

**Polyhalogenated aminobenzonitriles vs their co-crystals with 18-crown-6:
amino group position as a tool to control crystal packing and solid-state fluorescence**

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Table S1 Crystallographic data and structure refinement parameters of the aminobenzonitrile crystals and co-crystals

	B₂·cr	C₂·cr	D₂·cr	E₂·cr
Crystal data				
Chemical formula	2(C ₇ H ₃ F ₃ N ₂)·C ₁₂ H ₂₄ O ₆	2(C ₇ H ₃ F ₃ N ₂)·C ₁₂ H ₂₄ O ₆	2(C ₇ H ₂ ClF ₃ N)·C ₁₂ H ₂₄ O ₆	2(C ₇ H ₃ ClF ₂ N ₂)·C ₁₂ H ₂₄ O ₆
<i>M_r</i>	608.54	608.54	677.42	641.44
Crystal system, space group	Monoclinic, <i>C2/c</i>	Monoclinic, <i>C2/c</i>	Triclinic, <i>P</i> ⁻¹	Triclinic, <i>P</i> ⁻¹
Temperature (K)	296	296	296	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	14.4786 (6), 11.6381 (6), 34.8047 (16)	14.4590 (6), 11.6131 (6), 34.7535 (15)	9.4276 (6), 9.9092 (6), 10.3213 (7)	9.2760 (4), 9.8840 (5), 10.2679 (5)
α , β , γ (°)	90, 90.017 (3), 90	90, 90.333 (3), 90	111.749 (2), 97.219 (3), 116.798 (2)	111.106 (2), 98.506 (2), 116.108 (2)
<i>V</i> (Å ³)	5864.7 (5)	5835.5 (5)	747.91 (8)	734.00 (6)
<i>Z</i>	8	8	1	1
μ (mm ⁻¹)	0.12	0.12	0.30	0.29
Crystal size (mm)	0.58 × 0.20 × 0.15	0.59 × 0.11 × 0.06	0.57 × 0.39 × 0.31	0.58 × 0.52 × 0.16
Data collection				
<i>T</i> _{min} , <i>T</i> _{max}	0.863, 0.956	0.896, 0.954	0.806, 0.837	0.772, 0.837
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	16444, 5311, 2751	24213, 5505, 3834	20110, 3585, 3092	20065, 3547, 3009
<i>R</i> _{int}	0.029	0.059	0.023	0.023
(sin θ/λ) _{max} (Å ⁻¹)	0.600	0.612	0.659	0.661
Refinement				
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.130, 0.435, 1.48	0.088, 0.294, 0.95	0.036, 0.099, 1.03	0.037, 0.111, 1.03
No. of reflections	5311	5505	3585	3547
No. of parameters	378	385	207	198
No. of restraints	546	673	2	2
H-atom treatment	H-atom parameters constrained	H-atom parameters constrained	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
Δ _{max} , Δ _{min} (e Å ⁻³)	0.57, -0.41	0.56, -0.39	0.34, -0.34	0.33, -0.30
Absolute structure	–	–	–	–
Absolute structure parameter	–	–	–	–

Table S1 Crystallographic data and structure refinement parameters of the of the aminobenzonitrile crystals and co-crystals (continued)

	B	C	D	E
Crystal data				
Chemical formula	C ₇ H ₃ F ₃ N ₂	C ₇ H ₃ F ₃ N ₂	C ₇ H ₂ ClF ₃ N ₂	C ₇ H ₂ ClF ₂ N ₂
<i>M</i> _r	172.11	172.11	206.56	187.56
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>	Monoclinic, <i>P</i> 2 ₁	Monoclinic, <i>C</i> 2/ <i>m</i>	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>
Temperature (K)	296	200	296	296
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.5702 (5), 5.8303 (3), 15.8912 (11)	3.7360 (7), 8.4997 (17), 10.654 (2)	9.7777 (19), 7.7816 (15), 10.2460 (16)	7.6581 (3), 7.3941 (3), 13.4241 (6)
α, β, γ (°)	90, 96.846 (3), 90	90, 96.061 (7), 90	99.955 (8)	90, 98.090 (2), 90
<i>V</i> (Å ³)	696.38 (8)	336.44 (12)	767.8 (2)	752.57 (5)
<i>Z</i>	4	2	4	4
μ (mm ⁻¹)	0.16	0.16	0.50	0.48
Crystal size (mm)	0.61 × 0.28 × 0.08	0.37 × 0.27 × 0.12	0.66 × 0.42 × 0.38	0.51 × 0.19 × 0.14
Data collection				
<i>T</i> _{min} , <i>T</i> _{max}	0.852, 0.956	0.819, 0.971		0.833, 0.888
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	7627, 1587, 1084	2291, 1092, 990	3105, 799, 505	7523, 1792, 1445
<i>R</i> _{int}	0.027	0.033	0.023	0.048
(sin θ/λ) _{max} (Å ⁻¹)	0.650	0.613	0.620	0.658
Refinement				
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.046, 0.141, 1.03	0.033, 0.102, 0.82	0.096, 0.282, 1.02	0.040, 0.122, 1.06
No. of reflections	1587	1092	799	1792
No. of parameters	117	117	67	117
No. of restraints	2	3		2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement	H-atom parameters constrained	H atoms treated by a mixture of independent and constrained refinement
Δ _{max} , Δ _{min} (e Å ⁻³)	0.20, -0.15	0.16, -0.19	0.37, -0.41	0.27, -0.31
Absolute structure	–	Flack <i>x</i> determined using 353 quotients [(<i>I</i> ⁺)-(<i>I</i> ⁻)]/[(<i>I</i> ⁺)+(<i>I</i> ⁻)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).		–
Absolute structure parameter	–	-0.6 (6)		–

Short description of asymmetric units and co-formers geometry in the crystals.

The asymmetric units of isostructural crystals $\mathbf{B}_2 \cdot \mathbf{cr}$ and $\mathbf{C}_2 \cdot \mathbf{cr}$ have \mathbf{cr} molecules and two amine molecules in general positions. The asymmetric units of isostructural crystals $\mathbf{D}_2 \cdot \mathbf{cr}$ and $\mathbf{E}_2 \cdot \mathbf{cr}$ have one amine molecule in a general position and half of \mathbf{cr} molecules at the inversion centre in the $P-1$ structure. The asymmetric units of individual aminobenzonitriles \mathbf{B} , \mathbf{C} and \mathbf{E} have one molecule in general positions. The asymmetric unit of individual aminobenzonitrile \mathbf{D} has half of molecule at a mirror plane lying orthogonally in this $C2/m$ structure. Difference-map plots made with data on all the crystals confirm that all H atoms of the \mathbf{cr} and amines molecules were located correctly. The conformation of the 18-crown-6 molecules in the co-crystals $\mathbf{B}_2 \cdot \mathbf{cr}$ and $\mathbf{C}_2 \cdot \mathbf{cr}$ is close to the classical crown 3(TGT,T-GT), where T stands for trans, G stands for gauche; in the co-crystals $\mathbf{D}_2 \cdot \mathbf{cr}$ and $\mathbf{E}_2 \cdot \mathbf{cr}$ there is the centrosymmetrical conformation 2(TGT,TGT,GGT). The bond lengths in the individual and associated with crown ether arylamines $\mathbf{B} - \mathbf{E}$ are approximately the same. In all the individual arylamines and most co-crystals, the sum of 1,3-angles at the amino nitrogen atom is close to 360° , i.e. the amino group has a planar structure and is conjugated with an aromatic ring. A slight deviation from planarity is observed only in the co-crystals $\mathbf{D}_2 \cdot \mathbf{cr}$ and $\mathbf{E}_2 \cdot \mathbf{cr}$ (the angles sum is ~ 343 and 346°).

