SUPPLEMENTARY INFORMATION

Methyl Groups as Unconventional Lewis Bases in Chalcogen Bonding

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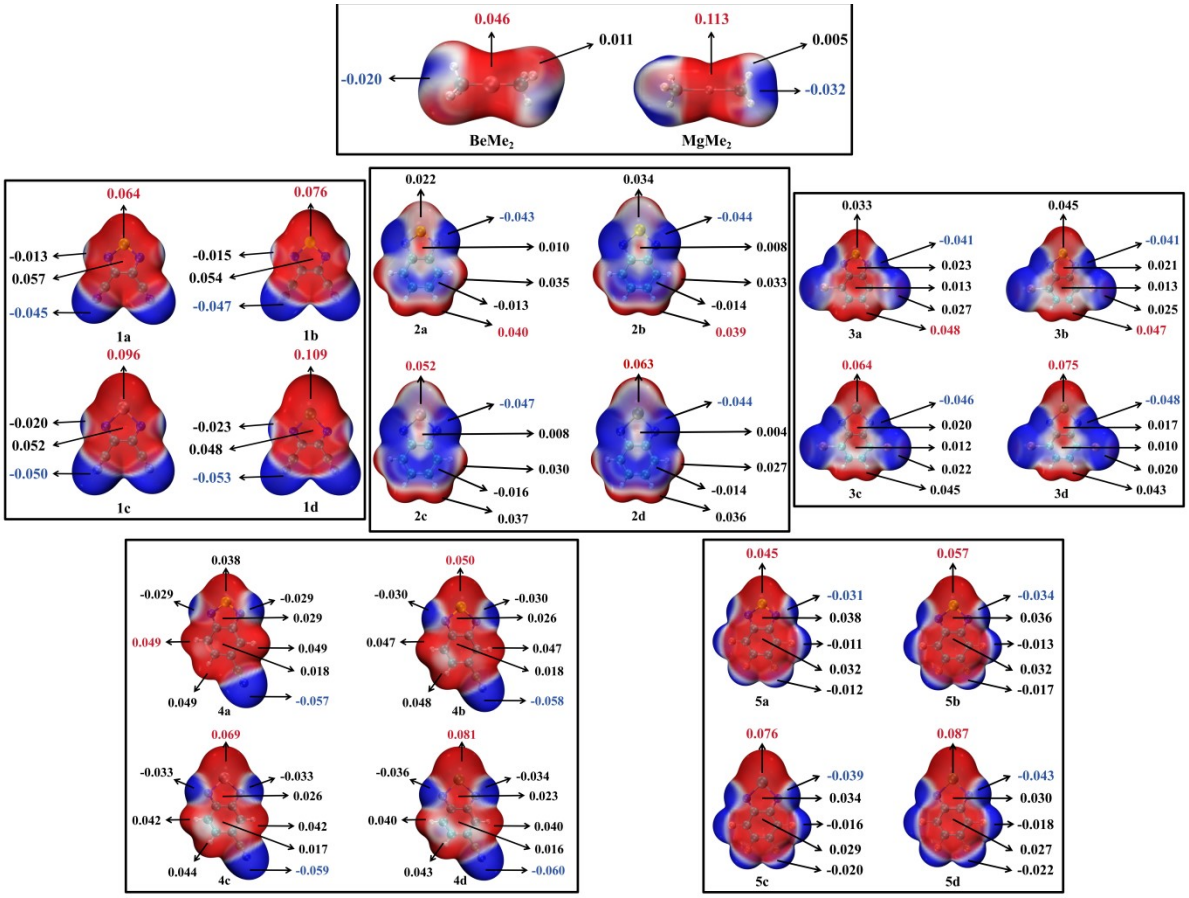

Fig. S1. Molecular electrostatic potentials (MEPs) of all monomers, calculated at the MP2/aug-cc-pVDZ level and mapped onto the 0.001 e Bohr^{-3} electron-density isosurface. Electron-rich regions (V_{min}) correspond to negative potential values, while electron-poor regions (V_{max}) correspond to positive values. The most positive MEP points are highlighted in red, and the most negative in blue. All potentials are reported in atomic units (a.u.).

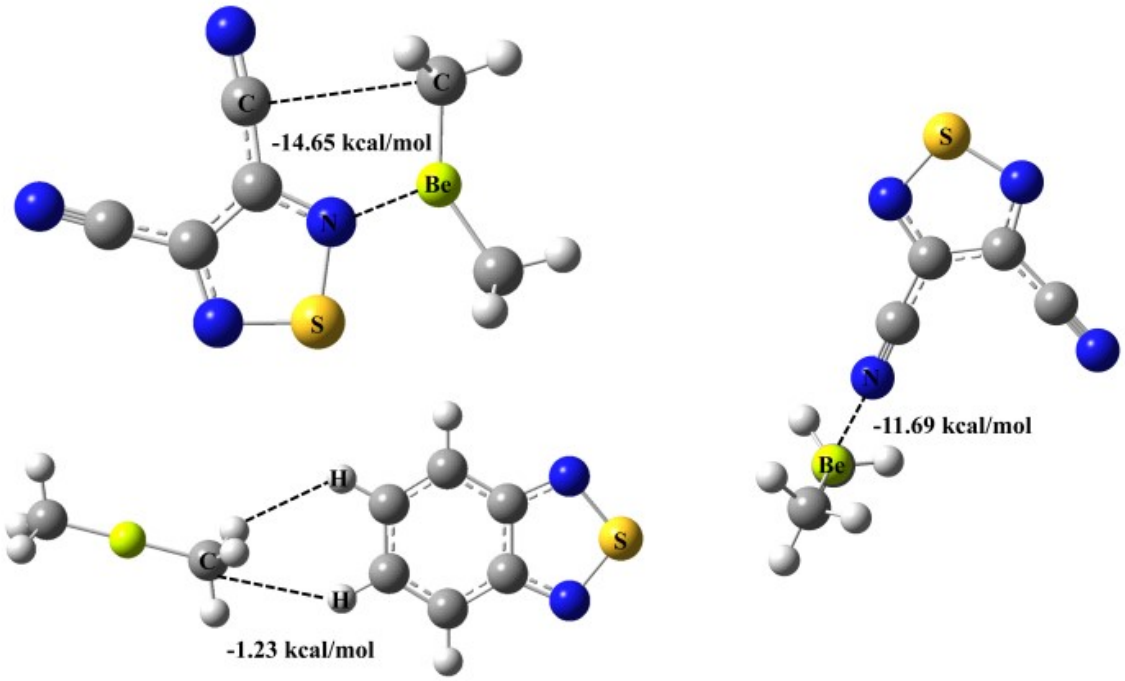

Fig. S2. Beryllium and hydrogen bonded complexes with interaction energies are shown.

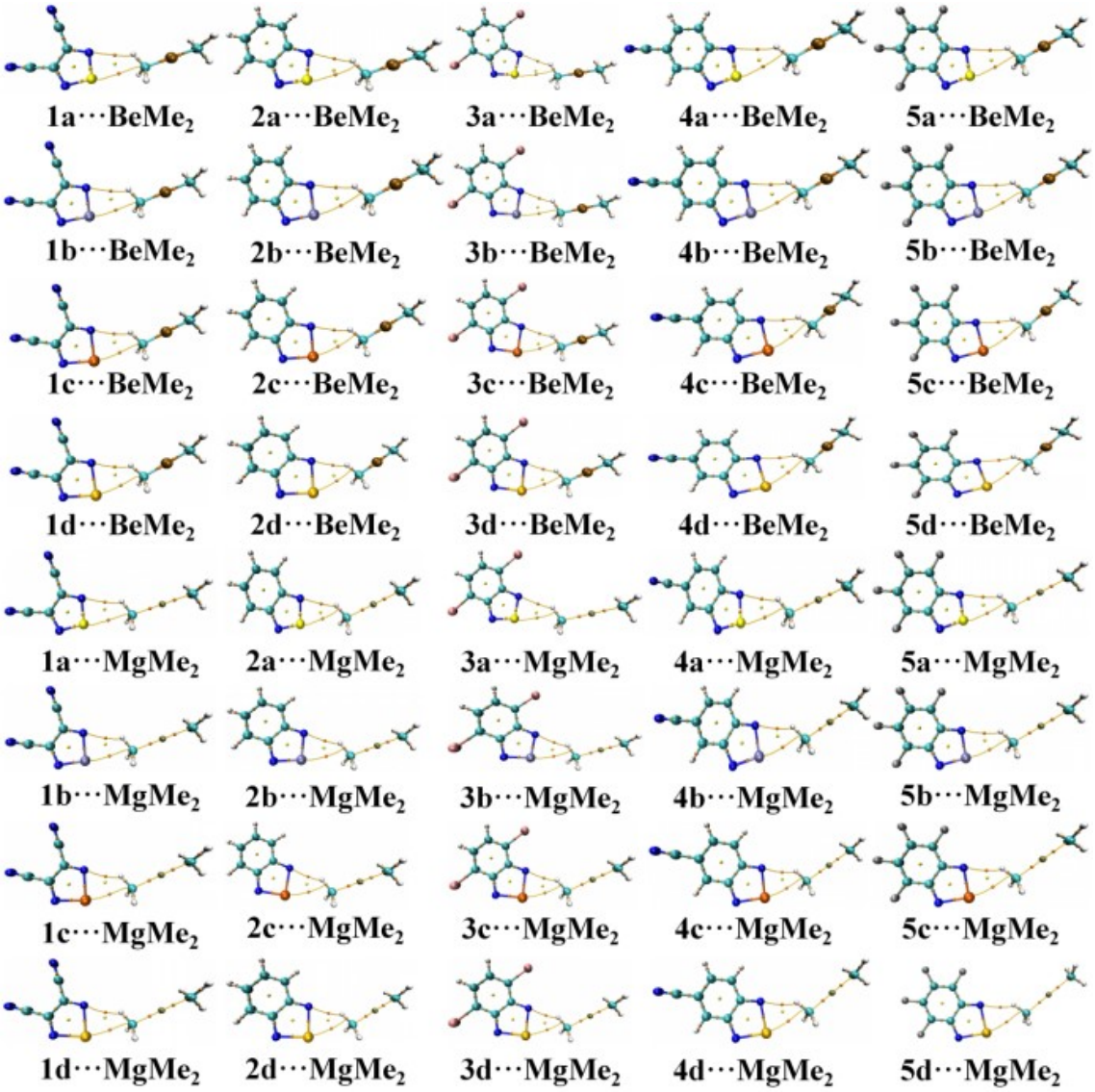

Fig. S3. AIM diagrams for all complexes.

