) | 0.057  | 0.292 |

|           |               |            |                           |        |       |
|-----------|---------------|------------|---------------------------|--------|-------|
| $u_{151}$ | C(2)...C(31)  | 4.806(7)   | 0.128(tied to $u_{145}$ ) | -0.017 | 0.106 |
| $u_{134}$ | H(9)...H(22)  | 4.814(108) | 0.408(fixed)              | 0.085  | 0.408 |
| $u_{155}$ | C(3)...H(26)  | 4.903(24)  | 0.318(tied to $u_{145}$ ) | 0.007  | 0.264 |
| $u_{168}$ | H(12)...H(35) | 4.931(53)  | 0.521(fixed)              | 0.131  | 0.521 |
| $u_{157}$ | C(2)...H(34)  | 4.932(22)  | 0.215(tied to $u_{145}$ ) | -0.037 | 0.178 |
| $u_{163}$ | C(5)...H(23)  | 4.996(33)  | 0.473(tied to $u_{145}$ ) | 0.077  | 0.392 |
| $u_{169}$ | C(3)...H(27)  | 5.003(25)  | 0.345(tied to $u_{145}$ ) | -0.042 | 0.286 |
| $u_{150}$ | C(4)...H(22)  | 5.018(75)  | 0.428(tied to $u_{145}$ ) | 0.048  | 0.355 |
| $u_{161}$ | H(8)...H(32)  | 5.021(96)  | 0.418(fixed)              | -0.073 | 0.418 |
| $u_{165}$ | H(9)...H(21)  | 5.038(27)  | 0.338(fixed)              | -0.014 | 0.338 |
| $u_{160}$ | C(4)...C(17)  | 5.058(49)  | 0.261(tied to $u_{145}$ ) | -0.012 | 0.216 |
| $u_{164}$ | C(2)...H(20)  | 5.084(16)  | 0.259(tied to $u_{145}$ ) | -0.008 | 0.215 |
| $u_{166}$ | C(2)...H(39)  | 5.104(22)  | 0.226(tied to $u_{145}$ ) | -0.012 | 0.188 |
| $u_{182}$ | H(8)...H(35)  | 5.109(104) | 0.393(fixed)              | 0.039  | 0.393 |
| $u_{174}$ | H(11)...H(37) | 5.112(87)  | 0.331(fixed)              | 0.017  | 0.331 |
| $u_{167}$ | C(2)...H(40)  | 5.124(19)  | 0.240(tied to $u_{145}$ ) | -0.035 | 0.199 |
| $u_{172}$ | C(3)...C(18)  | 5.149(16)  | 0.186(tied to $u_{145}$ ) | -0.015 | 0.154 |
| $u_{178}$ | C(4)...C(30)  | 5.164(39)  | 0.221(tied to $u_{145}$ ) | -0.003 | 0.183 |
| $u_{171}$ | C(5)...H(36)  | 5.195(38)  | 0.452(tied to $u_{145}$ ) | 0.095  | 0.375 |
| $u_{177}$ | H(9)...H(20)  | 5.211(47)  | 0.355(fixed)              | -0.018 | 0.355 |
| $u_{175}$ | H(6)...H(22)  | 5.211(58)  | 0.450(fixed)              | 0.131  | 0.450 |
| $u_{176}$ | C(3)...H(22)  | 5.243(31)  | 0.464(tied to $u_{145}$ ) | 0.084  | 0.385 |
| $u_{173}$ | C(2)...H(23)  | 5.257(22)  | 0.282(tied to $u_{145}$ ) | 0.006  | 0.234 |
| $u_{190}$ | H(9)...H(32)  | 5.267(42)  | 0.464(fixed)              | -0.095 | 0.464 |