Table S2 Hydrogen bonding in the aminobenzonitrile crystals and co-crystals

Associate ^a	Interaction D-H...A	<i>I</i> _{D-H} (Å)	<i>I</i> _{H...A} (Å)	<i>I</i> _{D...A} (Å)	Angle D-H...A (deg)	Symmetry code for acceptor
A₂·cr^{b,c}	N(1)-H(1A)...O(3)	0.88	2.22	2.89(2)	133	
	N(1)-H(1A)...O(4)	0.88	2.46	3.10(2)	131	
	N(1)-H(1B)...O(1)	0.88	2.53	3.37(3)	160	
	N(3)-H(3A)...O(2)	0.88	2.21	3.06(1)	162	1-x, 1-y, 1-z
	N(3)-H(3B)...O(4)	0.88	2.21	3.08(1)	169	1-x, 1-y, 1-z
	C(20)-H(20A)...F(1)	0.99	2.40	3.21(2)	138	
	C(25)-H(25B)...F(4)	0.99	2.32	3.14(2)	139	
	C(22)-H(22B)...F(5)	0.99	2.46	3.26(2)	137	1-x,1-y,1-z
	C(26)-H(26A)...F(5)	0.99	2.48	3.461(19)	170	3/2-x,1/2-y,1-z
	C(15)-H(15A)...F(8)	0.99	2.44	3.24(2)	138	1-x,1-y,1-z
	C(23)-H(23B)...F(8)	0.99	2.47	3.447(2)	169	1/2-x,1/2-y,1-z
B₂·cr^b	N(1)-H(1)...O(5)	0.86	2.34	3.150(13)	157	
	N(1)-H(2)...O(1)	0.86	2.15	2.990(11)	164	
	N(3)-H(3)...O(6)	0.86	2.21	3.000(8)	153	
	N(3)-H(4)...O(4)	0.86	2.30	3.149(15)	153	
	C(21)-H(21A)...F(2)	0.97	2.28	3.14(2)	148	
	C(26)-H(26B)...F(4)	0.97	2.46	3.357(19)	154	3/2-x,1/2+y,1/2-z
	C(26)-H(26A)...F(5)	0.97	1.98	2.95(2)	174	
C₂·cr^b	N(1)-H(1)...O(6)	0.86	2.38	3.220(6)	164	
	N(1)-H(2)...O(2)	0.86	2.18	3.027(6)	167	
	N(3)-H(3)...O(5)	0.86	2.27	3.098(7)	162	
	N(3)-H(4)...O(1)	0.86	2.22	3.066(5)	168	
	C(23)-H(23A)...F(2)	0.97	2.46	3.261(10)	140	
	C(21)-H(21B)...F(6)	0.97	2.41	3.235(8)	143	
D₂·cr	N(1)-H(1)...O(2)	0.854(18)	2.295(18)	3.1366(17)	168.9(19)	1-x,1-y,1-z
	N(1)-H(2)...O(2)	0.877(19)	2.28(2)	3.095(2)	155.7(18)	
	N(1)-H(2)...O(3)	0.877(19)	2.54(2)	3.118(2)	124.3(17)	
	C(12)-H(12B)...F(2)	0.97	2.55	3.137(8)	119	-1+x,-1+y,-1+z
E₂·cr	N(1)-H(1)...O(2)	0.868(19)	2.32(2)	3.118(2)	153.8(18)	x,-1+y,z
	N(1)-H(1)...O(3)	0.868(19)	2.55(2)	3.129(2)	125.0(16)	x,-1+y,z
	N(1)-H(2)...O(2)	0.863(18)	2.273(18)	3.1216(18)	167.7(19)	1-x,1-y,-z

Table S2 Hydrogen bonding in the aminobenzonitrile crystals and co-crystals (continued)

Associate ^a	Interaction D-H...A	<i>l</i> _{D-H} (Å)	<i>l</i> _{H...A} (Å)	<i>l</i> _{D...A} (Å)	Angle D-H...A (deg)	Symmetry code for acceptor
A ^d	N(1)-H(1A)...N(2')	1.00(2)	2.10(2)	3.100(4)	174(3)	x,3/2-y,-1/2+z
	N(1)-H(1B)...N(2)	1.00(2)	2.145(2)	3.136(4)	171(3)	1-x,-1/2+y,1/2-z
	N(1')-H(1C)...N(2')	0.991(12)	2.085(11)	3.072(4)	174.0(19)	2-x,-1/2+y,1/2-z
	N(1')-H(1D)...N(2)	1.00(2)	2.11(2)	3.111(4)	174(2)	1+x,3/2-y,-1/2+z
B	N(1)-H(1)...N(2)	0.90(3)	2.21(3)	3.081(4)	161(3)	x,1/2-y,-1/2+z
	N(1)-H(2)...F(2)	0.90(3)	2.38(3)	3.226(3)	157(3)	-x,2-y,-z
C	N(1)-H(1)...F(2)	0.89(3)	2.53(4)	3.218(4)	134(3)	-x,1/2+y,-z
	N(1)-H(2)...N(2)	0.88(3)	2.39(4)	3.143(4)	144(3)	-1+x,1+y,z
	C(6)-H(6)...N(2)	0.95	2.61	3.466(4)	150	2-x,1/2+y,1-z
D	N(2)-H(1)...F(1)	0.86	2.38	3.088(9)	140	x,-y,z
	N(2)-H(2)...N(2)	0.86	2.50	3.210(13)	141	1/2-x,-1/2+y,1-z
E	N(1)-H(1)...N(2)	0.87(2)	2.29(2)	3.152(2)	169(2)	-x,1-y,-z

^a Hydrogen bonds of the minor parts of amines are not shown.

^b N(1) belongs to the amine molecule (1), N(3) – to the amine molecule (2).

^c Data from *CrystEngComm*, 2018, **20**, 807–817.

^d Data from *ChemPhysChem*, 2005, **6**, 2307–2323.

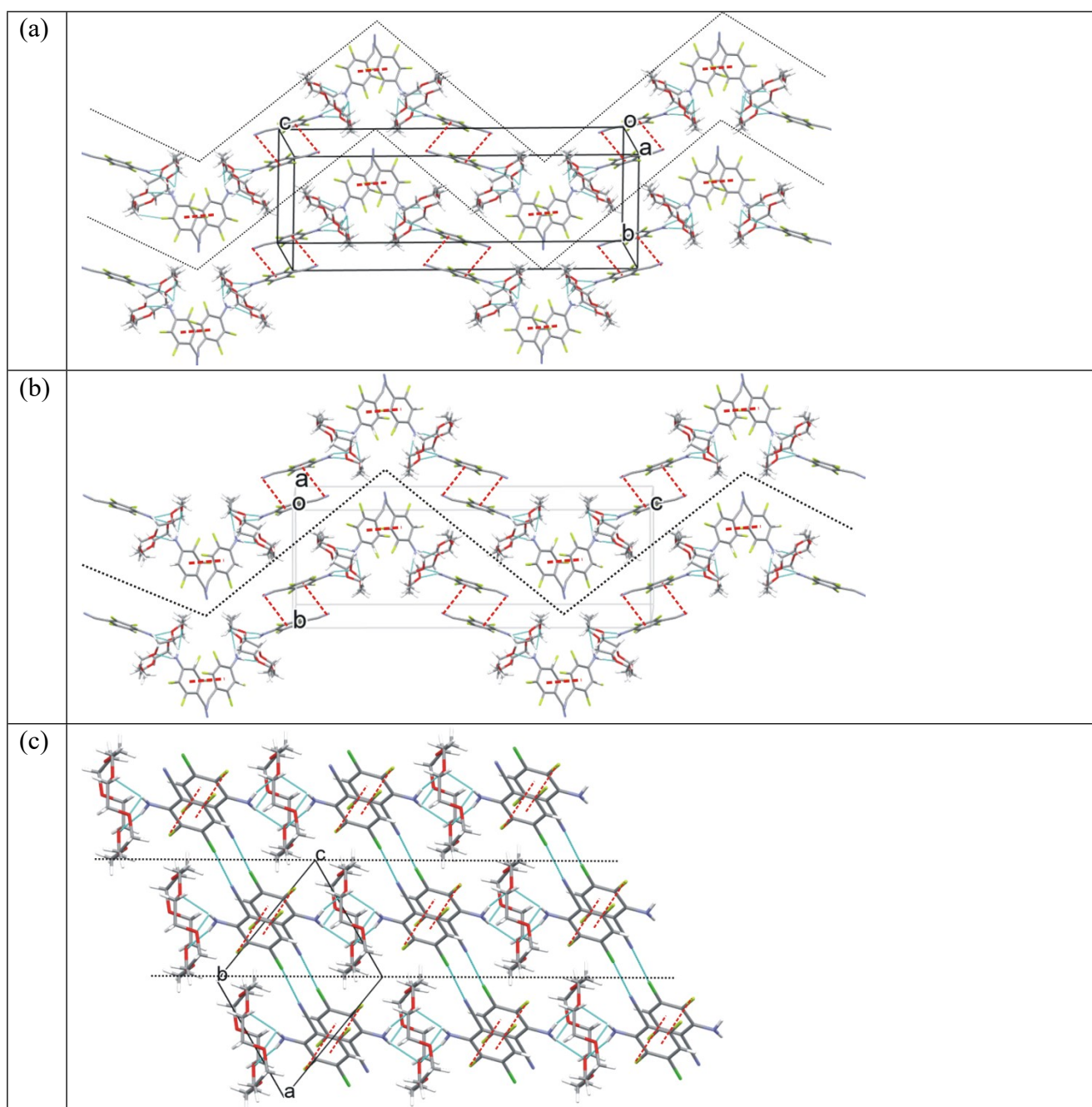
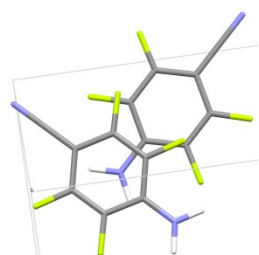
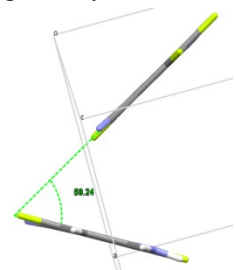


Fig. S1. Crystal packing in the associates $A_2 \cdot cr$ (a, without disorder), $B_2 \cdot cr$ (b, without disorder) and $E_2 \cdot cr$ (c); top view of the layers. H-bonded/ π -stacked rods are separated by dotted lines.