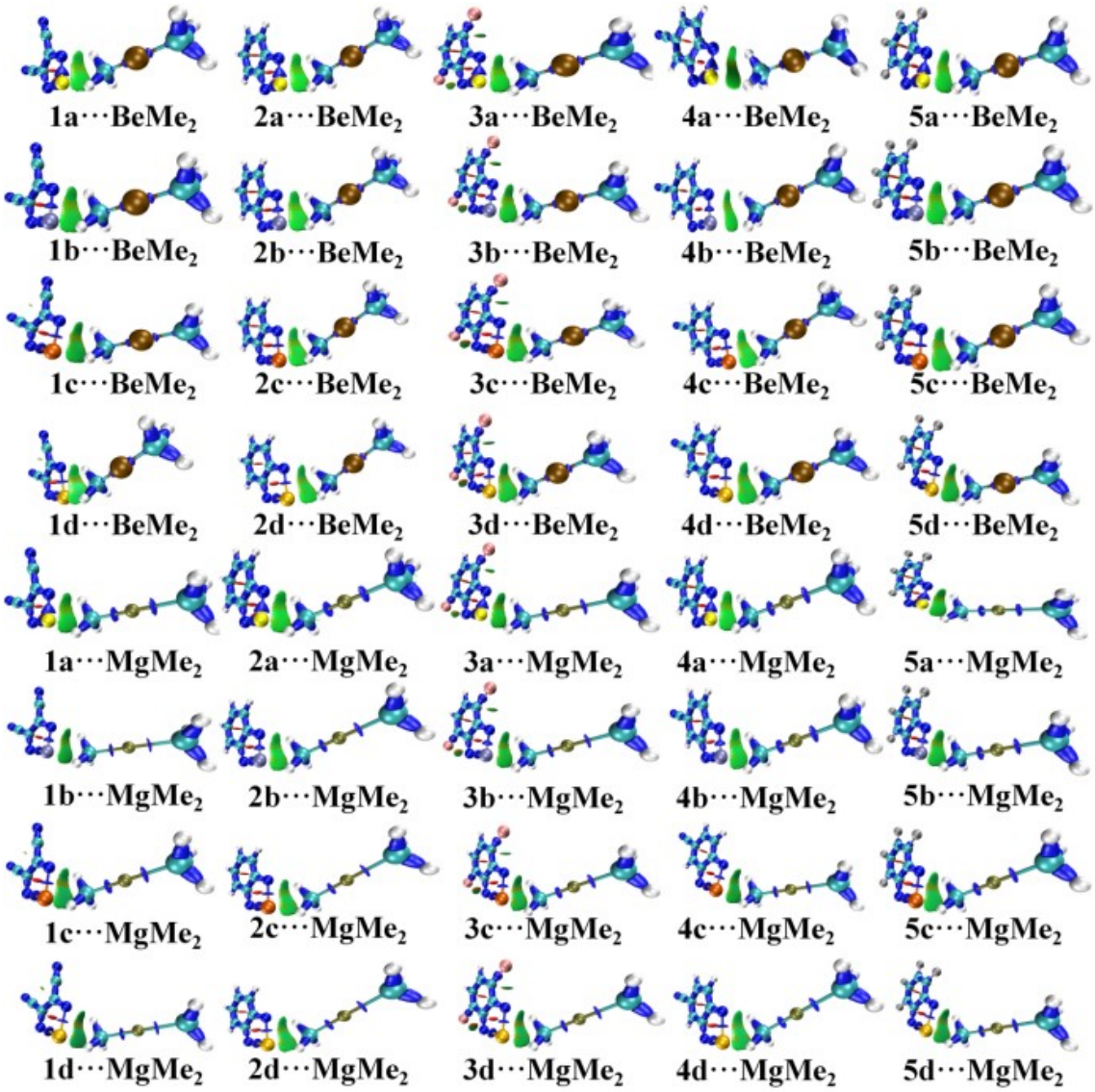

Fig. S4. NCI diagrams for all complexes. Blue indicates strong attractive interactions, red repulsive interactions, and green weak attractive interactions.

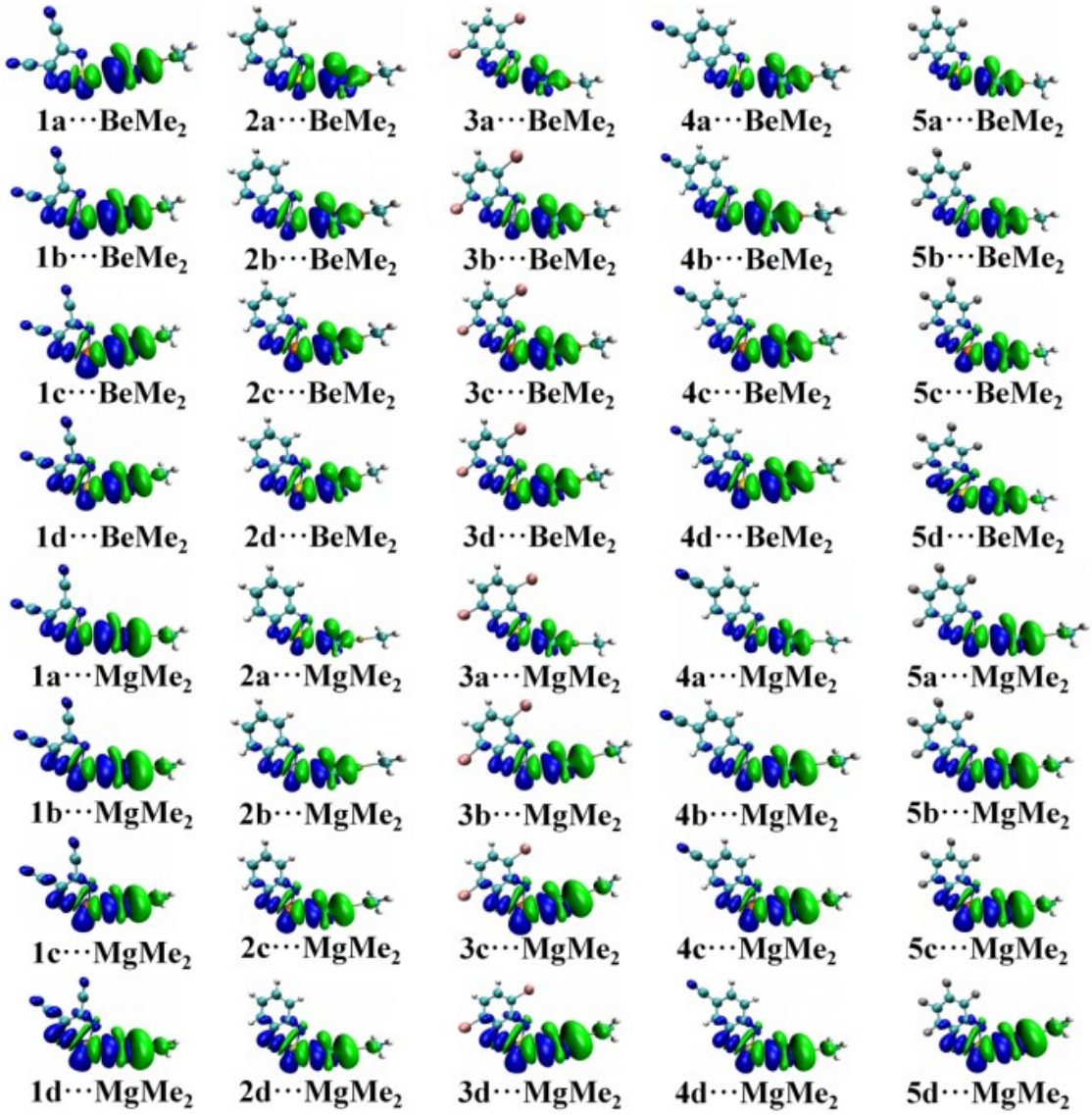

Fig. S5. NOCV diagrams for all complexes: the green electron cloud represents accepted electrons, while the blue electron cloud represents donated electrons.

Table S1. Condensed Fukui functions and derived local reactivity descriptors for electrophilic and nucleophilic attack at the most reactive site of each MMe_2, halcogenadiazoles, and benzochalcodiazoles

	$f^+(r)$	$f^-(r)$	$s^+(r)$	$h^+(r)$	$s^-(r)$	$h^-(r)$
$BeMe_2$	0.391	0.296	1.782	0.086	1.348	0.065
$MgMe_2$	0.412	0.306	2.328	0.073	1.728	0.054
1a	0.283	0.318	1.417	0.057	1.589	0.064
1b	0.325	0.435	1.724	0.061	2.310	0.082
1c	0.434	0.605	2.509	0.075	3.498	0.105
1d	0.511	0.682	3.015	0.086	4.026	0.115
2a	0.155	0.125	0.920	0.026	0.743	0.021
2b	0.228	0.177	1.412	0.037	1.097	0.029
2c	0.300	0.289	1.944	0.046	1.873	0.045
2d	0.336	0.346	2.209	0.051	2.271	0.053
3a	0.200	0.076	1.254	0.032	0.478	0.012
3b	0.244	0.118	1.591	0.037	0.768	0.018
3c	0.309	0.216	2.113	0.045	1.474	0.032
3d	0.339	0.268	2.346	0.049	1.855	0.039
4a	0.204	0.121	1.223	0.034	0.724	0.020
4b	0.260	0.172	1.621	0.042	1.075	0.028
4c	0.321	0.280	2.107	0.049	1.833	0.043
4d	0.351	0.332	2.351	0.052	2.227	0.050
5a	0.277	0.111	1.621	0.047	0.650	0.019
5b	0.309	0.163	1.892	0.051	0.998	0.027
5c	0.366	0.277	2.352	0.057	1.777	0.043
5d	0.398	0.332	2.593	0.061	2.163	0.051

Note: $f^+(r)$, $f^-(r)$: condensed Fukui functions for electrophilic and nucleophilic attack.

$s^+(r) = S \cdot f^+(r)$, $h^+(r) = \eta \cdot f^+(r)$: local softness and hardness for electrophilic attack.

$s^-(r) = S \cdot f^-(r)$, $h^-(r) = \eta \cdot f^-(r)$: local softness and hardness for nucleophilic attack.

All values in atomic units (au).

We evaluated the Fukui functions for all monomers to identify their most electrophilic ($f^-(r)$) and nucleophilic ($f^+(r)$) reactive sites. In the case of MMe_2, the maximum $f^+(r)$ value is localized on the M atom, indicating a strong electrophilic character, while the maximum $f^-(r)$ value resides on the carbon atoms of methyl groups, suggesting their role as electron donors.