| $u_{179}$ | H(7)...H(27)  | 5.370(52)  | 0.362(fixed)              | -0.034 | 0.362 |
| $u_{183}$ | H(6)...H(26)  | 5.377(54)  | 0.293(fixed)              | 0.023  | 0.293 |
| $u_{187}$ | H(10)...H(37) | 5.399(64)  | 0.337(fixed)              | 0.074  | 0.337 |
| $u_{201}$ | H(8)...H(36)  | 5.405(69)  | 0.348(fixed)              | 0.022  | 0.348 |
| $u_{196}$ | C(5)...H(19)  | 5.413(59)  | 0.310(tied to $u_{145}$ ) | -0.010 | 0.257 |
| $u_{191}$ | C(4)...H(20)  | 5.419(36)  | 0.359(tied to $u_{145}$ ) | -0.055 | 0.298 |
| $u_{170}$ | H(9)...H(23)  | 5.450(79)  | 0.322(fixed)              | 0.028  | 0.322 |
| $u_{200}$ | C(4)...H(35)  | 5.461(43)  | 0.360(tied to $u_{145}$ ) | 0.022  | 0.299 |
| $u_{185}$ | H(8)...H(34)  | 5.461(48)  | 0.263(fixed)              | -0.027 | 0.263 |
| $u_{181}$ | H(6)...H(38)  | 5.485(26)  | 0.299(fixed)              | 0.075  | 0.299 |
| $u_{194}$ | C(3)...C(17)  | 5.497(19)  | 0.272(tied to $u_{145}$ ) | 0.024  | 0.226 |
| $u_{193}$ | C(2)...H(21)  | 5.498(15)  | 0.190(tied to $u_{145}$ ) | -0.044 | 0.157 |
| $u_{186}$ | C(5)...H(32)  | 5.502(48)  | 0.350(tied to $u_{145}$ ) | -0.037 | 0.290 |
| $u_{189}$ | H(9)...H(37)  | 5.509(34)  | 0.317(fixed)              | 0.067  | 0.317 |
| $u_{209}$ | H(10)...H(19) | 5.510(60)  | 0.419(fixed)              | -0.076 | 0.419 |
| $u_{205}$ | H(10)...H(32) | 5.516(36)  | 0.452(fixed)              | -0.141 | 0.452 |
| $u_{198}$ | C(5)...H(39)  | 5.530(39)  | 0.369(tied to $u_{145}$ ) | 0.053  | 0.306 |
| $u_{180}$ | H(9)...H(24)  | 5.545(55)  | 0.299(fixed)              | 0.017  | 0.299 |
| $u_{204}$ | C(4)...H(21)  | 5.558(20)  | 0.321(tied to $u_{145}$ ) | -0.077 | 0.266 |
| $u_{206}$ | H(7)...H(38)  | 5.597(26)  | 0.316(fixed)              | -0.012 | 0.316 |
| $u_{184}$ | H(6)...H(40)  | 5.598(37)  | 0.302(fixed)              | 0.034  | 0.302 |
| $u_{192}$ | C(3)...H(40)  | 5.610(35)  | 0.282(tied to $u_{145}$ ) | -0.021 | 0.234 |
| $u_{207}$ | C(3)...H(39)  | 5.638(36)  | 0.240(tied to $u_{145}$ ) | -0.017 | 0.199 |
| $u_{199}$ | H(6)...H(24)  | 5.639(36)  | 0.389(fixed)              | 0.115  | 0.389 |
| $u_{188}$ | H(11)...H(22) | 5.643(66)  | 0.362(fixed)              | -0.002 | 0.362 |
| $u_{197}$ | C(4)...H(24)  | 5.663(35)  | 0.300(tied to $u_{145}$ ) | -0.014 | 0.249 |