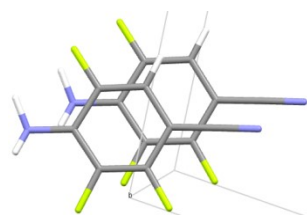
Crystals



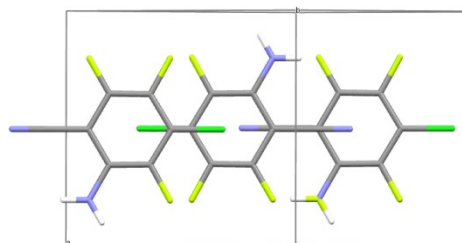
A (C–F $\cdots\pi_F$)
anti-parallel rotated
geometry



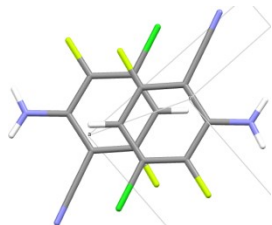
B (C \equiv N $\cdots\pi_F$) T-shaped edge-to-face geometry



C (C–F $\cdots\pi_F$ + $\pi_F\cdots\pi_F$)
parallel displaced geometry

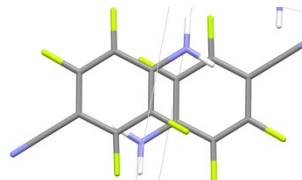


D (C–Cl $\cdots\pi_F$)₂ + (C \equiv N $\cdots\pi_F$)₂
anti-parallel slipped geometry

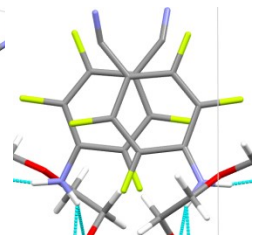
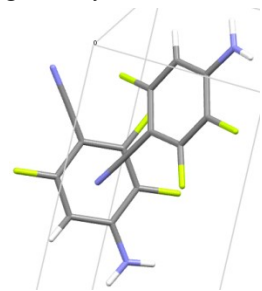


E ($\pi_F\cdots\pi_F$ + C–F $\cdots\pi_F$)
anti-parallel displaced geometry

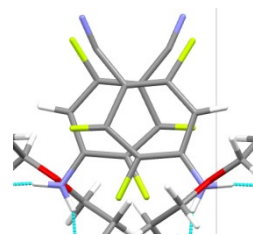
Co-crystals



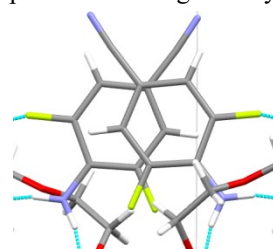
A (C–F $\cdots\pi_F$)₂
anti-parallel displaced
geometry



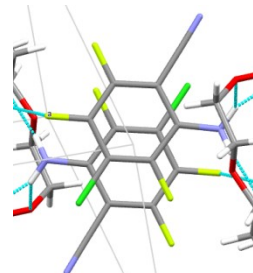
A₂·**cr** ($\pi_F\cdots\pi_F$)
parallel rotated geometry



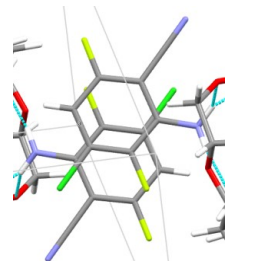
B₂·**cr** ($\pi_F\cdots\pi_F$)
parallel rotated geometry



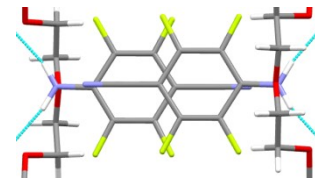
C₂·**cr** ($\pi_F\cdots\pi_F$)
parallel rotated geometry



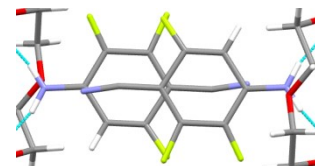
D₂·**cr** (C–F $\cdots\pi_F$ + $\pi_F\cdots\pi_F$)
anti-parallel displaced geometry



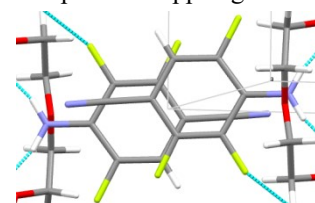
E₂·**cr** (C–F $\cdots\pi_F$)
anti-parallel displaced geometry



A₂·**cr** (C \equiv N $\cdots\pi_F$)
anti-parallel slipped geometry



B₂·**cr** (C \equiv N $\cdots\pi_F$)
anti-parallel slipped geometry



C₂·**cr** (C–F $\cdots\pi_F$)
anti-parallel displaced geometry

Fig. S2 Overlap of stacked molecules in the crystals; intermolecular interactions are shown in brackets.

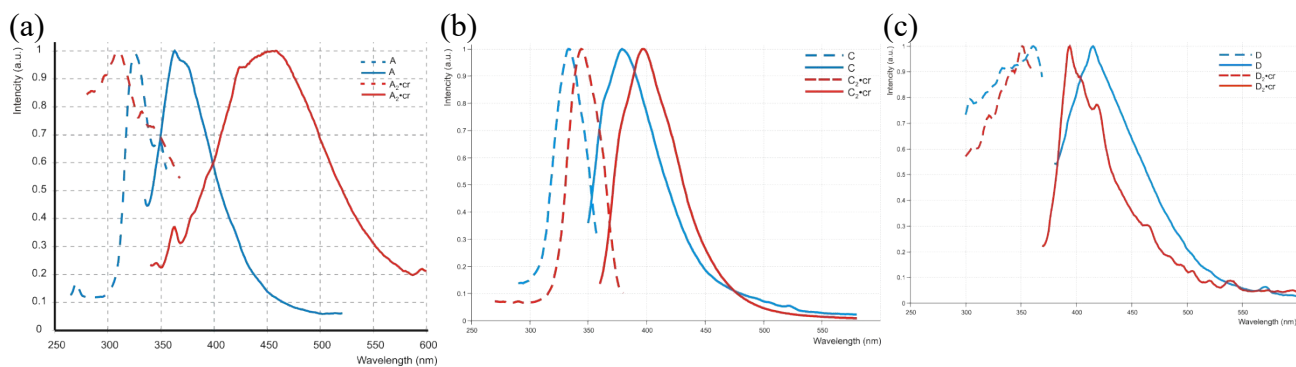


Fig. S3 Absorption (dashed lines) and fluorescence (solid lines) spectra of aminobenzonitriles (blue lines) and their co-crystals with 18-crown-6 (red lines): a) **A** and **A₂·cr**, b) **C** and **C₂·cr**, c) **D** and **D₂·cr**.

Table S3 Modulus of the Electric Dipole Moments (μ , in Debye) of molecules in isolated phase (is), crystal (hc) and co-crystal (cc) in the relaxed ground state (S_{0r}), vertically excited electronic state (S_{1v}), relaxed excited electronic state (S_{1r}) and vertically de-excited electronic state (S_{0v}).

Molecule	Phase	$\mu(S_{0r})$	$\mu(S_{1v})$	$\mu(S_{1r})$	$\mu(S_{0v})$
A	(is)	6.7	3.8	4.3	6.4
	(hc)	3.1	1.4	2.2	2.9
	(cc)	4.7	1.1	1.3	4.6
B	(is)	7.7	3.5	4.7	7.3
	(hc)	4.1	1.2	1.7	3.6
	(cc)	4.8	0.8	1.2	4.6
C	(is)	6.0	3.4	3.5	5.8
	(hc)	3.2	1.8	2.0	3.1
	(cc)	3.3	1.6	2.4	3.1
D	(is)	3.5	4.7	8.4	3.3
	(hc)	2.4	4.3	5.8	2.0
	(cc)	2.6	4.4	5.8	2.2
E	(is)	2.8	4.2	8.0	2.3
	(hc)	1.9	3.7	5.7	1.5
	(cc)	2.1	3.6	3.6	1.1