In our dataset of 20 Lewis acids (1a-5d), the maxima of the condensed Fukui functions $f^+(r)$ and $f^-(r)$ are overwhelmingly located on the chalcogen atom, confirming its role as the primary site for electrophilic and nucleophilic attack. However, five exceptions follow. These findings

illustrate that in the MMe_2 Lewis bases the metal center functions chiefly as an electron acceptor, whereas the methyl-carbon sites serve as electron donors. For chalcogenadiazoles and benzochalcodiazoles, the chalcogen atom remains, in nearly every case, the locus of greatest susceptibility to nucleophilic attack.

Table S2. Computed global reactivity descriptors for the monomers in the gas phase at the MP2/aug-cc-pVDZ level of theory.

	I	A	η	S	ω^+	ω^-
$BeMe_2$	0.414	-0.025	0.220	4.555	0.016	0.210
$MgMe_2$	0.338	-0.016	0.177	5.648	0.015	0.176
1a	0.411	0.011	0.200	5.002	0.031	0.242
1b	0.396	0.019	0.188	5.309	0.034	0.241
1c	0.368	0.022	0.173	5.783	0.034	0.229
1d	0.355	0.016	0.169	5.904	0.030	0.215
2a	0.323	-0.015	0.169	5.924	0.014	0.168
2b	0.317	-0.006	0.162	6.183	0.017	0.173
2c	0.309	0.000	0.154	6.474	0.019	0.174
2d	0.302	-0.003	0.152	6.566	0.018	0.167
3a	0.325	0.006	0.160	6.269	0.023	0.188
3b	0.320	0.014	0.153	6.529	0.027	0.193
3c	0.313	0.020	0.146	6.831	0.030	0.196
3d	0.307	0.018	0.145	6.917	0.028	0.191
4a	0.346	0.012	0.167	5.983	0.027	0.207
4b	0.340	0.020	0.160	6.242	0.031	0.211
4c	0.330	0.025	0.152	6.557	0.034	0.212
4d	0.322	0.023	0.149	6.702	0.032	0.205
5a	0.355	0.013	0.171	5.856	0.029	0.213
5b	0.348	0.022	0.163	6.121	0.033	0.218
5c	0.339	0.027	0.156	6.424	0.036	0.219
5d	0.332	0.025	0.153	6.517	0.034	0.212

Note: Ionization potential (I), electron nucleophilic potential (A), Global hardness (η), softness (S), electron-accepting power (ω^+) and electron-donating power (ω^-) (all in a.u.) were derived from the HOMO and LUMO energies ($I = -\varepsilon_{HOMO}$; $A = -\varepsilon_{LUMO}$) according to $\eta = (I - A)/2$, $S = 1/\eta$, $\omega^+ = (I + 3A)^2/(16 (I - A))$ and $\omega^- = (3I + A)^2/(16 (I - A))$.

We have computed the ionization potential (I), electron nucleophilic potential (A), global hardness (η), softness (S), and the electron-accepting (ω^+) and electron-donating (ω^-) powers for each monomer.

In $BeMe_2$ and $MgMe_2$, the highest-occupied molecular orbital is concentrated on the methyl carbons, which serve as the electron-donating sites, whereas the lowest-unoccupied orbital is centered on the metal, reflecting its electron-accepting character. In the series of twenty chalcogenadiazoles and benzochalcodiazoles, the LUMO almost always resides on the chalcogen atom, confirming it as the primary electrophilic center. The sole exceptions occur when regions of maximum positive electrostatic potential override this trend, yet in every case the HOMO remains localized at the point of most negative electrostatic potential.

As one moves from lighter to heavier chalcogens, the calculated global hardness steadily declines and the corresponding softness rises. This continuous shift demonstrates that the interactions become increasingly governed by polarizability and orbital overlap, in other words they acquire a progressively “soft–soft” character as the chalcogen atom grows larger and is more polarizable.

Cartesian Coordinates of Monomers

$BeMe_2$

C	0.00000000	0.00000000	1.69373000
H	-0.51128600	0.88746000	2.10781600
H	-0.51291900	-0.88651700	2.10781600
H	1.02420600	-0.00094300	2.10781600
C	0.00000000	0.00000000	-1.69373000
H	0.51128600	0.88746000	-2.10781600
H	0.51291900	-0.88651700	-2.10781600
H	-1.02420600	-0.00094300	-2.10781600
Be	0.00000000	0.00000000	0.00000000

$MgMe_2$

Mg	0.00000000	0.00000000	0.00000000
C	0.00000000	0.00000000	2.11957900
H	-0.51173000	0.88832700	2.53308700
H	-0.51344900	-0.88733500	2.53308700
H	1.02517900	-0.00099200	2.53308700
C	0.00000000	0.00000000	-2.11957900
H	0.51173000	0.88832700	-2.53308700
H	0.51344900	-0.88733500	-2.53308700
H	-1.02517900	-0.00099200	-2.53308700

1a

C	0.14202700	0.71366200	0.00007800
C	0.14202700	-0.71366200	0.00004200
S	-2.16365900	0.00000000	0.00074700
C	1.31896000	1.53687200	0.00002900
C	1.31896000	-1.53687200	0.00000400
N	-1.09533100	1.27256700	-0.00082000
N	-1.09533100	-1.27256700	-0.00074800
N	2.31580900	2.18614700	-0.00014000
N	2.31580900	-2.18614700	-0.00013000

1b

C	-0.62712600	0.71717400	0.00002100
C	-0.62712600	-0.71717500	-0.00003100

C	-1.82855500	1.50913500	0.00002500
C	-1.82855500	-1.50913500	-0.00002100
N	0.58112500	1.32977600	-0.00010800
N	0.58112500	-1.32977600	-0.00004800
N	-2.84060800	2.13570900	0.00000000
N	-2.84060800	-2.13570900	-0.00000700
Se	1.79708600	0.00000000	0.00003400

1c

C	-1.01195800	0.72262700	-0.00000600
C	-1.01195800	-0.72262700	-0.00002200
C	-2.24382800	1.47451600	-0.00002400
C	-2.24382800	-1.47451600	-0.00003000
N	0.15691100	1.39789500	-0.00020000
N	0.15691100	-1.39789500	-0.00018400
N	-3.27354300	2.07233800	-0.00005000
N	-3.27354200	-2.07233800	-0.00004200
Te	1.59042900	0.00000000	0.00007300

1d

C	-1.43550300	0.72660100	-0.00003000
C	-1.43550300	-0.72660000	-0.00002400
C	-2.68072800	1.46022000	-0.00004200
C	-2.68072800	-1.46022000	-0.00003700
N	-0.29057300	1.42878600	-0.00021200
N	-0.29057300	-1.42878500	-0.00021100
N	-3.71647300	2.04776300	-0.00006400
N	-3.71647200	-2.04776400	-0.00006100
Po	1.25587400	0.00000000	0.00005500

2a

C	0.00000000	0.72181500	-0.02506100
C	0.00000000	-0.72181500	-0.02506100
C	0.00000000	-1.44597400	-1.24628400
C	0.00000000	-0.71368500	-2.43382700
C	0.00000000	0.71368500	-2.43382700
C	0.00000000	1.44597400	-1.24628400

N	0.00000000	-1.28578200	1.23453900
N	0.00000000	1.28578200	1.23453900
S	0.00000000	0.00000000	2.27753400
H	0.00000000	2.53896100	-1.24083700
H	0.00000000	1.24522100	-3.39017500
H	0.00000000	-1.24522100	-3.39017500
H	0.00000000	-2.53896100	-1.24083700

2b

C	0.00000000	0.72360600	-0.52988400
C	0.00000000	-0.72360600	-0.52988400
C	0.00000000	-1.44000800	-1.75853100
C	0.00000000	-0.71326300	-2.94854100
C	0.00000000	0.71326300	-2.94854100
C	0.00000000	1.44000800	-1.75853100
N	0.00000000	-1.34497000	0.70380400
N	0.00000000	1.34497000	0.70380400
H	0.00000000	2.53328400	-1.75062200
H	0.00000000	1.24812900	-3.90312000
H	0.00000000	-1.24812900	-3.90312000
H	0.00000000	-2.53328400	-1.75062200
Se	0.00000000	0.00000000	1.89110900

2c

C	0.00000000	0.72613500	-0.93001300
C	0.00000000	-0.72613500	-0.93001300
C	0.00000000	-1.43248500	-2.16846500
C	0.00000000	-0.71272000	-3.36175800
C	0.00000000	0.71272000	-3.36175800
C	0.00000000	1.43248500	-2.16846500
N	0.00000000	-1.41665600	0.27004600
N	0.00000000	1.41665600	0.27004600
H	0.00000000	2.52610200	-2.15739000
H	0.00000000	1.25153300	-4.31426800
H	0.00000000	-1.25153300	-4.31426800
H	0.00000000	-2.52610200	-2.15739000
Te	0.00000000	0.00000000	1.66702900

2d

C	0.00000000	0.72681100	-1.36754600
C	0.00000000	-0.72681100	-1.36754600
C	0.00000000	-1.42916700	-2.61075900
C	0.00000000	-0.71266500	-3.80519400
C	0.00000000	0.71266500	-3.80519400
C	0.00000000	1.42916700	-2.61075900
N	0.00000000	-1.44768700	-0.18807500
N	0.00000000	1.44768700	-0.18807500
H	0.00000000	2.52293300	-2.59841900
H	0.00000000	1.25334400	-4.75669900
H	0.00000000	-1.25334400	-4.75669900
H	0.00000000	-2.52293300	-2.59841900
Po	0.00000000	0.00000000	1.31839600

3a

C	0.00000000	0.72454900	0.59290400
C	0.00000000	-0.72454900	0.59290400
C	0.00000000	-1.43903900	-0.63329700
C	0.00000000	-0.71036800	-1.82460700
C	0.00000000	0.71036800	-1.82460700
C	0.00000000	1.43903900	-0.63329700
N	0.00000000	-1.28589900	1.84857800
N	0.00000000	1.28589900	1.84857800
H	0.00000000	1.24559900	-2.77788300
H	0.00000000	-1.24559900	-2.77788300
Br	0.00000000	3.32441500	-0.63127700
Br	0.00000000	-3.32441500	-0.63127700
S	0.00000000	0.00000000	2.89031800

3b

C	0.00000000	0.72709300	0.24318500
C	0.00000000	-0.72709300	0.24318500
C	0.00000000	-1.43317900	-0.99094400
C	0.00000000	-0.70944600	-2.18479900
C	0.00000000	0.70944600	-2.18479900

C	0.00000000	1.43317900	-0.99094400
N	0.00000000	-1.34458800	1.47384400
N	0.00000000	1.34458800	1.47384400
Se	0.00000000	0.00000000	2.65871500
H	0.00000000	1.24752000	-3.13657700
H	0.00000000	-1.24752000	-3.13657700
Br	0.00000000	3.31948400	-0.99380400
Br	0.00000000	-3.31948400	-0.99380400