|                         |               |           |   |        |       |
|-------------------------|---------------|-----------|---|--------|-------|
| <i>u</i> <sub>203</sub> | H(7)...H(19)  | 5.665(43) | 0.445(fixed)                            | -0.032 | 0.445 |
| <i>u</i> <sub>202</sub> | C(2)...H(38)  | 5.677(8)  | 0.166(tied to <i>u</i> <sub>145</sub> ) | -0.016 | 0.137 |
| <i>u</i> <sub>215</sub> | H(6)...H(27)  | 5.704(36) | 0.289(fixed)                            | -0.034 | 0.289 |
| <i>u</i> <sub>213</sub> | C(3)...H(19)  | 5.719(22) | 0.406(tied to <i>u</i> <sub>145</sub> ) | -0.043 | 0.337 |
| <i>u</i> <sub>211</sub> | C(3)...H(24)  | 5.726(21) | 0.371(tied to <i>u</i> <sub>145</sub> ) | 0.049  | 0.308 |
| <i>u</i> <sub>210</sub> | C(5)...H(20)  | 5.734(23) | 0.275(tied to <i>u</i> <sub>145</sub> ) | 0.020  | 0.228 |
| <i>u</i> <sub>208</sub> | H(12)...H(24) | 5.771(54) | 0.437(fixed)                            | 0.066  | 0.437 |
| <i>u</i> <sub>216</sub> | C(3)...C(16)  | 5.782(11) | 0.215(tied to <i>u</i> <sub>145</sub> ) | -0.043 | 0.179 |
| <i>u</i> <sub>222</sub> | C(4)...H(34)  | 5.797(29) | 0.314(tied to <i>u</i> <sub>145</sub> ) | -0.103 | 0.261 |
| <i>u</i> <sub>214</sub> | C(3)...H(38)  | 5.809(15) | 0.229(tied to <i>u</i> <sub>145</sub> ) | 0.001  | 0.190 |
| <i>u</i> <sub>219</sub> | C(4)...H(40)  | 5.816(27) | 0.365(tied to <i>u</i> <sub>145</sub> ) | -0.087 | 0.303 |
| <i>u</i> <sub>225</sub> | H(11)...H(35) | 5.856(51) | 0.304(fixed)                            | -0.022 | 0.304 |
| <i>u</i> <sub>195</sub> | H(10)...H(22) | 5.858(79) | 0.424(fixed)                            | 0.071  | 0.424 |
| <i>u</i> <sub>212</sub> | C(4)...H(23)  | 5.865(54) | 0.298(tied to <i>u</i> <sub>145</sub> ) | -0.030 | 0.247 |
| <i>u</i> <sub>220</sub> | H(7)...H(22)  | 5.896(28) | 0.360(fixed)                            | 0.049  | 0.360 |
| <i>u</i> <sub>217</sub> | H(9)...H(35)  | 5.900(30) | 0.353(fixed)                            | 0.062  | 0.353 |
| <i>u</i> <sub>224</sub> | C(5)...H(21)  | 5.904(46) | 0.275(tied to <i>u</i> <sub>145</sub> ) | -0.002 | 0.228 |
| <i>u</i> <sub>227</sub> | C(5)...H(40)  | 5.958(16) | 0.279(tied to <i>u</i> <sub>145</sub> ) | -0.009 | 0.231 |
| <i>u</i> <sub>226</sub> | H(12)...H(23) | 5.958(37) | 0.431(fixed)                            | 0.046  | 0.431 |
| <i>u</i> <sub>218</sub> | C(5)...H(34)  | 6.013(50) | 0.325(tied to <i>u</i> <sub>145</sub> ) | 0.007  | 0.270 |
| <i>u</i> <sub>223</sub> | H(11)...H(24) | 6.014(26) | 0.305(fixed)                            | -0.044 | 0.305 |
| <i>u</i> <sub>221</sub> | H(8)...H(22)  | 6.040(37) | 0.437(fixed)                            | 0.095  | 0.437 |
| <i>u</i> <sub>228</sub> | H(7)...H(20)  | 6.061(26) | 0.377(fixed)                            | -0.008 | 0.377 |
| <i>u</i> <sub>229</sub> | C(3)...H(20)  | 6.079(13) | 0.309(tied to <i>u</i> <sub>145</sub> ) | -0.012 | 0.257 |