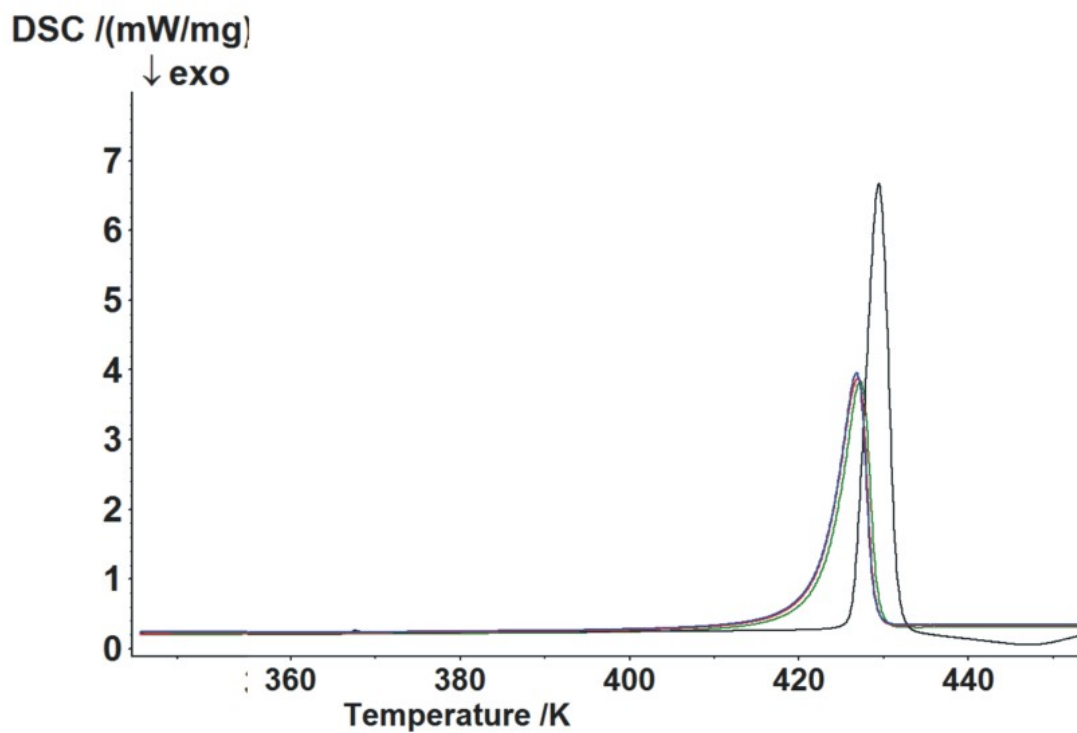


Fig. S4 DSC curves of the **A₂·cr** co-crystal, the first (black) and subsequent (red, green) heating runs.

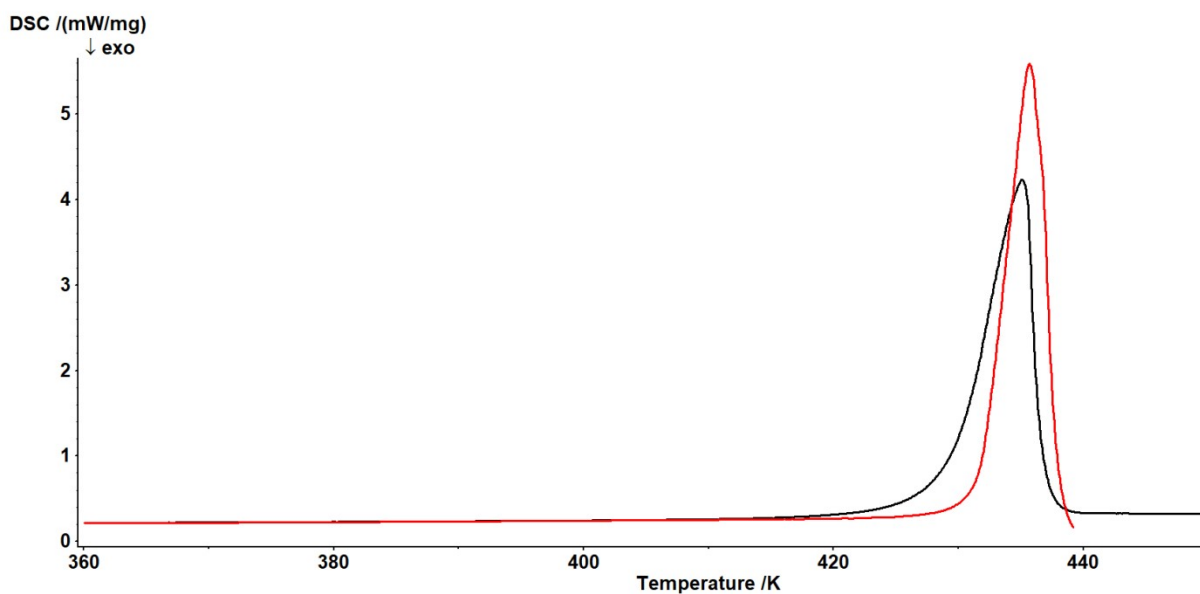


Fig. S5 DSC curves of the **B₂·cr** co-crystal, the first (red) and subsequent (black) heating runs.

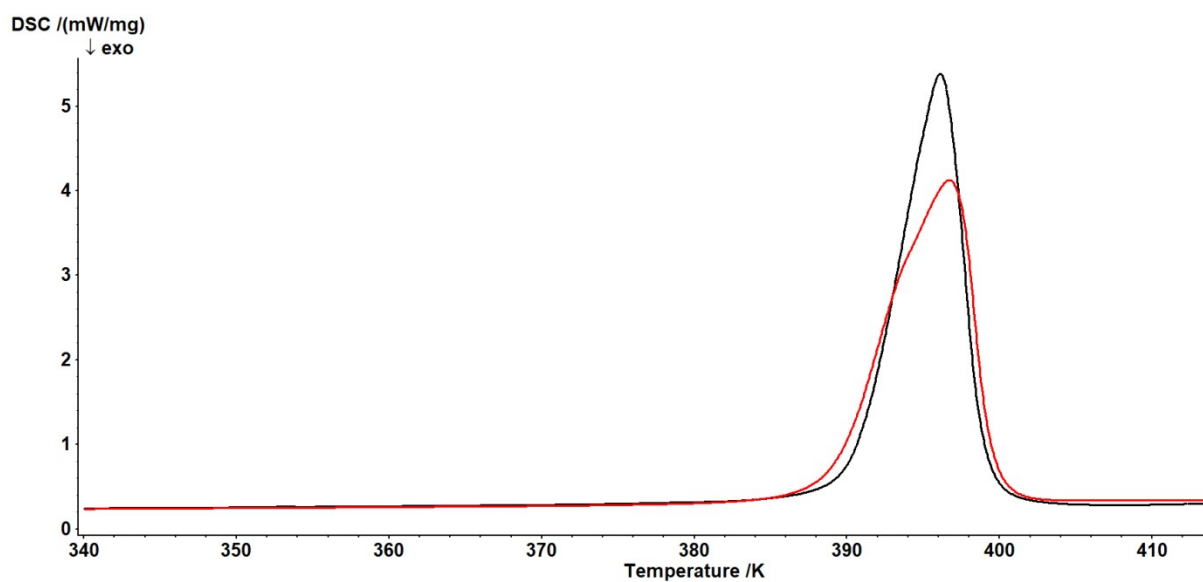


Fig. S6 DSC curves of the $E_2 \cdot cr$ co-crystal, the first (black) and subsequent (red) heating runs.

Computational Results

Optimised Geometries

molA_apfd

6	-0.002241	1.220370	-0.000000
6	-0.000810	0.496289	1.198091
6	-0.002353	-0.883420	1.194195
6	-0.006128	-1.613787	0.000000
6	-0.002353	-0.883420	-1.194195
6	-0.000810	0.496289	-1.198091
9	0.003702	1.139487	2.357759
9	0.005392	-1.563009	-2.349691
6	-0.001526	2.637314	-0.000000
7	-0.000474	3.792366	-0.000000
9	0.005392	-1.563009	2.349691
9	0.003702	1.139487	-2.357759
7	-0.051693	-2.972613	0.000000
1	0.147475	-3.459002	0.857966
1	0.147475	-3.459002	-0.857966

molA_b3lypd

6	-1.225628	0.000002	0.002241
6	-0.496045	1.197501	0.000830
6	0.883429	1.193636	0.002173
6	1.617896	-0.000001	0.006449
6	0.883426	-1.193638	0.002173
6	-0.496047	-1.197500	0.000830
9	-1.141919	2.364022	-0.003925
9	1.567000	-2.355543	-0.005991
6	-2.644206	0.000002	0.001773
7	-3.799120	-0.000000	0.000894
9	1.567004	2.355541	-0.005990
9	-1.141924	-2.364019	-0.003925
7	2.981588	-0.000003	0.052541
1	3.467161	0.859243	-0.147186
1	3.467158	-0.859251	-0.147185

molA_blyp

6	-0.003393	1.241276	-0.000000
6	-0.000978	0.500434	-1.206478
6	-0.000978	-0.890369	-1.201994
6	-0.005238	-1.634093	0.000000
6	-0.000978	-0.890369	1.201994
6	-0.000978	0.500434	1.206478
9	0.004005	1.152695	-2.390825
9	0.009060	-1.581966	2.381053
6	-0.005214	2.665111	-0.000000
7	-0.006104	3.833370	-0.000000
9	0.009060	-1.581966	-2.381053
9	0.004005	1.152695	2.390825
7	-0.057812	-3.009788	0.000000
1	0.159391	-3.496376	-0.863789

1	0.159391	-3.496376	0.863789
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molA_camb3lypd