3c

C	0.00000000	0.72964300	-0.07278900
C	0.00000000	-0.72964300	-0.07278900
C	0.00000000	-1.42576400	-1.31622200
C	0.00000000	-0.70794800	-2.51401000
C	0.00000000	0.70794800	-2.51401000
C	0.00000000	1.42576400	-1.31622200
N	0.00000000	-1.41562700	1.12726000
N	0.00000000	1.41562700	1.12726000
H	0.00000000	1.25000400	-3.46337600
H	0.00000000	-1.25000400	-3.46337600
Br	0.00000000	3.31468700	-1.32831200
Br	0.00000000	-3.31468700	-1.32831200
Te	0.00000000	0.00000000	2.51852200

3d

C	0.00000000	0.72918200	-0.49625100
C	0.00000000	-0.72918200	-0.49625100
C	0.00000000	-1.42147900	-1.74303800
C	0.00000000	-0.70705200	-2.94329100
C	0.00000000	0.70705200	-2.94329100
C	0.00000000	1.42147900	-1.74303800
N	0.00000000	-1.44718600	0.68693400
N	0.00000000	1.44718600	0.68693400
H	0.00000000	1.25131000	-3.89135100
H	0.00000000	-1.25131000	-3.89135100
Br	0.00000000	3.31151400	-1.75710400
Br	0.00000000	-3.31151400	-1.75710400

Po	0.00000000	0.00000000	2.18278400
4a			
C	-1.14379800	-0.11200700	0.00000000
C	0.00000000	0.76957500	0.00000000
C	1.31652900	0.24840700	0.00000000
C	1.45458000	-1.14631100	0.00000000
C	0.32262300	-2.02529300	0.00000000
C	-0.97528100	-1.52191900	0.00000000
H	2.18742800	0.90852200	0.00000000
H	0.49457800	-3.10491000	0.00000000
H	-1.84492300	-2.18361400	0.00000000
N	-0.32035800	2.11090500	0.00000000
N	-2.35703100	0.54064600	0.00000000
S	-1.97726900	2.15073200	0.00000000
C	2.77713600	-1.72588500	0.00000000
N	3.86146000	-2.21599400	0.00000000
4b			
C	-0.14566900	-0.92115200	0.00000000
C	0.00000000	0.51990100	0.00000000
C	1.28953900	1.10869400	0.00000000
C	2.40079000	0.25550200	0.00000000
C	2.26213800	-1.16979300	0.00000000
C	1.00265500	-1.76069200	0.00000000
H	1.40679700	2.19557200	0.00000000
H	3.16281900	-1.78960100	0.00000000
H	0.88310900	-2.84725900	0.00000000
N	-1.16372100	1.26304000	0.00000000
N	-1.43325700	-1.41336100	0.00000000
C	3.72872100	0.82146200	0.00000000
N	4.82907000	1.27496100	0.00000000
Se	-2.47960000	0.04250800	0.00000000
4c			
C	0.84737800	-0.50245300	0.00000000
C	0.00000000	0.67674300	0.00000000

C	0.58966200	1.96793800	0.00000000
C	1.98694600	2.07205900	0.00000000
C	2.82604800	0.91423400	0.00000000
C	2.26564200	-0.35873700	0.00000000
H	-0.04401900	2.85894500	0.00000000
H	3.91191900	1.04140800	0.00000000
H	2.89220000	-1.25479400	0.00000000
N	-1.37988300	0.53789600	0.00000000
N	0.27557500	-1.76180000	0.00000000
C	2.60172100	3.37758600	0.00000000
N	3.12156200	4.44841200	0.00000000
Te	-1.68433200	-1.42502600	0.00000000

4d

C	1.22077000	0.29748300	0.00000000
C	0.00000000	1.08199200	0.00000000
C	0.07945000	2.49985300	0.00000000
C	1.33937300	3.11332500	0.00000000
C	2.54449000	2.34606800	0.00000000
C	2.48640000	0.95651000	0.00000000
H	-0.83786900	3.09499400	0.00000000
H	3.50876100	2.86124400	0.00000000
H	3.39704600	0.35111700	0.00000000
N	-1.25003200	0.47791200	0.00000000
N	1.18822100	-1.08574400	0.00000000
C	1.42866600	4.55335400	0.00000000
N	1.51643700	5.74054100	0.00000000
Po	-0.84339600	-1.56342700	0.00000000

5a

C	0.00000000	0.72341400	0.75007500
C	0.00000000	-0.72341400	0.75007500
C	0.00000000	-1.43633500	-0.47355800
C	0.00000000	-0.71189500	-1.65780000
C	0.00000000	0.71189500	-1.65780000
C	0.00000000	1.43633500	-0.47355800
F	0.00000000	-1.34507700	-2.84635900

N	0.00000000	-1.28580600	2.00182900
N	0.00000000	1.28580600	2.00182900
S	0.00000000	0.00000000	3.04658500
F	0.00000000	-2.78200900	-0.49783900
F	0.00000000	1.34507700	-2.84635900
F	0.00000000	2.78200900	-0.49783900

5b

C	0.00000000	0.72574000	0.26666300
C	0.00000000	-0.72574000	0.26666300
C	0.00000000	-1.43148400	-0.96402100
C	0.00000000	-0.71123900	-2.15015300
C	0.00000000	0.71123900	-2.15015300
C	0.00000000	1.43148400	-0.96402100
F	0.00000000	-1.34650400	-3.33812500
N	0.00000000	-1.34490300	1.49252700
N	0.00000000	1.34490300	1.49252700
F	0.00000000	-2.77784300	-0.98916900
F	0.00000000	1.34650400	-3.33812500
F	0.00000000	2.77784300	-0.98916900
Se	0.00000000	0.00000000	2.68135500

5c

C	0.00000000	0.72827500	-0.14121200
C	0.00000000	-0.72827500	-0.14121200
C	0.00000000	-1.42467000	-1.38054600
C	0.00000000	-0.71006400	-2.56981500
C	0.00000000	0.71006400	-2.56981500
C	0.00000000	1.42467000	-1.38054600
F	0.00000000	-1.34957600	-3.75661000
N	0.00000000	-1.41563000	1.05265000
N	0.00000000	1.41563000	1.05265000
F	0.00000000	-2.77229900	-1.40868300
F	0.00000000	1.34957600	-3.75661000
F	0.00000000	2.77229900	-1.40868300
Te	0.00000000	0.00000000	2.44878900

5d

C	0.00000000	0.72796700	-0.64219900
C	0.00000000	-0.72796700	-0.64219900
C	0.00000000	-1.42132100	-1.88462100
C	0.00000000	-0.70927600	-3.07546600
C	0.00000000	0.70927600	-3.07546600
C	0.00000000	1.42132100	-1.88462100
F	0.00000000	-1.35079900	-4.26188900
N	0.00000000	-1.44726100	0.53412500
N	0.00000000	1.44726100	0.53412500
F	0.00000000	-2.76961800	-1.91356600
F	0.00000000	1.35079900	-4.26188900
F	0.00000000	2.76961800	-1.91356600
Po	0.00000000	0.00000000	2.03461800

Cartesian Coordinates of Dimers

1a···$BeMe_2$

C	-6.61099400	0.66259800	0.00102200
H	-6.82128500	1.28682100	-0.88582100
H	-7.35632800	-0.15276600	0.00117700
H	-6.82147900	1.28740800	0.88737100
C	-3.43440300	-0.51581000	0.00045900
H	-2.70211500	0.31113200	0.00017400
H	-3.23322300	-1.13848400	0.89103800
H	-3.23365700	-1.13876500	-0.89001600
Be	-5.02561000	0.07518300	0.00085000
C	1.33978800	0.64351900	-0.00056400
C	2.14994200	-0.53106500	0.00021900
S	-0.15776800	-1.25337900	-0.00130400
C	1.83941500	1.99016200	-0.00045000
C	3.58641100	-0.54148700	0.00126700
N	0.00347000	0.40297200	-0.00147100
N	1.44513300	-1.69099400	-0.00009400
N	2.28604100	3.09304800	-0.00034000
N	4.77590900	-0.51209900	0.00216600

1b···$BeMe_2$

C	-6.53533900	1.00870900	0.00115500
H	-6.72929900	1.63218600	-0.88985700
H	-7.30465900	0.21604200	0.00971500
H	-6.72415000	1.64631500	0.88323400
C	-3.39558700	-0.26550500	0.00239200
H	-2.64294100	0.54329900	0.00093300
H	-3.21862800	-0.89160600	0.89582900
H	-3.21927900	-0.89426300	-0.88931700
Be	-4.96899100	0.37496500	0.00177700
C	1.36402000	0.85227200	-0.00089200
C	2.20204400	-0.31023600	0.00071800
C	1.87294100	2.19836100	-0.00100300
C	3.64021800	-0.25065900	0.00245100
N	0.02486000	0.64525900	-0.00237100
N	1.57521300	-1.51062100	0.00060600
N	2.32250200	3.30047500	-0.00104000
N	4.82754800	-0.16799900	0.00384800
Se	-0.18899200	-1.14762600	-0.00158400

1c···$BeMe_2$

C	-6.36842400	1.47794700	-0.00028800
H	-6.50536800	2.12109700	-0.88782300
H	-7.20251700	0.75377700	0.00137700
H	-6.50439400	2.12405400	0.88524300
C	-3.34858400	-0.06121100	0.00027200
H	-2.54063500	0.69275500	-0.00151800
H	-3.23372800	-0.69661500	0.89717400
H	-3.23505800	-0.69954700	-0.89472100
Be	-4.86276000	0.71382900	0.00019100
C	1.35783000	1.05069800	0.00007400
C	2.27442300	-0.06670100	-0.00000100
C	1.83038100	2.41430500	0.00005500
C	3.70424300	0.13492800	-0.00011200
N	0.02594200	0.83315600	0.00009600
N	1.79183900	-1.32544100	-0.00007300
N	2.23924400	3.53272200	0.00008100
N	4.87983100	0.32370700	-0.00016900

Te	-0.20354700	-1.16153200	-0.00000100

1d···$BeMe_2$

C	-6.21357000	1.93213800	0.00019900
H	-6.31657200	2.58237500	-0.88671500
H	-7.08402800	1.25216600	0.00104300
H	-6.31573600	2.58350900	0.88637800
C	-3.27731800	0.23862000	0.00006600
H	-2.43743000	0.95711700	-0.00075200
H	-3.19895400	-0.40017900	0.89837400
H	-3.19964700	-0.40146000	-0.89738900
Be	-4.75003700	1.09153200	0.00002400
C	1.42684400	1.29653900	-0.00008500
C	2.34679000	0.16977000	0.00008400
C	1.92454200	2.65341100	-0.00013000
C	3.77596300	0.39355300	0.00021500
N	0.09694300	1.11779100	-0.00018400
N	1.89649800	-1.09218900	0.00013400
N	2.34882100	3.76621700	-0.00016700
N	4.94968400	0.59395800	0.00031300
Po	-0.20703100	-0.97314600	-0.00004500