| <i>u</i> <sub>231</sub> | H(7)...H(24)  | 6.112(26) | 0.312(fixed)                            | 0.031  | 0.312 |
| <i>u</i> <sub>230</sub> | C(4)...H(39)  | 6.114(12) | 0.263(tied to <i>u</i> <sub>145</sub> ) | -0.060 | 0.218 |
| <i>u</i> <sub>236</sub> | C(4)...H(36)  | 6.143(40) | 0.252(tied to <i>u</i> <sub>145</sub> ) | -0.045 | 0.209 |
| <i>u</i> <sub>237</sub> | H(10)...H(35) | 6.213(56) | 0.348(fixed)                            | 0.027  | 0.348 |
| <i>u</i> <sub>235</sub> | C(3)...H(25)  | 6.230(16) | 0.207(tied to <i>u</i> <sub>145</sub> ) | -0.037 | 0.172 |
| <i>u</i> <sub>233</sub> | H(6)...H(19)  | 6.255(22) | 0.343(fixed)                            | -0.024 | 0.343 |
| <i>u</i> <sub>239</sub> | H(11)...H(36) | 6.292(64) | 0.304(fixed)                            | -0.082 | 0.304 |
| <i>u</i> <sub>234</sub> | H(11)...H(23) | 6.301(58) | 0.333(fixed)                            | -0.074 | 0.333 |
| <i>u</i> <sub>232</sub> | H(6)...H(20)  | 6.342(24) | 0.293(fixed)                            | 0.036  | 0.293 |
| <i>u</i> <sub>238</sub> | C(5)...H(38)  | 6.388(22) | 0.329(tied to <i>u</i> <sub>145</sub> ) | 0.043  | 0.273 |
| <i>u</i> <sub>243</sub> | H(9)...H(34)  | 6.485(36) | 0.299(fixed)                            | -0.103 | 0.299 |
| <i>u</i> <sub>241</sub> | C(3)...H(23)  | 6.514(19) | 0.281(tied to <i>u</i> <sub>145</sub> ) | -0.008 | 0.233 |
| <i>u</i> <sub>248</sub> | H(10)...H(21) | 6.579(22) | 0.281(fixed)                            | -0.102 | 0.281 |
| <i>u</i> <sub>246</sub> | H(8)...H(19)  | 6.579(28) | 0.357(fixed)                            | -0.072 | 0.357 |
| <i>u</i> <sub>247</sub> | H(6)...H(23)  | 6.607(41) | 0.315(fixed)                            | 0.041  | 0.315 |
| <i>u</i> <sub>240</sub> | H(10)...H(24) | 6.639(39) | 0.296(fixed)                            | -0.012 | 0.296 |
| <i>u</i> <sub>249</sub> | C(4)...H(38)  | 6.673(13) | 0.234(tied to <i>u</i> <sub>145</sub> ) | -0.079 | 0.194 |
| <i>u</i> <sub>242</sub> | H(8)...H(24)  | 6.686(24) | 0.345(fixed)                            | 0.040  | 0.345 |
| <i>u</i> <sub>244</sub> | H(7)...H(25)  | 6.688(35) | 0.246(fixed)                            | -0.050 | 0.246 |
| <i>u</i> <sub>250</sub> | H(6)...H(25)  | 6.725(38) | 0.219(fixed)                            | -0.012 | 0.219 |
| <i>u</i> <sub>252</sub> | C(3)...H(21)  | 6.759(10) | 0.213(tied to <i>u</i> <sub>145</sub> ) | -0.067 | 0.177 |
| <i>u</i> <sub>251</sub> | H(9)...H(36)  | 6.761(23) | 0.235(fixed)                            | -0.028 | 0.235 |
| <i>u</i> <sub>245</sub> | H(10)...H(23) | 6.790(55) | 0.307(fixed)                            | -0.025 | 0.307 |
| <i>u</i> <sub>253</sub> | H(8)...H(25)  | 6.850(15) | 0.215(fixed)                            | -0.048 | 0.215 |
| <i>u</i> <sub>255</sub> | H(10)...H(36) | 6.854(47) | 0.259(fixed)                            | -0.044 | 0.259 |
| <i>u</i> <sub>254</sub> | H(7)...H(21)  | 6.892(28) | 0.302(fixed)                            | -0.077 | 0.302 |