6	-0.001781	1.218903	0.000000
6	-0.000825	0.493894	1.191622
6	-0.002149	-0.880460	1.188358
6	-0.005660	-1.611672	-0.000000
6	-0.002149	-0.880460	-1.188358
6	-0.000825	0.493894	-1.191622
9	0.002823	1.135703	2.353050
9	0.004232	-1.560514	-2.345180
6	-0.000881	2.639894	0.000000
7	0.000231	3.787983	0.000000
9	0.004232	-1.560514	2.345180
9	0.002823	1.135703	-2.353050
7	-0.040829	-2.969861	-0.000000
1	0.119585	-3.462218	0.862245
1	0.119585	-3.462218	-0.862246

molA_m062x

6	-1.216326	0.000001	0.002351
6	-0.493551	1.194856	0.001892
6	0.883780	1.191445	0.005665
6	1.613743	-0.000002	0.009755
6	0.883778	-1.191447	0.005665
6	-0.493553	-1.194855	0.001892
9	-1.134860	2.352906	-0.003513
9	1.562470	-2.343846	-0.001489
6	-2.641505	0.000002	-0.001365
7	-3.791101	0.000003	-0.004820
9	1.562474	2.343843	-0.001489
9	-1.134864	-2.352904	-0.003513
7	2.976241	-0.000003	0.060481
1	3.456524	0.858254	-0.157906
1	3.456523	-0.858260	-0.157906

molA_mp2

6	-1.219605	-0.000037	0.028708
6	-0.495667	1.200610	-0.001165
6	0.891347	1.194814	0.039345
6	1.623583	0.000013	0.012227
6	0.891427	-1.194821	0.039099
6	-0.495783	-1.200685	-0.001073
9	-1.142688	2.367094	-0.006717
9	1.568720	-2.352853	0.022325
6	-2.645411	-0.000217	-0.013212
7	-3.822807	-0.000438	-0.044048
9	1.568637	2.352899	0.022577
9	-1.142515	-2.367257	-0.006884
7	3.002328	0.000277	0.099516
1	3.453923	0.847123	-0.217705
1	3.454285	-0.846529	-0.217291

molA_pbe0d			
6	-0.003717	1.219879	0.000000
6	-0.001449	0.494968	-1.195749
6	-0.001702	-0.882044	-1.191800
6	-0.004838	-1.612753	-0.000000
6	-0.001702	-0.882044	1.191800
6	-0.001449	0.494968	1.195749
9	0.002644	1.136352	-2.352884
9	0.007355	-1.560781	2.344073
6	-0.004383	2.635891	0.000000
7	-0.004452	3.790102	0.000000
9	0.007355	-1.560781	-2.344073
9	0.002644	1.136352	2.352884
7	-0.050222	-2.971068	-0.000000
1	0.157305	-3.453462	-0.857946
1	0.157305	-3.453462	0.857946

molA_pbe			
6	-0.003901	1.234710	-0.000000
6	-0.001183	0.499477	-1.204864
6	-0.001183	-0.888635	-1.200188
6	-0.005165	-1.627710	0.000000
6	-0.001183	-0.888635	1.200188
6	-0.001183	0.499477	1.204864
9	0.003768	1.147835	-2.378920
9	0.009370	-1.576342	2.368383
6	-0.005869	2.653326	-0.000000
7	-0.006877	3.822416	-0.000000
9	0.009370	-1.576342	-2.368383
9	0.003768	1.147835	2.378920
7	-0.056770	-2.996352	0.000000
1	0.163504	-3.480692	-0.864112
1	0.163504	-3.480692	0.864112

molA_rtpss			
6	-0.005614	1.233295	0.000000
6	-0.001569	0.497975	-1.201692
6	-0.001569	-0.887092	-1.196543
6	-0.004352	-1.624822	-0.000000
6	-0.001569	-0.887092	1.196543
6	-0.001569	0.497975	1.201692
9	0.004423	1.146694	-2.376549
9	0.012182	-1.575354	2.365522
6	-0.007807	2.652316	0.000000
7	-0.008948	3.819220	0.000000
9	0.012182	-1.575354	-2.365522
9	0.004423	1.146694	2.376549
7	-0.072393	-2.998090	-0.000000
1	0.207397	-3.463676	-0.857223
1	0.207397	-3.463676	0.857223

molA_wb97xd

6	-0.002274	1.218789	-0.000000
6	-0.000835	0.494865	1.194704
6	-0.002594	-0.882889	1.191183
6	-0.005862	-1.613927	0.000000
6	-0.002594	-0.882889	-1.191183
6	-0.000835	0.494865	-1.194704
9	0.003255	1.136885	2.352886
9	0.005109	-1.560331	-2.346339
6	-0.001057	2.641620	-0.000000
7	0.000359	3.792608	-0.000000
9	0.005109	-1.560331	2.346339
9	0.003255	1.136885	-2.352886
7	-0.052054	-2.975642	0.000000
1	0.151950	-3.459854	0.857367
1	0.151950	-3.459854	-0.857367

molA_x3lyp

6	-0.003064	1.226476	0.000000
6	-0.001175	0.495887	-1.196634
6	-0.001315	-0.883351	-1.192789
6	-0.004827	-1.618636	-0.000000
6	-0.001315	-0.883351	1.192789
6	-0.001175	0.495887	1.196634
9	0.002796	1.139500	-2.363194
9	0.006854	-1.565337	2.354399
6	-0.003732	2.646164	0.000000
7	-0.003816	3.800423	0.000000
9	0.006854	-1.565337	-2.354399
9	0.002796	1.139500	2.363194
7	-0.048240	-2.981876	-0.000000
1	0.143705	-3.469687	-0.859552
1	0.143705	-3.469687	0.859552

molB_apfd

6	1.098969	-0.042821	0.001367
6	0.670232	1.289019	-0.000307
6	-0.659615	1.647905	0.001375
6	-1.647546	0.653485	0.004414
6	-1.235479	-0.686284	0.003719
6	0.100435	-1.025759	0.002429
9	1.595862	2.249023	-0.003096
9	-2.173027	-1.648285	-0.003116
6	2.472356	-0.390397	-0.000438
7	3.592439	-0.673378	-0.002372
9	0.439984	-2.307605	-0.001620
7	-2.979290	0.943531	0.047427
1	-3.280110	1.874508	-0.184132
1	-3.636662	0.205020	-0.141095
1	-0.925020	2.698675	0.006571

molB_b3lypd

6	1.103381	-0.043672	0.001449
6	0.669168	1.288448	-0.000317

6	-0.660273	1.650090	0.001527
6	-1.650903	0.654708	0.004737
6	-1.234884	-0.685050	0.003752
6	0.100547	-1.025419	0.002524
9	1.598291	2.256040	-0.003267
9	-2.178937	-1.651552	-0.003892
6	2.478651	-0.390527	-0.000332
7	3.598772	-0.672767	-0.002284
9	0.441112	-2.314523	-0.001929
7	-2.987773	0.946608	0.049169
1	-3.287177	1.876940	-0.190889
1	-3.643139	0.205893	-0.142449
1	-0.924984	2.699132	0.006898

molB_blyp

6	1.115746	-0.045595	0.000773
6	0.672694	1.297914	-0.005140
6	-0.665878	1.664247	-0.020117
6	-1.667391	0.663490	-0.029510
6	-1.246882	-0.686923	-0.020620
6	0.099140	-1.032160	-0.006338
9	1.613482	2.281669	0.003744
9	-2.203811	-1.667307	-0.017437
6	2.495766	-0.394849	0.015630
7	3.628527	-0.681105	0.028359
9	0.439999	-2.340621	0.006013
7	-3.014918	0.961533	-0.094375
1	-3.315129	1.897177	0.157816
1	-3.676643	0.218216	0.107332
1	-0.929868	2.720468	-0.031244

molB_camb3lypd

6	1.097090	-0.042277	0.001067
6	0.665678	1.282868	-0.000056
6	-0.659239	1.644388	0.001887
6	-1.644905	0.652166	0.004644
6	-1.229668	-0.681897	0.003534
6	0.100547	-1.020186	0.002142
9	1.590541	2.245319	-0.002282
9	-2.169296	-1.644150	-0.002716
6	2.474864	-0.388789	-0.000776
7	3.588489	-0.668971	-0.002703
9	0.439064	-2.303066	-0.001450
7	-2.977507	0.937516	0.039388
1	-3.287418	1.872307	-0.160897
1	-3.636390	0.193805	-0.119499
1	-0.922039	2.693505	0.006991

molB_m062x

6	1.094595	-0.041614	0.001308
6	0.667803	1.286993	0.000563
6	-0.660117	1.650659	0.003896
6	-1.646722	0.656231	0.006959