2a···$BeMe_2$

C	6.61753000	1.08692300	0.00036600
H	6.73971300	1.73470800	0.88692400
H	7.46861400	0.38252100	0.00053200
H	6.73980500	1.73440900	-0.88639700
C	3.63316700	-0.51480000	0.00050200
H	2.79198200	0.20124700	0.00040500
H	3.51123900	-1.16089300	-0.88779300
H	3.51119300	-1.16071300	0.88892200
Be	5.12633200	0.28470900	0.00046300
C	-1.23013500	0.52259800	-0.00048900
C	-2.03535800	-0.67511100	0.00020800
C	-3.45287400	-0.59480400	0.00086000
C	-4.03007900	0.67550600	0.00077900
C	-3.23374900	1.86019400	0.00008100

C	-1.83958800	1.80500100	-0.00054700
H	-4.05794600	-1.50504900	0.00139000
H	-3.73091400	2.83488700	0.00003100
H	-1.22536500	2.70914800	-0.00108800
N	-1.30239400	-1.84374800	0.00017900
N	0.12962800	0.28959300	-0.00106900
S	0.28140800	-1.36193700	-0.00064700
H	-5.12028800	0.76792900	0.00125200

2b···$BeMe_2$

C	6.52874500	1.42271200	0.00039500
H	6.63667900	2.08459300	0.87829900
H	7.38841500	0.72904900	0.01631600
H	6.64880800	2.05892300	-0.89474500
C	3.56405700	-0.21568500	0.00389300
H	2.71854200	0.49566000	-0.01184900
H	3.45876500	-0.87460700	-0.87715500
H	3.44675400	-0.84844600	0.90244000
Be	5.04816900	0.60290800	0.00214300
C	-1.28973100	0.74526300	-0.00160000
C	-2.11055300	-0.44627000	0.00111600
C	-3.52853900	-0.33872700	0.00329100
C	-4.09631500	0.93516600	0.00272600
C	-3.28716000	2.10991000	0.00004400
C	-1.89470400	2.03247800	-0.00210600
H	-4.14247000	-1.24341600	0.00534000
H	-3.76981300	3.09198500	-0.00031500
H	-1.26782300	2.92825900	-0.00415700
N	-1.44309300	-1.65528900	0.00138000
N	0.07872900	0.55896800	-0.00351500
H	-5.18586700	1.03634800	0.00436300
Se	0.29738500	-1.22543600	-0.00172700

2c···$BeMe_2$

C	6.31814300	1.91460500	-0.00126500
H	6.37192100	2.57520300	0.88251500
H	7.23634000	1.30038400	0.00302500

H	6.37498700	2.56739800	-0.89063300
C	3.51198300	0.01650400	0.00254500
H	2.61361900	0.66067600	-0.00118900
H	3.46461300	-0.63764100	-0.88708200
H	3.46238500	-0.63014900	0.89755800
Be	4.91727700	0.96656700	0.00051400
C	-1.30102900	0.94681300	-0.00007500
C	-2.20317700	-0.19109500	-0.00002800
C	-3.61189000	0.02611100	0.00009000
C	-4.09969300	1.33196200	0.00018900
C	-3.21424800	2.44893800	0.00014600
C	-1.83194700	2.27005100	0.00002000
H	-4.28304700	-0.83749600	0.00012200
H	-3.62571400	3.46306900	0.00023300
H	-1.14360200	3.12002500	-0.00001300
N	-1.68547000	-1.47494600	-0.00012100
N	0.06793800	0.74377000	-0.00017200
H	-5.18085100	1.50180700	0.00029200
Te	0.28757900	-1.23874300	-0.00028000

2d···$BeMe_2$

C	6.13415000	2.38805000	-0.00231500
H	6.15918600	3.04966700	0.88195000
H	7.07946500	1.81647400	-0.00030200
H	6.15918500	3.04343200	-0.89120900
C	3.41758800	0.36361200	0.00482400
H	2.49488800	0.97278900	0.00271900
H	3.40038100	-0.28954300	-0.88662000
H	3.40011400	-0.28323800	0.90083300
Be	4.77850300	1.37725700	0.00128000
C	-1.39303400	1.19783100	-0.00013600
C	-2.28957300	0.05409700	0.00008000
C	-3.70092400	0.27047000	0.00034500
C	-4.19822900	1.57177000	0.00039200
C	-3.31887500	2.69381800	0.00017200
C	-1.93709300	2.51858400	-0.00009300
H	-4.36641000	-0.59766500	0.00051300

H	-3.73400600	3.70647500	0.00021800
H	-1.25177300	3.37120200	-0.00025900
N	-1.79929000	-1.23826600	-0.00002500
N	-0.02086200	1.03857700	-0.00035500
H	-5.28059700	1.73409100	0.00061000
Po	0.27717300	-1.03552700	-0.00036300

3a···$BeMe_2$

C	-7.59768300	-1.59915000	-0.00051300
H	-7.92416600	-1.02853100	-0.88837700
H	-8.17160500	-2.54311000	0.00072400
H	-7.92544300	-1.02541400	0.88486500
C	-4.25317700	-2.13549800	0.00309900
H	-3.69717000	-1.18095100	0.00221900
H	-3.92863000	-2.70385100	0.89364400
H	-3.92678800	-2.70667700	-0.88495900
Be	-5.92664500	-1.86883400	0.00098700
C	0.01054700	0.27764100	-0.00053000
C	1.15081600	-0.61547500	-0.00045200
C	2.46914600	-0.08998500	0.00020400
C	2.63009500	1.29736200	0.00073700
C	1.51137800	2.17356600	0.00063900
C	0.20374800	1.68339300	0.00001300
N	0.81536900	-1.94856000	-0.00102000
N	-1.20590200	-0.36231700	-0.00117400
S	-0.83966900	-1.97908000	-0.00161500
H	1.67736200	3.25419300	0.00106500
H	3.63937400	1.71770700	0.00124200
Br	-1.28400800	2.84263700	-0.00012300
Br	3.95209000	-1.25457300	0.00034200

3b···$BeMe_2$

C	-7.53642400	-1.07384500	0.00490200
H	-7.83572100	-0.48879200	-0.88309200
H	-8.15655500	-1.98806500	0.00864700
H	-7.83315500	-0.48326600	0.89009400
C	-4.22261900	-1.77681700	0.00231500

H	-3.62568300	-0.84689000	-0.00138100
H	-3.92874300	-2.35881300	0.89481200
H	-3.93127200	-2.36450800	-0.88727400
Be	-5.88175700	-1.42582200	0.00360200
C	0.11305100	0.46676100	-0.00109500
C	1.24555500	-0.44344600	-0.00047300
C	2.56843900	0.07692300	0.00118700
C	2.75202400	1.46135700	0.00212300
C	1.64600000	2.35024200	0.00148600
C	0.33452100	1.87086500	-0.00011000
N	0.95131800	-1.78843700	-0.00154100
N	-1.14018900	-0.10320900	-0.00262600
H	1.82179200	3.42927000	0.00225200
H	3.76781000	1.86568800	0.00337800
Br	-1.13672400	3.05361300	-0.00094500
Br	4.04155000	-1.10259900	0.00203200
Se	-0.83828100	-1.87345800	-0.00331500

3c···$BeMe_2$

C	-7.36784600	-0.38588500	0.00109700
H	-7.59116300	0.23432000	-0.88532400
H	-8.09554800	-1.21699200	0.00107700
H	-7.59089200	0.23403900	0.88778300
C	-4.16555400	-1.49288700	0.00042400
H	-3.47144200	-0.63249800	0.00010700
H	-3.95240900	-2.10724500	0.89419300
H	-3.95285400	-2.10758600	-0.89321000
Be	-5.76985900	-0.93794500	0.00075800
C	0.18933700	0.61147900	-0.00016700
C	1.36236500	-0.25649600	-0.00001400
C	2.66005300	0.33159800	0.00023400
C	2.79451700	1.72194400	0.00032600
C	1.65609300	2.56410300	0.00017400
C	0.36788900	2.02488400	-0.00006300
N	1.19270700	-1.62724700	-0.00011000
N	-1.07516200	0.05637300	-0.00039600
H	1.78388100	3.64983500	0.00025000

H	3.79487600	2.16305700	0.00051300
Br	-1.14681200	3.15589900	-0.00025900
Br	4.18738700	-0.78085100	0.00043900
Te	-0.77055900	-1.90977200	-0.00044700

3d···$BeMe_2$

C	-7.19132500	0.40143100	0.00220500
H	-7.35886900	1.03933300	-0.88392000
H	-7.98950200	-0.36220300	0.00190200
H	-7.35852300	1.03826400	0.88916600
C	-4.09876800	-0.98317900	0.00083100
H	-3.33783300	-0.18098000	0.00058100
H	-3.94216400	-1.61249700	0.89589300
H	-3.94288500	-1.61240200	-0.89442300
Be	-5.64860700	-0.28887700	0.00149900
C	0.34835300	0.87522400	-0.00023300
C	1.48623800	-0.03811000	0.00009600
C	2.80463900	0.50503100	0.00045400
C	2.99665600	1.88894000	0.00052000
C	1.89345500	2.77409200	0.00020900
C	0.58657600	2.28104200	-0.00014100
N	1.29770200	-1.40764900	0.00003100
N	-0.95036900	0.40249100	-0.00058500
H	2.06098700	3.85435600	0.00026100
H	4.01429600	2.28856900	0.00079500
Br	-0.88268900	3.47258800	-0.00055100
Br	4.29024200	-0.66449400	0.00086500
Po	-0.76430600	-1.67584500	-0.00056000

4a···$BeMe_2$

C	-7.33035100	-1.24547500	0.00042800
H	-7.44948500	-1.89255700	0.88787200
H	-8.18521500	-0.54572600	-0.00081500
H	-7.44875600	-1.89483400	-0.88544300
C	-4.35456100	0.37282600	-0.00020000
H	-3.50963500	-0.33879000	0.00027500
H	-4.23840000	1.01871500	-0.88940000

H	-4.23859300	1.01969700	0.88831100
Be	-5.84469600	-0.43510700	0.00008400
C	0.55011900	-0.41486200	-0.00004200
C	1.28004300	0.83075300	-0.00007800
C	2.69602800	0.84101800	-0.00002000
C	3.34697800	-0.40024300	0.00007800
C	2.62700500	-1.63947700	0.00012500
C	1.23497300	-1.65883000	0.00006200
H	3.25592800	1.77948100	-0.00006600
H	3.19109300	-2.57595100	0.00021300
H	0.67688800	-2.59835600	0.00011000
N	0.47821700	1.95183700	-0.00023300
N	-0.81897400	-0.26628200	-0.00005000
C	4.79033600	-0.44193800	0.00013300
N	5.97917500	-0.48965300	0.00018300
S	-1.07421200	1.37092500	-0.00022600