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|                         |              |           |              |        |       |
|-------------------------|--------------|-----------|--------------|--------|-------|
| <i>u</i> <sub>256</sub> | H(7)...H(23) | 7.000(15) | 0.232(fixed) | -0.034 | 0.232 |
| <i>u</i> <sub>257</sub> | H(8)...H(20) | 7.068(14) | 0.260(fixed) | -0.042 | 0.260 |
| <i>u</i> <sub>258</sub> | H(6)...H(21) | 7.156(15) | 0.217(fixed) | -0.028 | 0.217 |
| <i>u</i> <sub>259</sub> | H(8)...H(23) | 7.348(24) | 0.291(fixed) | -0.010 | 0.291 |
| <i>u</i> <sub>260</sub> | H(8)...H(21) | 7.624(14) | 0.198(fixed) | -0.090 | 0.198 |

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**Table S7** Least-squares correlation matrix ( $\times 100$ ) for the GED refinement of  $\text{Al}(\text{Bu}^t)_3 \cdot \mathbf{1}^a$

|           | $p_1$ | $p_2$ | $p_3$ | $p_4$ | $p_5$ | $p_6$ | $p_7$ | $p_8$ | $p_9$ | $p_{10}$ | $p_{11}$ | $p_{12}$ | $u_7$ | $u_{10}$ | $u_{22}$ | $u_{24}$ | $u_{37}$ | $u_{40}$ | $u_{55}$ | $u_{81}$ | $u_{124}$ | $u_{144}$ | $u_{154}$ | $u_{171}$ | $u_{192}$ | $k_1$ | $k_2$ |  |
|-----------|-------|-------|-------|-------|-------|-------|-------|-------|-------|----------|----------|----------|-------|----------|----------|----------|----------|----------|----------|----------|-----------|-----------|-----------|-----------|-----------|-------|-------|--|
| $p_1$     | 100   |       |       |       |       |       |       |       |       |          |          |          |       |          |          |          |          |          |          |          |           |           |           |           |           |       |       |  |
| $p_2$     |       | 100   |       |       |       |       |       |       |       |          |          |          |       |          |          |          |          |          |          |          |           |           |           |           |           |       |       |  |
| $p_3$     |       |       | 100   |       |       |       |       |       |       |          |          |          |       |          |          |          |          |          |          |          |           |           |           |           |           |       |       |  |
| $p_4$     |       |       |       | 100   |       |       |       |       |       |          |          |          |       |          |          |          |          |          |          |          |           |           |           |           |           |       |       |  |
| $p_5$     |       |       |       |       | 100   |       |       |       |       |          |          |          |       |          |          |          |          |          |          |          |           |           |           |           |           |       |       |  |
| $p_6$     |       |       |       |       |       | 100   |       |       |       |          |          |          |       |          |          |          |          |          |          |          |           |           |           |           |           |       |       |  |
| $p_7$     |       |       |       |       |       |       | 100   |       |       |          |          |          |       |          |          |          |          |          |          |          |           |           |           |           |           |       |       |  |
| $p_8$     |       |       |       |       |       |       |       | 100   |       |          |          |          |       |          |          |          |          |          |          |          |           |           |           |           |           |       |       |  |
| $p_9$     |       |       |       |       |       |       |       |       | 100   |          |          |          |       |          |          |          |          |          |          |          |           |           |           |           |           |       |       |  |
| $p_{10}$  |       |       |       |       |       |       |       |       |       | 100      |          |          |       |          |          |          |          |          |          |          |           |           |           |           |           |       |       |  |
| $p_{11}$  |       |       |       |       |       |       |       |       |       |          | 100      |          |       |          |          |          |          |          |          |          |           |           |           |           |           |       |       |  |
| $p_{12}$  |       |       |       |       |       |       |       |       |       |          |          | 100      |       |          |          |          |          |          |          |          |           |           |           |           |           |       |       |  |
| $u_7$     |       |       |       |       |       |       |       |       |       |          |          |          | 100   |          |          |          |          |          |          |          |           |           |           |           |           |       |       |  |
| $u_{10}$  |       |       |       |       |       |       |       |       |       |          |          |          |       | 100      |          |          |          |          |          |          |           |           |           |           |           |       |       |  |
| $u_{22}$  |       |       |       |       |       |       |       |       |       |          |          |          |       |          | 100      |          |          |          |          |          |           |           |           |           |           |       |       |  |
| $u_{24}$  |       |       |       |       |       |       |       |       |       |          |          |          |       |          |          | 100      |          |          |          |          |           |           |           |           |           |       |       |  |
| $u_{37}$  |       |       |       |       |       |       |       |       |       |          |          |          |       |          |          |          | 100      |          |          |          |           |           |           |           |           |       |       |  |
| $u_{40}$  |       |       |       |       |       |       |       |       |       |          |          |          |       |          |          |          |          | 100      |          |          |           |           |           |           |           |       |       |  |
| $u_{55}$  |       |       |       |       |       |       |       |       |       |          |          |          |       |          |          |          |          |          | 100      |          |           |           |           |           |           |       |       |  |
| $u_{81}$  |       |       |       |       |       |       |       |       |       |          |          |          |       |          |          |          |          |          |          | 100      |           |           |           |           |           |       |       |  |
| $u_{124}$ |       |       |       |       |       |       |       |       |       |          |          |          |       |          |          |          |          |          |          |          | 100       |           |           |           |           |       |       |  |
| $u_{144}$ |       |       |       |       |       |       |       |       |       |          |          |          |       |          |          |          |          |          |          |          |           | 100       |           |           |           |       |       |  |
| $u_{154}$ |       |       |       |       |       |       |       |       |       |          |          |          |       |          |          |          |          |          |          |          |           |           | 100       |           |           |       |       |  |
| $u_{171}$ |       |       |       |       |       |       |       |       |       |          |          |          |       |          |          |          |          |          |          |          |           |           |           | 100       |           |       |       |  |
| $u_{192}$ |       |       |       |       |       |       |       |       |       |          |          |          |       |          |          |          |          |          |          |          |           |           |           |           | 100       |       |       |  |
| $k_1$     |       |       |       |       |       |       |       |       |       |          |          |          |       |          |          |          |          |          |          |          |           |           |           |           |           | 100   |       |  |
| $k_2$     |       |       |       |       |       |       |       |       |       |          |          |          |       |          |          |          |          |          |          |          |           |           |           |           |           |       | 100   |  |