6	-1.234621	-0.681170	0.006036
6	0.098033	-1.021783	0.003033
9	1.593808	2.242807	-0.002590
9	-2.172418	-1.638702	-0.000573
6	2.475932	-0.391201	-0.002603
7	3.590688	-0.673054	-0.006264
9	0.435190	-2.301648	-0.001768
7	-2.983203	0.941282	0.053501
1	-3.283256	1.868433	-0.197660
1	-3.631276	0.196723	-0.149363
1	-0.922584	2.700393	0.010221

molB_mp2

6	1.098539	-0.042306	0.030965
6	0.670869	1.292179	0.002519
6	-0.667200	1.650690	0.038063
6	-1.657518	0.655150	0.011377
6	-1.243529	-0.684579	0.041364
6	0.100145	-1.027038	0.002027
9	1.601314	2.258174	-0.000661
9	-2.178144	-1.650372	0.023173
6	2.480564	-0.391701	-0.017725
7	3.621676	-0.680610	-0.053129
9	0.441254	-2.316390	-0.006798
7	-3.008115	0.955367	0.092074
1	-3.272098	1.858608	-0.275493
1	-3.631924	0.214376	-0.197688
1	-0.933983	2.702801	0.034630

molB_pbe0d

6	1.098809	-0.042197	0.001446
6	0.667374	1.286912	-0.000193
6	-0.660391	1.645349	0.001720
6	-1.647004	0.651388	0.004808
6	-1.232292	-0.685502	0.004000
6	0.101063	-1.023784	0.002506
9	1.588782	2.246217	-0.003017
9	-2.168117	-1.644786	-0.003529
6	2.471728	-0.387673	-0.000540
7	3.591360	-0.669003	-0.002631
9	0.440426	-2.302338	-0.001937
7	-2.978570	0.938132	0.048722
1	-3.279753	1.866295	-0.191909
1	-3.629631	0.195486	-0.144044
1	-0.925689	2.695515	0.007173

molB_pbe

6	1.112205	-0.044898	0.001670
6	0.672992	1.295628	-0.000807
6	-0.663519	1.658755	0.000747
6	-1.660553	0.659934	0.004348
6	-1.242316	-0.687553	0.003758
6	0.101309	-1.031265	0.002643

9	1.607118	2.269217	-0.004245
9	-2.191668	-1.659142	-0.005041
6	2.487299	-0.392498	0.000417
7	3.621042	-0.678522	-0.001136
9	0.441331	-2.328612	-0.002450
7	-3.001871	0.951643	0.054230
1	-3.303194	1.885780	-0.200149
1	-3.657815	0.203764	-0.148437
1	-0.928723	2.716819	0.005889

molB_rtpss

6	1.110345	-0.045330	0.002413
6	0.670393	1.292006	-0.001066
6	-0.663312	1.659422	0.000601
6	-1.656588	0.659863	0.003833
6	-1.239420	-0.683698	0.004464
6	0.100567	-1.028588	0.003237
9	1.607468	2.264718	-0.005379
9	-2.190652	-1.655073	-0.006688
6	2.486037	-0.392333	0.000844
7	3.617727	-0.677581	-0.001012
9	0.439874	-2.327007	-0.002966
7	-3.003449	0.950101	0.069238
1	-3.292093	1.868097	-0.250495
1	-3.637914	0.198849	-0.183304
1	-0.928280	2.713611	0.005552

molB_wb97xd

6	1.097465	-0.040721	0.001252
6	0.665383	1.286656	-0.000100
6	-0.663396	1.644134	0.002036
6	-1.648093	0.648776	0.004756
6	-1.232104	-0.687370	0.003925
6	0.102460	-1.023491	0.002350
9	1.585675	2.249193	-0.002533
9	-2.166789	-1.650462	-0.003133
6	2.477477	-0.385839	-0.000911
7	3.594398	-0.664815	-0.003142
9	0.444518	-2.302575	-0.001500
7	-2.982611	0.939100	0.047820
1	-3.280197	1.868662	-0.191017
1	-3.637361	0.200162	-0.145114
1	-0.930739	2.692896	0.008042

molB_x3llyp

6	1.104333	-0.043364	0.001342
6	0.668351	1.287980	-0.000342
6	-0.661153	1.649157	0.001390
6	-1.651912	0.654027	0.004423
6	-1.234117	-0.684918	0.003497
6	0.101226	-1.024556	0.002374
9	1.595156	2.256245	-0.003087
9	-2.176122	-1.651947	-0.003702

6	2.480856	-0.389799	-0.000325
7	3.600482	-0.671337	-0.002150
9	0.440247	-2.312949	-0.001826
7	-2.988638	0.944141	0.047508
1	-3.291725	1.875299	-0.183704
1	-3.645358	0.203085	-0.137074
1	-0.924857	2.698687	0.006659

molC_apfd

6	1.264071	-0.448127	0.001608
6	0.355901	-1.516953	-0.000132
6	-0.991944	-1.259553	0.001507
6	-1.523999	0.038220	0.006255
6	-0.598685	1.085142	0.002560
6	0.765546	0.855943	0.000958
9	-1.066861	2.341194	-0.004967
6	2.665567	-0.678760	0.000586
7	3.802793	-0.883358	-0.000816
9	1.591002	1.896645	-0.003371
7	-2.865420	0.269953	0.056190
1	-3.483447	-0.493676	-0.162054
1	-3.196728	1.194775	-0.162181
9	-1.879463	-2.274412	-0.007204
1	0.710543	-2.540206	-0.003900

molC_b3lypd

6	1.269803	-0.446310	0.001690
6	0.359026	-1.517555	-0.000128
6	-0.989091	-1.259519	0.001404
6	-1.527414	0.036833	0.006678
6	-0.600574	1.084623	0.002512
6	0.763504	0.856907	0.001037
9	-1.073795	2.346851	-0.005465
6	2.672760	-0.677351	0.000761
7	3.809267	-0.885332	-0.000585
9	1.591814	1.904976	-0.003569
7	-2.874370	0.266109	0.057252
1	-3.489696	-0.500605	-0.161580
1	-3.206960	1.191068	-0.162328
9	-1.878955	-2.283217	-0.007890
1	0.712710	-2.539161	-0.004166

molC_blyp

6	1.285032	-0.451037	0.001702
6	0.362758	-1.529856	-0.000614
6	-0.995025	-1.268120	0.000682
6	-1.542644	0.037232	0.006421
6	-0.605403	1.092246	0.001987
6	0.769624	0.863164	0.000863
9	-1.084297	2.372676	-0.006946
6	2.692866	-0.684824	0.001609
7	3.842059	-0.897326	0.000874
9	1.607275	1.927681	-0.004204

7	-2.900812	0.267475	0.063424
1	-3.518744	-0.504434	-0.166116
1	-3.235986	1.197563	-0.166683
9	-1.895664	-2.309108	-0.009738
1	0.716920	-2.558246	-0.005199

molC_camb3lypd

6	1.262675	-0.444884	0.001465
6	0.357290	-1.511696	0.000127
6	-0.985928	-1.254332	0.001706
6	-1.521397	0.036828	0.006317
6	-0.599103	1.079353	0.002561
6	0.760183	0.851513	0.000980
9	-1.068870	2.336134	-0.004194
6	2.668678	-0.673644	0.000218
7	3.798873	-0.878172	-0.001286
9	1.583844	1.895139	-0.002868
7	-2.863698	0.265080	0.048289
1	-3.484468	-0.503196	-0.142742
1	-3.201009	1.193215	-0.143825
9	-1.873200	-2.271638	-0.006219
1	0.708898	-2.533924	-0.003162

molC_m062x

6	1.260165	-0.447200	0.001486
6	0.355960	-1.517589	0.000983
6	-0.990432	-1.258371	0.005181
6	-1.523450	0.036588	0.010640
6	-0.601213	1.081506	0.006320
6	0.761054	0.852277	0.002044
9	-1.069133	2.334103	-0.000366
6	2.671326	-0.672085	-0.002691
7	3.803964	-0.871386	-0.006671
9	1.583658	1.892431	-0.003389
7	-2.869720	0.266556	0.066513
1	-3.478906	-0.499240	-0.174070
1	-3.195373	1.189330	-0.174100
9	-1.878061	-2.268316	-0.002723
1	0.708189	-2.540287	-0.003532

molC_mp2

6	1.265260	-0.447217	0.021945
6	0.358417	-1.523947	-0.001924
6	-0.998868	-1.261046	0.029719
6	-1.534237	0.037019	0.009270
6	-0.607359	1.085420	0.034969
6	0.764778	0.858988	-0.002321
9	-1.074605	2.342946	0.022738
6	2.676294	-0.675528	-0.012787
7	3.835964	-0.880027	-0.040372
9	1.592603	1.907342	-0.005451
7	-2.894715	0.271128	0.100740
1	-3.478816	-0.487477	-0.223652

1	-3.196268	1.179840	-0.223758
9	-1.882554	-2.280099	0.016425
1	0.712136	-2.549024	0.000084

molC_pbe0d

6	1.264277	-0.444813	0.001735
6	0.357623	-1.513755	-0.000068
6	-0.988262	-1.257743	0.001771
6	-1.523344	0.036572	0.006748
6	-0.599993	1.082613	0.002883
6	0.761970	0.855843	0.001068
9	-1.069532	2.334602	-0.005161
6	2.665104	-0.673639	0.000533
7	3.801439	-0.878425	-0.001027
9	1.583407	1.895843	-0.003515
7	-2.864808	0.265137	0.057903
1	-3.477012	-0.500781	-0.167556
1	-3.194681	1.188274	-0.168466
9	-1.871801	-2.271391	-0.007550
1	0.712366	-2.536420	-0.004095

molC_pbe

6	1.278357	-0.451184	0.001773
6	0.359949	-1.526663	-0.000561
6	-0.994932	-1.265768	0.001046
6	-1.537289	0.037960	0.006802
6	-0.603341	1.090537	0.002381
6	0.768960	0.861043	0.000919
9	-1.078413	2.360152	-0.006751
6	2.681413	-0.682322	0.001455
7	3.832138	-0.890748	0.000523
9	1.601193	1.915605	-0.004239
7	-2.887928	0.268337	0.062885
1	-3.504729	-0.503934	-0.167833
1	-3.220587	1.198781	-0.168656
9	-1.891483	-2.293845	-0.009560
1	0.715471	-2.556808	-0.005299

molC_rtpss

6	1.275750	-0.452156	0.002486
6	0.359563	-1.527891	-0.000765
6	-0.992972	-1.261549	0.001290
6	-1.533823	0.038426	0.006531
6	-0.601901	1.087358	0.002983
6	0.766938	0.857271	0.001105
9	-1.076296	2.358238	-0.008486
6	2.679816	-0.681327	0.001994
7	3.828582	-0.888559	0.000784
9	1.600838	1.911781	-0.005119
7	-2.889111	0.269526	0.079055
1	-3.486580	-0.499013	-0.208300
1	-3.204571	1.190171	-0.209081
9	-1.893319	-2.288303	-0.011831