4b···$BeMe_2$

C	-7.08814000	1.69553600	-0.00035900
H	-7.18355000	2.34381100	-0.88975700
H	-7.96971800	1.02984000	0.00501700
H	-7.17886800	2.35201500	0.88347400
C	-4.17771400	-0.03815400	-0.00083600
H	-3.30924500	0.64503100	-0.00278700
H	-4.08978200	-0.68555800	0.89060500
H	-4.09169700	-0.68828600	-0.89047800
Be	-5.63591500	0.82853500	-0.00050700
C	0.72815100	0.59524800	0.00044500
C	1.45615700	-0.65568200	-0.00009400
C	2.87375800	-0.65850300	-0.00046700
C	3.53296700	0.57802100	-0.00020500
C	2.81756300	1.81837100	0.00041200
C	1.42608200	1.83471000	0.00075900
H	3.43007400	-1.59940300	-0.00090900
H	3.38109100	2.75521500	0.00064300
H	0.86782200	2.77447000	0.00122400
N	0.70003000	-1.81080200	-0.00018200

N	-0.64805800	0.51327200	0.00080400
C	4.97622700	0.61165600	-0.00055700
N	6.16546500	0.65374700	-0.00084600
Se	-1.00308300	-1.24770600	0.00035200

4c···$BeMe_2$

C	6.69628600	2.38386300	0.00005200
H	6.70786200	3.04254400	0.88677100
H	7.65339600	1.83231500	-0.00023200
H	6.70756400	3.04294100	-0.88637800
C	4.02306300	0.30188200	-0.00004000
H	3.08278700	0.88294000	0.00001300
H	4.02258600	-0.34930200	-0.89312900
H	4.02259400	-0.34947000	0.89292500
Be	5.36298200	1.34479100	0.00004500
C	-0.86193200	0.72442900	-0.00001800
C	-1.62762000	-0.50953700	0.00001500
C	-3.04627900	-0.45669100	0.00002500
C	-3.67617600	0.79495400	0.00000500
C	-2.92719200	2.01305100	-0.00002800
C	-1.53651600	1.98036100	-0.00004100
H	-3.62792300	-1.38252900	0.00005200
H	-3.45960100	2.96799200	-0.00004100
H	-0.94796300	2.90192900	-0.00006500
N	-0.96623600	-1.72718600	0.00003800
N	0.51955100	0.67864000	-0.00003000
C	-5.11774500	0.86467500	0.00002000
N	-6.30579000	0.93638300	0.00003200
Te	0.96343800	-1.26471800	-0.00000600

4d···$BeMe_2$

C	6.31399800	2.97439400	0.00011500
H	6.27996500	3.63211100	0.88692500
H	7.30690500	2.49025000	-0.00028700
H	6.27954400	3.63271600	-0.88623100
C	3.79174800	0.71165500	-0.00003800
H	2.81686700	1.23297700	0.00002800

H	3.83752400	0.06397900	-0.89447000
H	3.83759300	0.06388100	0.89432100
Be	5.05649700	1.84554900	-0.00000100
C	-1.09240700	0.93770400	-0.00003900
C	-1.82552300	-0.31567900	0.00003900
C	-3.24606200	-0.29253700	0.00006000
C	-3.91029200	0.94108900	0.00001000
C	-3.19395000	2.17756400	-0.00006900
C	-1.80319800	2.17548000	-0.00009600
H	-3.80342000	-1.23330900	0.00012400
H	-3.74859700	3.11972400	-0.00010200
H	-1.23606200	3.11058800	-0.00015500
N	-1.16398000	-1.53403800	0.00009500
N	0.28936600	0.96321100	-0.00006900
C	-5.35311400	0.97175000	0.00004600
N	-6.54269600	1.01170100	0.00007100
Po	0.85759100	-1.05083000	-0.00001200

5a···$BeMe_2$

C	-7.55515000	1.09717900	0.01226600
H	-7.67938500	1.74249200	-0.87575400
H	-8.41009800	0.39758900	0.02032600
H	-7.66774800	1.74859500	0.89740000
C	-4.58029000	-0.52317300	-0.00073400
H	-3.73661400	0.18980900	-0.00433200
H	-4.46228400	-1.16911800	0.88816900
H	-4.47004500	-1.16905400	-0.89068400
Be	-6.06941700	0.28768700	0.00571000
C	0.30052400	0.19559500	-0.00517400
C	1.01462400	-1.06205200	-0.00082500
C	2.43082700	-1.07744400	0.00407600
C	3.10295500	0.13738300	0.00470700
C	2.39987800	1.37556400	0.00040900
C	1.01235000	1.41978800	-0.00440800
F	4.44930100	0.17372400	0.00932300
N	0.20130300	-2.16638700	-0.00204500
N	-1.06537900	0.06923700	-0.00963000

S	-1.34373200	-1.56702800	-0.00821000
F	3.11708700	-2.23553300	0.00816500
F	3.12062200	2.51347200	0.00124500
F	0.36829800	2.60215900	-0.00837600

5b···$BeMe_2$

C	-7.27795200	1.63033400	0.00397100
H	-7.36406800	2.28132000	-0.88437400
H	-8.16859700	0.97681900	0.00830000
H	-7.35941600	2.28673000	0.88876500
C	-4.39287600	-0.14562100	0.00185400
H	-3.51683000	0.52776000	-0.00218500
H	-4.31461600	-0.79212400	0.89485300
H	-4.31903700	-0.79731200	-0.88774400
Be	-5.83770400	0.74425900	0.00287500
C	0.48825800	0.36869000	-0.00163800
C	1.18901200	-0.90120700	0.00018000
C	2.60738500	-0.92349700	0.00192500
C	3.29801000	0.28041100	0.00181200
C	2.61078400	1.52568800	0.00001700
C	1.22414800	1.58124000	-0.00170000
F	4.64537200	0.29763300	0.00341700
N	0.41033300	-2.03214100	0.00009800
N	-0.88438700	0.32153000	-0.00320500
F	3.28141200	-2.08990200	0.00363800
F	3.34304100	2.65708900	0.00001900
F	0.59445300	2.77244900	-0.00337800
Se	-1.28080400	-1.43287100	-0.00232700

5c···$BeMe_2$

C	-6.82015400	2.37466900	0.00020300
H	-6.81161800	3.03231200	-0.88729500
H	-7.79387900	1.85303500	0.00198800
H	-6.80977500	3.03494200	0.88572700
C	-4.21397300	0.20884700	0.00070900
H	-3.25930100	0.76595200	-0.00078800
H	-4.23468300	-0.43947900	0.89560300

H	-4.23622900	-0.44182600	-0.89244200
Be	-5.51937500	1.29584900	0.00045500
C	0.63967700	0.49369600	-0.00018300
C	1.37041700	-0.76614300	0.00004000
C	2.79174000	-0.74531500	0.00024200
C	3.46160300	0.47015300	0.00019900
C	2.74934200	1.69854000	-0.00002300
C	1.36193700	1.71781600	-0.00022100
F	4.80937200	0.51259900	0.00038100
N	0.67598100	-1.95467900	0.00005900
N	-0.73721200	0.49155900	-0.00035800
F	3.49454000	-1.89617000	0.00045700
F	3.45452600	2.84839500	-0.00004300
F	0.70919500	2.89828000	-0.00043100
Te	-1.24232000	-1.43707700	-0.00022300

5d···$BeMe_2$

C	-6.33125500	3.11632300	0.00045200
H	-6.26117600	3.76953800	-0.88755400
H	-7.34980800	2.68886300	0.00331100
H	-6.25775200	3.77324700	0.88543900
C	-3.94046700	0.71459700	0.00084000
H	-2.94089700	1.18683600	-0.00156900
H	-4.02329600	0.07400500	0.89769300
H	-4.02622500	0.07076400	-0.89341600
Be	-5.13815900	1.92031300	0.00065700
C	0.90559600	0.69303800	-0.00101200
C	1.57345000	-0.60138000	0.00080000
C	2.99568700	-0.64538200	-0.00026900
C	3.72642400	0.53451900	0.00079400
C	3.07614300	1.79531300	-0.00057700
C	1.69123200	1.87915100	0.00035600
F	5.07511900	0.50929300	0.00084500
N	0.85110700	-1.77391900	0.00081800
N	-0.46824400	0.79427900	-0.00109600
F	3.64302900	-1.82910700	0.00035600
F	3.83576500	2.91085400	-0.00044100

F	1.09731800	3.09103600	-0.00027300
Po	-1.14655000	-1.18384200	-0.00020600

1a···$MgMe_2$

C	-6.88858700	0.68383500	0.00010100
H	-7.12001800	1.30019500	-0.88761200
H	-7.60249600	-0.15993700	-0.00015000
H	-7.12053300	1.30010800	0.88773800
C	-2.86533000	-0.65932300	0.00099800
H	-2.16495600	0.19538900	0.00124400
H	-2.64460400	-1.27442200	0.89284700
H	-2.64419300	-1.27421800	-0.89089100
C	1.85511500	0.65443800	-0.00017500
C	2.68768900	-0.50386200	-0.00034700
S	0.39180400	-1.27081400	-0.00008700
C	2.32780800	2.01087000	-0.00017600
C	4.12423700	-0.48675000	-0.00053900
N	0.52353400	0.38880700	0.00000600
N	2.00434900	-1.67630300	-0.00027900
N	2.75113300	3.12291200	-0.00018000
N	5.31296600	-0.43473800	-0.00069000
Mg	-4.88012700	0.02049300	0.00058800

1b···$MgMe_2$

C	-6.86578700	0.96591200	0.00016200
H	-7.07391200	1.59001500	-0.88777500
H	-7.61001600	0.14886000	0.00039500
H	-7.07396900	1.59057300	0.88769400
C	-2.89668800	-0.53324100	0.00074800
H	-2.17662300	0.30514100	0.00053400
H	-2.70334900	-1.15305800	0.89548900
H	-2.70328500	-1.15356000	-0.89363100
C	1.75490500	0.87314300	-0.00007400
C	2.64598900	-0.24854000	-0.00033100
C	2.19919600	2.24203900	-0.00003700
C	4.08009100	-0.12165700	-0.00053500
N	0.42669200	0.60461100	0.00007500

N	2.07439100	-1.47567600	-0.00029500
N	2.59381500	3.36502400	-0.00002100
N	5.26233700	0.01572800	-0.00068300
Mg	-4.88523200	0.22865800	0.00046200
Se	0.29285400	-1.19722400	-0.00004100