<sup>a</sup>  $k_1$  and  $k_2$  are scale factors.

**Table S8** Least-squares correlation matrix ( $\times 100$ ) for the GED refinement of  $\text{Ga}(\text{Bu})_3 \cdot 2^a$ .

|           | $p_1$ | $p_2$ | $p_3$ | $p_4$ | $p_5$ | $p_6$ | $p_7$ | $p_8$ | $p_9$ | $p_{10}$ | $p_{11}$ | $p_{12}$ | $u_1$ | $u_{10}$ | $u_{22}$ | $u_{24}$ | $u_{34}$ | $u_{51}$ | $u_{74}$ | $u_{86}$ | $u_{95}$ | $u_{130}$ | $u_{144}$ | $k_1$ | $k_2$ |
|-----------|-------|-------|-------|-------|-------|-------|-------|-------|-------|----------|----------|----------|-------|----------|----------|----------|----------|----------|----------|----------|----------|-----------|-----------|-------|-------|
| $p_1$     | 100   | 28    | -17   | -24   | 2     | 18    | -5    | -9    | 0     | -3       | 0        | 6        | 11    | -29      | -1       | -12      | 1        | 13       | 3        | -2       | -2       | -3        | 1         | 16    | -12   |
| $p_2$     |       | 100   | -44   | 4     | 3     | 27    | -7    | -13   | -3    | -15      | 7        | 6        | 34    | 4        | -27      | -39      | -10      | 21       | 16       | -1       | -1       | -8        | -1        | 26    | 6     |
| $p_3$     |       |       | 100   | -7    | 5     | -67   | -17   | -26   | 4     | -2       | -4       | 14       | -16   | 5        | 41       | 83       | 6        | 17       | -6       | -19      | -8       | -1        | -5        | -28   | 1     |
| $p_4$     |       |       |       | 100   | -15   | -30   | 18    | 8     | 5     | 5        | 1        | -15      | -18   | 24       | -66      | -16      | -1       | -22      | 0        | 8        | -7       | 2         | -7        | -31   | -4    |
| $p_5$     |       |       |       |       | 100   | -8    | -1    | 3     | -5    | -3       | 0        | 2        | 0     | 1        | 1        | 1        | -5       | -11      | -1       | 23       | 13       | 2         | -1        | 0     | -1    |
| $p_6$     |       |       |       |       |       | 100   | 35    | 0     | 4     | 11       | 4        | 4        | 17    | -13      | -5       | -42      | 23       | -17      | 18       | 12       | 15       | -1        | 11        | 31    | 2     |
| $p_7$     |       |       |       |       |       |       | 100   | -21   | 1     | 2        | -13      | 14       | -9    | 0        | -17      | -19      | -8       | -69      | -18      | 2        | 26       | 14        | -13       | -11   | -1    |
| $p_8$     |       |       |       |       |       |       |       | 100   | 5     | 2        | -18      | -57      | -6    | 1        | -13      | -29      | 9        | -44      | -14      | 6        | -16      | -1        | -1        | -10   | 3     |
| $p_9$     |       |       |       |       |       |       |       |       | 100   | -36      | -19      | -9       | -5    | -2       | -5       | -1       | 57       | -4       | 1        | 21       | -9       | -4        | 30        | -9    | -6    |
| $p_{10}$  |       |       |       |       |       |       |       |       |       | 100      | 29       | 14       | -7    | -3       | 0        | -1       | 26       | -4       | 5        | 20       | -8       | -2        | 29        | -8    | -4    |
| $p_{11}$  |       |       |       |       |       |       |       |       |       |          | 100      | -8       | 1     | -1       | -4       | 0        | 2        | 22       | -17      | -35      | 53       | -22       | 14        | 0     | -2    |
| $p_{12}$  |       |       |       |       |       |       |       |       |       |          |          | 100      | 4     | -3       | 14       | 16       | -4       | 22       | 27       | 28       | -25      | -31       | 13        | 8     | -4    |
| $u_1$     |       |       |       |       |       |       |       |       |       |          |          |          | 100   | 22       | 11       | -14      | -1       | 24       | 5        | -6       | 1        | -4        | 4         | 51    | 35    |
| $u_{10}$  |       |       |       |       |       |       |       |       |       |          |          |          |       | 100      | -8       | -3       | 2        | 10       | 1        | -2       | 0        | 0         | 0         | 33    | 55    |
| $u_{22}$  |       |       |       |       |       |       |       |       |       |          |          |          |       |          | 100      | 50       | 6        | 24       | -9       | -19      | -1       | -2        | 6         | 30    | 17    |
| $u_{24}$  |       |       |       |       |       |       |       |       |       |          |          |          |       |          |          | 100      | 21       | 24       | -3       | -22      | -8       | -3        | -2        | -15   | 0     |
| $u_{34}$  |       |       |       |       |       |       |       |       |       |          |          |          |       |          |          |          | 100      | 8        | 11       | 22       | -14      | -8        | 41        | 5     | 11    |
| $u_{51}$  |       |       |       |       |       |       |       |       |       |          |          |          |       |          |          |          |          | 100      | 38       | 1        | -7       | -10       | 13        | 39    | 13    |
| $u_{74}$  |       |       |       |       |       |       |       |       |       |          |          |          |       |          |          |          |          |          | 100      | 55       | 0        | 4         | 1         | 3     | 1     |
| $u_{86}$  |       |       |       |       |       |       |       |       |       |          |          |          |       |          |          |          |          |          |          | 100      | -20      | 5         | 7         | -8    | -7    |
| $u_{95}$  |       |       |       |       |       |       |       |       |       |          |          |          |       |          |          |          |          |          |          |          | 100      | 40        | 4         | 2     | 4     |
| $u_{130}$ |       |       |       |       |       |       |       |       |       |          |          |          |       |          |          |          |          |          |          |          |          | 100       | 22        | -6    | 1     |
| $u_{144}$ |       |       |       |       |       |       |       |       |       |          |          |          |       |          |          |          |          |          |          |          |          |           | 100       | 10    | 1     |
| $k_1$     |       |       |       |       |       |       |       |       |       |          |          |          |       |          |          |          |          |          |          |          |          |           |           | 100   | 41    |
| $k_2$     |       |       |       |       |       |       |       |       |       |          |          |          |       |          |          |          |          |          |          |          |          |           |           |       | 100   |

<sup>a</sup>  $k_1$  and  $k_2$  are scale factors.