1	0.713630	-2.554185	-0.006316
molC_wb97xd			
6	1.263473	-0.441516	0.001680
6	0.360408	-1.511820	0.000008
6	-0.986366	-1.257891	0.001872
6	-1.524183	0.035008	0.006155
6	-0.603046	1.082015	0.002816
6	0.760355	0.856913	0.000932
9	-1.073055	2.335732	-0.004726
6	2.671309	-0.671303	0.000274
7	3.804176	-0.877373	-0.001422
9	1.581353	1.899022	-0.003070
7	-2.870077	0.261550	0.057401
1	-3.481389	-0.504503	-0.168771
1	-3.202384	1.183239	-0.170083
9	-1.866367	-2.277305	-0.006875
1	0.716009	-2.533451	-0.003385
molC_x3lyp			
6	1.270700	-0.445733	0.001590
6	0.359600	-1.516615	-0.000142
6	-0.988516	-1.259238	0.001265
6	-1.528313	0.036245	0.006304
6	-0.601380	1.083469	0.002312
6	0.762654	0.856504	0.000957
9	-1.073662	2.344897	-0.005235
6	2.674936	-0.675975	0.000732
7	3.810938	-0.883040	-0.000514
9	1.588121	1.905468	-0.003413
7	-2.875000	0.264813	0.055612
1	-3.492197	-0.502053	-0.156566
1	-3.210161	1.190220	-0.157330
9	-1.876605	-2.282986	-0.007569
1	0.712021	-2.538925	-0.003958
molD_apfd			
6	-1.467317	-0.071548	0.006116
6	-0.712993	-1.248911	0.005093
6	0.667134	-1.212440	0.004286
6	1.318709	0.023826	0.000544
6	0.572016	1.189351	0.003197
6	-0.826767	1.185381	0.010213
7	-1.518241	2.356236	0.057191
9	-1.333472	-2.422690	0.002317
9	1.188180	2.379976	-0.004406
17	3.028429	0.089480	-0.008243
6	-2.883765	-0.121358	-0.005917
7	-4.039168	-0.079617	-0.021922
1	-1.028579	3.212441	-0.139727
1	-2.509645	2.344449	-0.122280
9	1.365301	-2.344434	0.003921

molD_b3lypd				
6	-1.475352	-0.075063	0.005914	
6	-0.713356	-1.249485	0.004891	
6	0.666778	-1.211831	0.004310	
6	1.320907	0.024946	0.000730	
6	0.568538	1.188138	0.003081	
6	-0.831672	1.184650	0.010165	
7	-1.526062	2.359746	0.057668	
9	-1.334556	-2.431401	0.001947	
9	1.182768	2.388770	-0.005155	
17	3.045495	0.093486	-0.008223	
6	-2.893169	-0.124525	-0.005543	
7	-4.048233	-0.078898	-0.021237	
1	-1.032965	3.215474	-0.136767	
1	-2.516971	2.349282	-0.127549	
9	1.367404	-2.350805	0.004074	

molD_blyp				
6	-1.494658	-0.069314	-0.005555	
6	-0.725261	-1.254050	-0.005194	
6	0.667075	-1.221396	-0.004929	
6	1.333003	0.021748	-0.000683	
6	0.575563	1.195724	-0.002723	
6	-0.836210	1.199988	-0.010468	
7	-1.529535	2.389249	-0.065235	
9	-1.355802	-2.452180	-0.002194	
9	1.202445	2.411729	0.006807	
17	3.076616	0.085377	0.009210	
6	-2.917846	-0.118632	0.007186	
7	-4.086550	-0.078709	0.023807	
1	-1.028092	3.246149	0.143555	
1	-2.525394	2.384203	0.135954	
9	1.370425	-2.379544	-0.005933	

molD_camb3lypd				
6	-1.466886	-0.072251	0.004725	
6	-0.710217	-1.242864	0.003508	
6	0.663731	-1.207197	0.003078	
6	1.316647	0.023689	0.000729	
6	0.568254	1.181300	0.002727	
6	-0.827417	1.179661	0.008059	
7	-1.513902	2.353691	0.043462	
9	-1.329915	-2.418303	0.001100	
9	1.179027	2.376804	-0.003601	
17	3.032397	0.091033	-0.005938	
6	-2.887258	-0.123182	-0.003376	
7	-4.035656	-0.081715	-0.015152	
1	-1.015699	3.213797	-0.108138	
1	-2.509829	2.354731	-0.104445	
9	1.359838	-2.342373	0.002351	

molD_m062x

6	-1.467327	-0.073534	0.008229
6	-0.711958	-1.246925	0.004091
6	0.665143	-1.208755	0.002729
6	1.315824	0.025886	0.001262
6	0.566502	1.186459	0.006451
6	-0.831275	1.181224	0.013307
7	-1.523207	2.356507	0.066272
9	-1.329269	-2.419757	-0.000623
9	1.175282	2.377527	0.000357
17	3.028912	0.094861	-0.008156
6	-2.892146	-0.123516	-0.001969
7	-4.041957	-0.079390	-0.017107
1	-1.026509	3.206388	-0.146742
1	-2.510772	2.344341	-0.139014
9	1.362311	-2.338831	-0.000781

mo1D_mp2

6	-1.469400	-0.072205	0.040472
6	-0.714684	-1.251622	-0.007898
6	0.672804	-1.210760	0.008309
6	1.331736	0.025232	-0.021833
6	0.571173	1.192526	0.034664
6	-0.828861	1.187174	0.016520
7	-1.536501	2.371647	0.116342
9	-1.336898	-2.432826	-0.011697
9	1.184994	2.386478	0.028333
17	3.042878	0.095770	-0.013818
6	-2.895038	-0.120354	0.015317
7	-4.072718	-0.074346	-0.009704
1	-1.040111	3.197005	-0.190490
1	-2.497307	2.336230	-0.199969
9	1.367486	-2.347466	-0.016242

mo1D_pbe0d

6	-1.466533	-0.076556	-0.006563
6	-0.708396	-1.249347	-0.005281
6	0.669011	-1.209943	-0.004459
6	1.318556	0.025923	-0.000600
6	0.567875	1.187180	-0.003446
6	-0.828988	1.180823	-0.010721
7	-1.522842	2.349393	-0.059039
9	-1.324497	-2.421969	-0.002354
9	1.176908	2.377818	0.004828
17	3.027226	0.096158	0.008717
6	-2.881798	-0.125706	0.005771
7	-4.036266	-0.081483	0.022462
1	-1.031996	3.203312	0.143480
1	-2.512209	2.333892	0.129441
9	1.367228	-2.338238	-0.003950

mo1D_pbe

6	-1.484027	-0.076804	-0.006551
6	-0.716100	-1.257597	-0.005904

6	0.673317	-1.218611	-0.005216
6	1.330354	0.025768	-0.000523
6	0.571583	1.195695	-0.003217
6	-0.836054	1.191818	-0.011572
7	-1.534024	2.369191	-0.065387
9	-1.338355	-2.447506	-0.002860
9	1.189253	2.402998	0.006447
17	3.053891	0.095992	0.010044
6	-2.901734	-0.124823	0.007773
7	-4.071085	-0.077842	0.025997
1	-1.039314	3.229052	0.146347
1	-2.530967	2.352505	0.130758
9	1.378642	-2.362774	-0.005907

molD_rtpss

6	-1.481715	-0.074828	-0.008201
6	-0.715354	-1.253600	-0.007545
6	0.670869	-1.216150	-0.006999
6	1.327915	0.024497	-0.000730
6	0.570028	1.191747	-0.003912
6	-0.833424	1.189801	-0.012921
7	-1.531691	2.372835	-0.086593
9	-1.339520	-2.443544	-0.003725
9	1.189490	2.399191	0.008442
17	3.051624	0.094345	0.012769
6	-2.900357	-0.122554	0.010013
7	-4.067531	-0.079200	0.033133
1	-1.032604	3.211087	0.191860
1	-2.513517	2.345707	0.174013
9	1.376174	-2.361155	-0.007712

molD_wb97xd

6	-1.466868	-0.072000	0.005999
6	-0.711525	-1.246127	0.004454
6	0.665825	-1.209979	0.003830
6	1.318382	0.023700	0.000597
6	0.569960	1.185259	0.003178
6	-0.828097	1.182119	0.009310
7	-1.519644	2.356326	0.055902
9	-1.331151	-2.418340	0.001829
9	1.181223	2.376997	-0.004341
17	3.035850	0.091143	-0.007499
6	-2.889128	-0.123079	-0.004484
7	-4.040559	-0.083793	-0.019505
1	-1.026199	3.210115	-0.139162
1	-2.509110	2.348300	-0.130397
9	1.360592	-2.342539	0.003064

molD_x31yp

6	-1.476533	-0.070127	-0.005323
6	-0.716158	-1.245708	-0.004428
6	0.663687	-1.211852	-0.003997
6	1.321462	0.022355	-0.000684