1c···$MgMe_2$

C	-6.74521000	1.32490400	0.00015500
H	-6.91181600	1.96042100	-0.88822700
H	-7.53952700	0.55667900	0.00109200
H	-6.91101300	1.96176200	0.88772700
C	-2.88187500	-0.43654200	-0.00017100
H	-2.13275900	0.37564200	-0.00102800
H	-2.74168700	-1.06144300	0.90007600
H	-2.74232900	-1.06277700	-0.89958700
C	1.63901100	1.09098400	-0.00000600
C	2.63105300	0.04024500	0.00003700
C	2.01308600	2.48487800	-0.00003800
C	4.04374200	0.34237800	0.00004100
N	0.32593400	0.78131500	-0.00001900
N	2.23477300	-1.24675500	0.00005800
N	2.33833700	3.63048000	-0.00005200
N	5.20339400	0.61221600	0.00004900
Mg	-4.81841200	0.46267700	-0.00005300
Te	0.22854200	-1.22700500	0.00000400

1d···$MgMe_2$

C	-6.74517100	1.61625100	-0.00008500
H	-6.90070300	2.25729800	-0.88641900
H	-7.54972300	0.85883100	-0.00368900
H	-6.90349300	2.25180400	0.88970600
C	-2.90934000	-0.20606300	0.00060600
H	-2.15445400	0.60086200	0.00431200
H	-2.78696400	-0.83396100	0.90109400
H	-2.78418600	-0.82819500	-0.90350100
C	1.58857700	1.37136700	-0.00018200
C	2.61088400	0.33510200	-0.00015800

C	1.95523900	2.76946600	-0.00045300
C	4.01288100	0.69534900	-0.00039900
N	0.28249100	1.06858400	-0.00009000
N	2.27852500	-0.96045100	-0.00006600
N	2.26883400	3.91845900	-0.00060400
N	5.16236500	1.00581900	-0.00055500
Mg	-4.83158900	0.72749200	0.00016800
Po	0.16707900	-1.04467000	0.00011600

2a···$MgMe_2$

C	6.87247800	-1.10595100	0.00069600
H	7.00870300	-1.75722300	0.88352600
H	7.01666200	-1.74289800	-0.89126700
H	7.70366500	-0.37709400	0.01031700
C	3.08584000	0.80012400	-0.00042100
H	2.94185300	1.43990300	0.88966900
H	2.94286700	1.44095700	-0.88992000
H	2.27392900	0.05047900	-0.00133100
C	-1.72923700	-0.53058400	-0.00043900
C	-2.58235200	0.63338700	0.00032300
C	-3.99548000	0.49554800	0.00090000
C	-4.52111900	-0.79703500	0.00070100
C	-3.67752300	-1.94848100	-0.00005200
C	-2.28670300	-1.83646000	-0.00062200
H	-4.63691400	1.38059500	0.00147500
H	-4.13474400	-2.94257200	-0.00017700
H	-1.63646500	-2.71511300	-0.00120000
N	-1.89662400	1.82997200	0.00040300
N	-0.38003500	-0.24317400	-0.00092000
S	-0.29355500	1.41364400	-0.00042400
H	-5.60672800	-0.93344500	0.00112200
Mg	4.98043700	-0.15273000	0.00014000

2b···$MgMe_2$

C	6.87268800	1.34091700	-0.00018800
H	7.01050500	1.98560800	0.88708100
H	7.70534700	0.61381500	0.00021000

H	7.01073100	1.98489300	-0.88794200
C	3.09228100	-0.57982200	0.00010500
H	2.28597800	0.17625600	-0.00022800
H	2.95322400	-1.21857900	-0.89141200
H	2.95306700	-1.21795600	0.89204400
C	-1.67329400	0.76572800	-0.00003100
C	-2.56507300	-0.37355600	0.00003500
C	-3.97385900	-0.17971200	-0.00001400
C	-4.46355600	1.12634600	-0.00011800
C	-3.58458400	2.24967800	-0.00018700
C	-2.19934900	2.08714600	-0.00015000
H	-4.64169700	-1.04543000	0.00004400
H	-4.00648400	3.25938000	-0.00026400
H	-1.51932000	2.94336200	-0.00020000
N	-1.97113600	-1.61996800	0.00015600
N	-0.31872700	0.49717100	0.00001300
H	-5.54500300	1.29343200	-0.00014300
Mg	4.98415100	0.38342500	-0.00004300
Se	-0.20643100	-1.29813600	0.00010100

2c···$MgMe_2$

C	6.73539100	1.70095100	-0.00001300
H	6.83142800	2.35274400	0.88742400
H	7.61175300	1.02734100	0.00042800
H	6.83186300	2.35214600	-0.88784200
C	3.08446200	-0.45758100	-0.00021200
H	2.25042300	0.26810000	-0.00057700
H	2.98817200	-1.09912800	-0.89506500
H	2.98783000	-1.09858900	0.89499400
C	-1.57781300	0.98995600	0.00019100
C	-2.57013700	-0.07063600	0.00003200
C	-3.95622000	0.26204400	0.00000500
C	-4.33580900	1.60349200	0.00013800
C	-3.36212700	2.64434100	0.00029700
C	-1.99918300	2.35212300	0.00031900
H	-4.69597700	-0.54365300	-0.00011200
H	-3.68906400	3.68883300	0.00040700

H	-1.24367600	3.14312200	0.00044500
N	-2.15683000	-1.39098100	-0.00008700
N	-0.23056800	0.67577500	0.00021800
H	-5.39950400	1.86120600	0.00013000
Mg	4.91252300	0.62707600	-0.00010100
Te	-0.16967500	-1.31959100	-0.00008600

2d···$MgMe_2$

C	6.73232400	1.98996800	-0.00014700
H	6.82564000	2.64192900	0.88739300
H	7.61116100	1.31964200	0.00012400
H	6.82586400	2.64150400	-0.88797500
C	3.09338500	-0.18997400	-0.00012400
H	2.25870800	0.53506200	-0.00030900
H	3.00491500	-0.83033100	-0.89657300
H	3.00478800	-0.82997400	0.89657300
C	-1.54832300	1.28034000	0.00025300
C	-2.56142900	0.23725100	-0.00009100
C	-3.94177200	0.60367900	-0.00015600
C	-4.29822700	1.95039100	0.00010200
C	-3.30495300	2.97309900	0.00044600
C	-1.94982800	2.65142000	0.00052300
H	-4.69586700	-0.18877200	-0.00042400
H	-3.61033000	4.02411700	0.00063900
H	-1.17790500	3.42664300	0.00078200
N	-2.20840900	-1.09790900	-0.00035200
N	-0.20167900	0.97662300	0.00032400
H	-5.35728800	2.22681300	0.00004000
Mg	4.91470300	0.90874900	-0.00012300
Po	-0.12050700	-1.11904400	-0.00004100

3a···$MgMe_2$

C	8.10310200	-0.82985200	0.00042300
H	8.37575600	-0.23047100	0.88831100
H	8.76128300	-1.71802600	-0.00024400
H	8.37563200	-0.22922900	-0.88666400
C	3.99992800	-1.89735200	0.00000700

H	3.36947000	-0.98988000	0.00024700
H	3.72634000	-2.49199800	-0.89095200
H	3.72629500	-2.49249800	0.89061700
C	-0.38189300	0.33417500	-0.00006700
C	-1.46404300	-0.62853200	0.00010300
C	-2.81261800	-0.18642300	0.00005500
C	-3.06076100	1.18808200	-0.00015700
C	-1.99926500	2.13267000	-0.00032400
C	-0.66364800	1.72479600	-0.00028200
H	-2.23252700	3.20076900	-0.00048800
N	-1.04475300	-1.93725000	0.00028900
N	0.87230900	-0.22776300	0.00000400
Mg	6.05320000	-1.36147000	0.00019700
H	-4.09443200	1.54415600	-0.00019700
Br	0.74789300	2.97653600	-0.00050200
Br	-4.21994600	-1.44168800	0.00027000
S	0.60987200	-1.86532200	0.00028100

3b···$MgMe_2$

C	7.99402500	-0.45313400	0.00037800
H	8.24530600	0.15547200	0.88815700
H	8.68170500	-1.31856100	0.00010200
H	8.24536900	0.15608700	-0.88696100
C	3.93068400	-1.66701800	0.00007500
H	3.28088100	-0.77289100	-0.00016800
H	3.68045000	-2.26893600	-0.89279200
H	3.68032500	-2.26853700	0.89317600
C	-0.44165600	0.49600000	-0.00006100
C	-1.53839300	-0.45700100	0.00001900
C	-2.88010800	0.01269800	-0.00001200
C	-3.11739100	1.38902800	-0.00011900
C	-2.04650400	2.31983600	-0.00019700
C	-0.71787400	1.89023400	-0.00017100
H	-2.26329000	3.39137100	-0.00028100
N	-1.19113800	-1.78871300	0.00011900
N	0.83252100	-0.02474800	-0.00002800
Mg	5.96498400	-1.05442900	0.00009100

H	-4.14808600	1.75368000	-0.00014300
Br	0.70644800	3.13025100	-0.00027600
Br	-4.30722400	-1.22259400	0.00009100
Se	0.60171600	-1.80682900	0.00012300

3c···$MgMe_2$

C	7.76215000	0.06696500	0.00008900
H	7.95513700	0.69621200	0.88788800
H	8.52623400	-0.73164000	-0.00011200
H	7.95499600	0.69652100	-0.88752300
C	3.82931700	-1.52392800	0.00046300
H	3.12520100	-0.67175000	0.00011000
H	3.63983300	-2.14173300	-0.89611300
H	3.63986300	-2.14096400	0.89757700
C	-0.46832300	0.62564500	-0.00000900
C	-1.62808000	-0.26072100	-0.00011900
C	-2.93409100	0.30878800	-0.00024500
C	-3.09038100	1.69694800	-0.00025900
C	-1.96525300	2.55670100	-0.00015300
C	-0.66956100	2.03579800	-0.00003200
H	-2.10929400	3.64037500	-0.00017200
N	-1.43426000	-1.62701000	-0.00012600
N	0.80372900	0.09014700	0.00008800
Mg	5.79915000	-0.71837700	0.00008300
H	-4.09746300	2.12242200	-0.00036000
Br	0.82751300	3.19191000	0.00009600
Br	-4.44509400	-0.82650900	-0.00040300
Te	0.53442500	-1.88302100	0.00019800

3d···$MgMe_2$

C	7.63441100	0.61992800	0.00030200
H	7.79934200	1.25671000	0.88831500
H	8.43245700	-0.14469000	-0.00006300
H	7.79924100	1.25745300	-0.88719600
C	3.77860000	-1.15048300	0.00002800
H	3.04087900	-0.32711000	-0.00018000
H	3.62188500	-1.77490700	-0.89827800