**Table S9** Coordinates (in Å) from the GED-refined structure of Al(Bu')<sub>3</sub>, **1**.

|       | <i>x</i> | <i>y</i> | <i>z</i> |
|-------|----------|----------|----------|
| Al(1) | 0.0000   | 0.0000   | 0.0000   |
| C(2)  | 1.9961   | -0.2201  | 0.0000   |
| C(3)  | 2.2351   | -1.6068  | 0.6522   |
| C(4)  | 2.6647   | -0.1999  | -1.3894  |
| C(5)  | 2.7251   | 0.8850   | 0.7965   |
| H(6)  | 1.8356   | -1.6603  | 1.6866   |
| H(7)  | 1.7509   | -2.4285  | 0.0842   |
| H(8)  | 3.3247   | -1.8153  | 0.6946   |
| H(9)  | 2.4852   | 0.7533   | -1.9293  |
| H(10) | 3.7615   | -0.3285  | -1.2764  |
| H(11) | 2.2907   | -1.0111  | -2.0485  |
| H(12) | 3.8206   | 0.7092   | 0.7596   |
| H(13) | 2.5267   | 1.8984   | 0.3891   |
| H(14) | 2.4175   | 0.9080   | 1.8629   |
| C(15) | -0.9980  | -0.2201  | 1.7286   |
| C(16) | -0.1291  | -0.1999  | 3.0024   |
| C(17) | -2.0524  | 0.8850   | 1.9617   |
| C(18) | -1.6824  | -1.6068  | 1.6096   |
| H(19) | 0.6287   | -1.0111  | 3.0081   |
| H(20) | 0.4282   | 0.7533   | 3.1169   |
| H(21) | -0.7753  | -0.3285  | 3.8958   |
| H(22) | -2.8221  | 0.9080   | 1.1621   |
| H(23) | -2.5681  | 0.7092   | 2.9289   |
| H(24) | -1.6003  | 1.8984   | 1.9936   |
| H(25) | -2.2639  | -1.8153  | 2.5320   |
| H(26) | -2.3784  | -1.6603  | 0.7464   |
| H(27) | -0.9484  | -2.4285  | 1.4742   |
| C(28) | -0.9980  | -0.2201  | -1.7286  |
| C(29) | -2.5356  | -0.1999  | -1.6130  |
| C(30) | -0.6727  | 0.8850   | -2.7583  |
| C(31) | -0.5527  | -1.6068  | -2.2618  |
| H(32) | -2.9194  | -1.0111  | -0.9595  |
| H(33) | -2.9134  | 0.7533   | -1.1876  |
| H(34) | -2.9862  | -0.3285  | -2.6194  |
| H(35) | 0.4046   | 0.9080   | -3.0251  |
| H(36) | -1.2524  | 0.7092   | -3.6885  |
| H(37) | -0.9264  | 1.8984   | -2.3827  |
| H(38) | -1.0608  | -1.8153  | -3.2266  |
| H(39) | 0.5428   | -1.6603  | -2.4329  |
| H(40) | -0.8025  | -2.4285  | -1.5584  |

**Table S10** Coordinates (in Å) from the GED-refined structure of Ga(Bu<sup>t</sup>)<sub>3</sub>, **2**.

|       | <i>x</i> | <i>y</i> | <i>z</i> |
|-------|----------|----------|----------|
| Ga(1) | 0.0000   | 0.0000   | 0.0000   |
| C(2)  | 2.0253   | -0.1680  | 0.0000   |
| C(3)  | 2.6302   | -0.1246  | -1.4118  |
| C(4)  | 2.6635   | 0.9549   | 0.8379   |
| C(5)  | 2.2840   | -1.5609  | 0.6155   |
| H(6)  | 2.2849   | -0.9233  | -2.0960  |
| H(7)  | 2.4281   | 0.8027   | -1.9815  |
| H(8)  | 3.7331   | -0.2170  | -1.3983  |
| H(9)  | 2.3612   | 0.9768   | 1.9025   |
| H(10) | 3.7682   | 0.8883   | 0.8558   |
| H(11) | 2.4447   | 1.9828   | 0.4906   |
| H(12) | 3.3635   | -1.7962  | 0.6809   |
| H(13) | 1.8985   | -1.6994  | 1.6438   |
| H(14) | 1.8395   | -2.4097  | 0.0612   |
| C(15) | -1.0126  | -0.1680  | 1.7540   |
| C(16) | -2.0574  | 0.9549   | 1.8877   |
| C(17) | -1.6750  | -1.5609  | 1.6702   |
| C(18) | -0.0924  | -0.1246  | 2.9837   |
| H(19) | -1.6473  | 1.9828   | 1.8719   |
| H(20) | -2.8282  | 0.9768   | 1.0937   |
| H(21) | -2.6252  | 0.8883   | 2.8354   |
| H(22) | -0.9727  | -2.4097  | 1.5625   |
| H(23) | -2.2714  | -1.7962  | 2.5725   |
| H(24) | -2.3728  | -1.6994  | 0.8223   |
| H(25) | -0.6556  | -0.2170  | 3.9321   |
| H(26) | 0.6727   | -0.9233  | 3.0268   |
| H(27) | 0.5020   | 0.8027   | 3.0936   |
| C(28) | -1.0127  | -0.1680  | -1.7540  |
| C(29) | -0.6061  | 0.9549   | -2.7256  |
| C(30) | -0.6090  | -1.5609  | -2.2857  |
| C(31) | -2.5378  | -0.1246  | -1.5719  |
| H(32) | -0.7975  | 1.9828   | -2.3625  |
| H(33) | 0.4670   | 0.9768   | -2.9961  |
| H(34) | -1.1430  | 0.8883   | -3.6912  |
| H(35) | -0.8668  | -2.4097  | -1.6237  |
| H(36) | -1.0921  | -1.7962  | -3.2534  |
| H(37) | 0.4743   | -1.6994  | -2.4660  |
| H(38) | -3.0775  | -0.2170  | -2.5338  |
| H(39) | -2.9576  | -0.9233  | -0.9308  |
| H(40) | -2.9301  | 0.8027   | -1.1120  |

**Table S11** Unrefined molecular-scattering intensity data for the longer nozzle-to-film distance.<sup>a</sup>

| <i>s</i> | intensity |
|----------|-----------|
| 2.0      | -52.309   |
| 2.2      | -7.486    |
| 2.4      | 12.824    |
| 2.6      | 23.196    |
| 2.8      | 1.372     |
| 3.0      | -45.348   |
| 3.2      | -92.906   |
| 3.4      | -122.162  |
| 3.6      | -119.344  |
| 3.8      | -113.777  |
| 4.0      | -104.920  |
| 4.2      | -100.676  |
| 4.4      | -92.732   |
| 4.6      | -69.950   |
| 4.8      | -21.180   |
| 5.0      | 33.125    |
| 5.2      | 82.019    |
| 5.4      | 108.452   |
| 5.6      | 93.099    |
| 5.8      | 50.817    |
| 6.0      | -2.806    |
| 6.2      | -31.257   |
| 6.4      | -24.997   |
| 6.6      | 5.268     |
| 6.8      | 36.435    |
| 7.0      | 44.986    |
| 7.2      | 36.789    |
| 7.4      | 20.643    |
| 7.6      | 2.000     |
| 7.8      | -10.878   |
| 8.0      | -11.480   |
| 8.2      | -4.195    |
| 8.4      | 15.422    |
| 8.6      | 37.120    |
| 8.8      | 51.799    |
| 9.0      | 57.716    |
| 9.2      | 52.126    |
| 9.4      | 37.100    |
| 9.6      | 16.940    |
| 9.8      | -10.000   |
| 10.0     | -31.886   |
| 10.2     | -51.012   |
| 10.4     | -59.015   |
| 10.6     | -58.609   |
| 10.8     | -53.773   |
| 11.0     | -51.172   |
| 11.2     | -57.236   |

|      |         |
|------|---------|
| 11.4 | -70.321 |
| 11.6 | -79.494 |
| 11.8 | -78.983 |
| 12.0 | -62.571 |
| 12.2 | -28.836 |
| 12.4 | 15.343  |
| 12.6 | 65.389  |
| 12.8 | 111.367 |
| 13.0 | 146.034 |
| 13.2 | 157.838 |
| 13.4 | 143.959 |
| 13.6 | 107.770 |
| 13.8 | 55.939  |
| 14.0 | 4.560   |
| 14.2 | -36.822 |
| 14.4 | -60.424 |
| 14.6 | -70.628 |
| 14.8 | -68.785 |
| 15.0 | -64.348 |

<sup>a</sup>  $s$  in  $\text{\AA}^{-1}$ . Intensity in arbitrary units.

**Table S12** Unrefined molecular-scattering intensity data for the shorter nozzle-to-film distance.<sup>a</sup>

| $s$  | intensity |
|------|-----------|
| 10.0 | -47.868   |
| 10.4 | -66.229   |
| 10.8 | -65.090   |
| 11.2 | -73.606   |
| 11.6 | -92.451   |
| 12.0 | -67.008   |
| 12.4 | 20.969    |
| 12.8 | 136.800   |
| 13.2 | 187.230   |
| 13.6 | 127.661   |
| 14.0 | 7.668     |
| 14.4 | -74.165   |
| 14.8 | -92.770   |
| 15.2 | -83.365   |
| 15.6 | -68.716   |
| 16.0 | -35.688   |
| 16.4 | 6.467     |
| 16.8 | 35.945    |
| 17.2 | 54.873    |
| 17.6 | 51.086    |
| 18.0 | 28.735    |
| 18.4 | 9.058     |
| 18.8 | -10.921   |
| 19.2 | -30.151   |
| 19.6 | -31.562   |
| 20.0 | -17.467   |

|      |         |
|------|---------|
| 20.4 | 1.407   |
| 20.8 | 11.876  |
| 21.2 | 17.786  |
| 21.6 | 13.496  |
| 22.0 | 7.848   |
| 22.4 | -3.492  |
| 22.8 | -10.951 |
| 23.2 | -14.546 |
| 23.6 | -22.482 |
| 24.0 | -17.916 |
| 24.4 | -5.710  |
| 24.8 | 16.355  |
| 25.2 | 32.973  |
| 25.6 | 36.170  |
| 26.0 | 22.512  |
| 26.4 | 2.253   |
| 26.8 | -25.266 |
| 27.2 | -35.721 |
| 27.6 | -30.977 |
| 28.0 | -13.184 |
| 28.4 | 3.934   |
| 28.8 | 17.526  |
| 29.2 | 19.622  |
| 29.6 | 12.336  |
| 30.0 | 7.192   |

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<sup>a</sup>  $s$  in  $\text{\AA}^{-1}$ . Intensity in arbitrary units.