H	3.62173400	-1.77458000	0.89853500
C	-0.56802000	0.87894500	-0.00013600
C	-1.71717800	-0.02184300	0.00000500
C	-3.02833300	0.53927900	-0.00005700
C	-3.20396600	1.92539100	-0.00025500
C	-2.09052800	2.79764900	-0.00039300
C	-0.79041700	2.28724100	-0.00033700
H	-2.24467400	3.87987000	-0.00054700
N	-1.54166200	-1.39139400	0.00020200
N	0.72384200	0.39073500	-0.00008000
Mg	5.70862400	-0.25058700	0.00004500
Po	0.51843600	-1.68771100	0.00020500
H	-4.21676100	2.33698700	-0.00030000
Br	0.69289700	3.46316900	-0.00052300
Br	-4.52915100	-0.61137000	0.00012800

4a···$MgMe_2$

C	-7.63056800	-1.21273700	0.00037100
H	-7.78135000	-1.85345800	0.88843600
H	-8.44944400	-0.47016100	-0.00066000
H	-7.78070500	-1.85521100	-0.88653500
C	-3.81158000	0.62884500	-0.00008400
H	-3.00742400	-0.12921700	0.00016900
H	-3.66284600	1.26735800	-0.89038200
H	-3.66289200	1.26790600	0.88982700
C	1.06179900	-0.39582900	0.00006400
C	1.82660200	0.82855600	-0.00018400
C	3.24235600	0.79871700	-0.00020800
C	3.85834300	-0.46033200	0.00001600
C	3.10381200	-1.67875400	0.00026000
C	1.71170300	-1.65841000	0.00028700
H	3.82851300	1.72104000	-0.00038900
H	3.64119200	-2.63082200	0.00042700
H	1.12743400	-2.58191400	0.00047000
N	1.05597000	1.97082300	-0.00036700
N	-0.30253600	-0.20942600	0.00004500
C	5.29996700	-0.54248900	0.00000500

N	6.48698900	-0.62384100	-0.00000300
S	-0.51347900	1.43477800	-0.00025100
Mg	-5.72453200	-0.29168900	0.00014600

4b···$MgMe_2$

C	7.45599200	1.60694300	-0.00073600
H	7.57843100	2.25426000	0.88675200
H	8.30534200	0.89959400	-0.00097700
H	7.57777300	2.25407300	-0.88845200
C	3.72066200	-0.40151600	0.00086100
H	2.89259500	0.33071000	0.00039100
H	3.60198400	-1.04432200	-0.89081300
H	3.60208400	-1.04308100	0.89344300
C	-1.12875800	0.56961800	0.00017600
C	-1.91782600	-0.64363800	-0.00012400
C	-3.33387300	-0.57579300	-0.00024800
C	-3.93122700	0.69184200	-0.00006800
C	-3.15534700	1.89519400	0.00022900
C	-1.76468300	1.84195600	0.00035100
H	-3.93614000	-1.48799800	-0.00047300
H	-3.67172200	2.85885000	0.00036000
H	-1.16051600	2.75292600	0.00057600
N	-1.21870200	-1.83362900	-0.00027400
N	0.24167200	0.42013200	0.00027500
C	-5.37105800	0.79702600	-0.00018300
N	-6.55671200	0.89843500	-0.00027500
Mg	5.59207600	0.60566000	0.00006200
Se	0.51171000	-1.35668500	-0.00003500

4c···$MgMe_2$

C	7.12534200	2.20485600	0.00024300
H	7.17694000	2.86041700	0.88846500
H	8.04519600	1.59219100	-0.00073700
H	7.17595200	2.86177400	-0.88703200
C	3.62766600	-0.19647700	0.00037800
H	2.74279400	0.46614800	0.00065900
H	3.58194300	-0.84231400	-0.89545800

H	3.58222800	-0.84270700	0.89594400
C	-1.16227600	0.70633900	-0.00002900
C	-2.01449700	-0.46987700	-0.00013500
C	-3.42583100	-0.31424200	-0.00016000
C	-3.96436400	0.97934800	-0.00008400
C	-3.13009600	2.14061200	0.00002100
C	-1.74533200	2.00730000	0.00005100
H	-4.07265500	-1.19580500	-0.00024600
H	-3.59243100	3.13138800	0.00007200
H	-1.09224200	2.88440300	0.00012600
N	-1.43991300	-1.72955900	-0.00022300
N	0.21184200	0.56170500	-0.00000400
C	-5.39723700	1.15274300	-0.00012200
N	-6.57694800	1.31043600	-0.00014900
Mg	5.38142500	1.01006200	0.00030600
Te	0.51980900	-1.40957500	-0.00007300

4d···$MgMe_2$

C	6.92212800	2.68138400	0.00017200
H	6.94955500	3.33827700	0.88841600
H	7.86345800	2.10232400	-0.00075500
H	6.94855000	3.33948800	-0.88720500
C	3.51807600	0.14813000	0.00040000
H	2.61137200	0.78067600	0.00060700
H	3.50059800	-0.49716300	-0.89680400
H	3.50084300	-0.49741500	0.89742400
C	-1.28694700	0.95117700	-0.00014500
C	-2.13069600	-0.23154800	-0.00009200
C	-3.54366900	-0.07788300	-0.00013900
C	-4.09306600	1.21077000	-0.00023700
C	-3.26773000	2.37745900	-0.00029100
C	-1.88304800	2.24825600	-0.00024500
H	-4.18438700	-0.96401200	-0.00009800
H	-3.73459200	3.36606800	-0.00036800
H	-1.23341600	3.12815500	-0.00028600
N	-1.58003400	-1.50201400	0.00000000
N	0.09058000	0.85142300	-0.00009800

C	-5.52719900	1.37287100	-0.00028600
N	-6.70809400	1.52170200	-0.00032600
Mg	5.22374100	1.42402500	0.00028100
Po	0.47891500	-1.20674000	0.00004600

5a···$MgMe_2$

C	-7.88167500	1.11703600	-0.00058200
H	-8.02132400	1.76039600	-0.88849500
H	-8.71207200	0.38740500	-0.00019000
H	-8.02139900	1.76143500	0.88656500
C	-4.09815600	-0.79711800	0.00057400
H	-3.28308300	-0.05094300	0.00010400
H	-3.96224000	-1.43734200	0.89165400
H	-3.96228300	-1.43840700	-0.88974500
C	0.74555000	0.17518000	0.00007300
C	1.50176700	-1.05744100	-0.00004100
C	2.91775800	-1.02474600	-0.00012900
C	3.54876300	0.21193500	-0.00010300
C	2.80431100	1.42556600	0.00001000
C	1.41610800	1.42244700	0.00009800
N	0.72546400	-2.18765200	-0.00004500
N	-0.61525100	0.00342600	0.00015100
S	-0.84034800	-1.64175600	0.00005200
Mg	-5.99075800	0.16586200	0.00006000
F	3.48617000	2.58764000	0.00003200
F	4.89347300	0.29365100	-0.00018100
F	3.64316500	-2.15908400	-0.00023400
F	0.73263800	2.58308700	0.00020600

5b···$MgMe_2$

C	-7.64709500	1.55920600	0.00007000
H	-7.75214400	2.20941700	-0.88748200
H	-8.51419100	0.87373500	-0.00004300
H	-7.75224700	2.20925500	0.88772900
C	-3.97130800	-0.55698900	-0.00005300
H	-3.12729800	0.15659900	-0.00000200
H	-3.87244000	-1.20109500	0.89299400

H	-3.87246900	-1.20093500	-0.89321800
C	0.84160600	0.34125900	0.00013500
C	1.61908800	-0.88284100	-0.00012700
C	3.03622200	-0.81726400	-0.00019500
C	3.65174500	0.42676400	0.00000700
C	2.88920100	1.62724100	0.00026200
C	1.50182800	1.59659800	0.00032200
N	0.91039400	-2.05837300	-0.00028300
N	-0.52546800	0.21040200	0.00016900
Mg	-5.80995800	0.51077200	0.00008700
F	3.55021400	2.80223200	0.00048200
F	4.99586500	0.52685400	-0.00000200
F	3.78145600	-1.93997300	-0.00041300
F	0.79998300	2.74754500	0.00057600
Se	-0.81645900	-1.56571200	-0.00025100

5c···$MgMe_2$

C	-7.27015200	2.15850500	0.00054300
H	-7.30586900	2.81634900	-0.88669800
H	-8.20340200	1.56647400	-0.00001800
H	-7.30603500	2.81493200	0.88882600
C	-3.83890200	-0.33784700	-0.00099700
H	-2.94178300	0.30780000	-0.00040600
H	-3.81391400	-0.98349200	0.89564100
H	-3.81367800	-0.98219700	-0.89855900
C	0.91110900	0.47705100	-0.00004000
C	1.74615800	-0.71632100	0.00016200
C	3.16061700	-0.57305000	0.00029200
C	3.72471500	0.69501000	0.00023400
C	2.91056900	1.85818300	0.00003900
C	1.52674800	1.75805800	-0.00009300
N	1.15322000	-1.95733300	0.00021700
N	-0.46002000	0.35785300	-0.00017300
Mg	-5.55411800	0.92532500	-0.00031500
F	3.51492500	3.06484100	-0.00001200
F	5.06439000	0.85215600	0.00035800
F	3.96039800	-1.65944800	0.00047700

F	0.77557600	2.87958000	-0.00027800
Te	-0.80540500	-1.60767500	-0.00002000

5d···$MgMe_2$

C	-6.97922600	2.75370800	0.00026200
H	-6.97884400	3.41211400	-0.88720800
H	-7.94288900	2.21266700	-0.00038900
H	-6.97951500	3.41116700	0.88843400
C	-3.69311100	0.06830500	-0.00032600
H	-2.76493200	0.66857600	0.00023300
H	-3.70840800	-0.57503500	0.89811200
H	-3.70804800	-0.57391500	-0.89957000
C	1.07805300	0.71145900	-0.00000200
C	1.88690200	-0.50074200	-0.00004200
C	3.30532400	-0.38235100	0.00004500
C	3.89860800	0.87227100	0.00014600
C	3.11083000	2.05202200	0.00018600
C	1.72554800	1.97835900	0.00011000
N	1.29855100	-1.74402200	-0.00015900
N	-0.29757200	0.65756100	-0.00007800
Mg	-5.33329900	1.42980700	0.00018900
F	3.74013600	3.24677800	0.00026900
F	5.24195100	0.99924600	0.00019800
F	4.08358800	-1.48513600	-0.00000200
F	0.99874100	3.11659600	0.00013700
Po	-0.75597600	-1.38480400	-0.00009400