6	0.571231	1.186363	-0.002775
6	-0.829230	1.187685	-0.009303
7	-1.516906	2.366506	-0.055123
9	-1.338249	-2.425892	-0.001693
9	1.187465	2.384917	0.004937
17	3.046273	0.087013	0.007565
6	-2.895668	-0.120774	0.005091
7	-4.050367	-0.082394	0.019459
1	-1.018929	3.221221	0.130594
1	-2.508703	2.364717	0.124256
9	1.359580	-2.352537	-0.003834

molE_apfd

6	-1.378126	-0.097816	0.004863
6	-0.770543	-1.357430	0.004564
6	0.595823	-1.523823	0.003972
6	1.390196	-0.375373	0.000985
6	0.817846	0.881800	0.002499
6	-0.571848	1.061568	0.007852
7	-1.098768	2.310222	0.041173
9	-1.559931	-2.433421	0.002854
9	1.580764	1.987181	-0.003570
17	3.106120	-0.512605	-0.005719
1	1.033866	-2.512921	0.004021
6	-2.787779	0.046075	-0.004507
7	-3.926689	0.247028	-0.016821
1	-0.497924	3.103259	-0.101606
1	-2.089108	2.438072	-0.089293

molE_b3lypd

6	-1.385641	-0.102032	0.005058
6	-0.768272	-1.358292	0.004732
6	0.598860	-1.522703	0.004257
6	1.392256	-0.370967	0.001185
6	0.812493	0.883565	0.002616
6	-0.578693	1.061585	0.008308
7	-1.110526	2.314103	0.044419
9	-1.556123	-2.445374	0.002786
9	1.573489	2.000118	-0.004350
17	3.123013	-0.511401	-0.006061
1	1.038728	-2.508781	0.004374
6	-2.796970	0.038945	-0.004485
7	-3.935518	0.240708	-0.017398
1	-0.508259	3.105601	-0.106886
1	-2.099863	2.440022	-0.099551

molE_blyp

6	-1.403862	-0.097443	-0.005208
6	-0.777828	-1.363377	-0.005658
6	0.599698	-1.533656	-0.005477
6	1.402848	-0.376445	-0.001479
6	0.818996	0.889097	-0.002513
6	-0.582695	1.074683	-0.009011

7	-1.113462	2.340838	-0.053587
9	-1.575121	-2.467923	-0.003682
9	1.593363	2.019935	0.006093
17	3.153065	-0.523804	0.006976
1	1.037712	-2.527829	-0.006544
6	-2.820791	0.042218	0.006059
7	-3.973947	0.237912	0.020716
1	-0.503811	3.132040	0.121336
1	-2.106525	2.470637	0.114741

molE_camb3lypd

6	-1.377347	-0.099480	0.002430
6	-0.765464	-1.351960	0.002031
6	0.595420	-1.518973	0.001782
6	1.387502	-0.372077	0.000577
6	0.811337	0.876508	0.001404
6	-0.575231	1.056767	0.004097
7	-1.098267	2.306854	0.020189
9	-1.553493	-2.430705	0.001031
9	1.568841	1.988211	-0.001855
17	3.109069	-0.510248	-0.002750
1	1.032599	-2.506002	0.001634
6	-2.791188	0.041070	-0.001748
7	-3.923537	0.239017	-0.007639
1	-0.490018	3.103556	-0.050366
1	-2.092428	2.446859	-0.048393

molE_m062x

6	-1.377613	-0.101737	0.006247
6	-0.766676	-1.356913	0.004139
6	0.598153	-1.521457	0.003212
6	1.387852	-0.369607	0.001430
6	0.810380	0.881727	0.004472
6	-0.579017	1.057976	0.009888
7	-1.107607	2.309409	0.048555
9	-1.553461	-2.431454	0.001260
9	1.563981	1.989935	-0.001163
17	3.107559	-0.499229	-0.005931
1	1.038576	-2.507846	0.001853
6	-2.795736	0.040272	-0.002406
7	-3.929071	0.241265	-0.014819
1	-0.502476	3.097378	-0.112079
1	-2.095871	2.435379	-0.105655

molE_mp2

6	-1.379788	-0.099004	0.046510
6	-0.771074	-1.360187	-0.005389
6	0.603880	-1.521218	0.008278
6	1.404383	-0.371747	-0.018577
6	0.815849	0.887736	0.040621
6	-0.575534	1.062909	0.023483
7	-1.118550	2.327910	0.117384
9	-1.560999	-2.445080	-0.012662

9	1.573850	1.998117	0.032512
17	3.120497	-0.505271	-0.017395
1	1.043149	-2.511390	-0.024581
6	-2.799020	0.044894	0.016851
7	-3.959538	0.249494	-0.009874
1	-0.517562	3.085089	-0.176675
1	-2.080568	2.422846	-0.181479

molE_pbe0d

6	-1.377694	-0.102988	-0.005333
6	-0.765013	-1.357997	-0.004832
6	0.599587	-1.520277	-0.004201
6	1.390747	-0.370718	-0.001054
6	0.813135	0.882134	-0.002780
6	-0.575187	1.057866	-0.008467
7	-1.105618	2.304046	-0.043631
9	-1.547956	-2.434433	-0.002955
9	1.567843	1.989203	0.003961
17	3.105260	-0.506274	0.006238
1	1.041240	-2.507062	-0.004123
6	-2.786144	0.040335	0.004524
7	-3.923926	0.242844	0.017687
1	-0.504542	3.095142	0.106892
1	-2.094881	2.427304	0.096611

molE_pbe

6	-1.394226	-0.102701	-0.005780
6	-0.771846	-1.366172	-0.005988
6	0.603205	-1.531368	-0.005502
6	1.401877	-0.375352	-0.001329
6	0.818326	0.887653	-0.002809
6	-0.580009	1.067632	-0.009561
7	-1.113510	2.323724	-0.051516
9	-1.563178	-2.460031	-0.004036
9	1.584007	2.009746	0.005562
17	3.132110	-0.512906	0.007392
1	1.046034	-2.525801	-0.006295
6	-2.805092	0.041805	0.006295
7	-3.957297	0.248326	0.021647
1	-0.507639	3.118645	0.118057
1	-2.109478	2.445783	0.105979

molE_rtpss

6	-1.391166	-0.100228	-0.008098
6	-0.770820	-1.361721	-0.008579
6	0.601786	-1.533684	-0.008209
6	1.397948	-0.377722	-0.001977
6	0.816027	0.883000	-0.003825
6	-0.577373	1.065870	-0.012018
7	-1.109593	2.327883	-0.076671
9	-1.567317	-2.453619	-0.005861
9	1.584757	2.004227	0.008226
17	3.129078	-0.512870	0.010459

1	1.042469	-2.524646	-0.009271
6	-2.802946	0.044683	0.009084
7	-3.953415	0.247705	0.030890
1	-0.501888	3.099820	0.174021
1	-2.091547	2.437845	0.158356

molE_wb97xd

6	-1.377759	-0.100649	0.004680
6	-0.765410	-1.355590	0.003896
6	0.598743	-1.518832	0.003399
6	1.389735	-0.369379	0.000890
6	0.812637	0.882399	0.002471
6	-0.577085	1.058848	0.007168
7	-1.106750	2.308974	0.039590
9	-1.548774	-2.433686	0.002271
9	1.568136	1.991547	-0.003461
17	3.112831	-0.509496	-0.005220
1	1.038719	-2.505547	0.003154
6	-2.793610	0.038462	-0.003467
7	-3.929518	0.233202	-0.014841
1	-0.504822	3.101215	-0.098733
1	-2.095927	2.438225	-0.092433

molE_x31yp

6	-1.386772	-0.098070	-0.004419
6	-0.770427	-1.354998	-0.004180
6	0.596098	-1.522445	-0.003824
6	1.392073	-0.372885	-0.001070
6	0.813759	0.881764	-0.002287
6	-0.577221	1.063700	-0.007376
7	-1.102672	2.318600	-0.040951
9	-1.558676	-2.440345	-0.002446
9	1.575718	1.996539	0.004019
17	3.122728	-0.515344	0.005388
1	1.032509	-2.510299	-0.003996
6	-2.799643	0.041071	0.004005
7	-3.938924	0.234948	0.015446
1	-0.496272	3.108990	0.098399
1	-2.092041	2.452751	0.093290

Internal Coordinates

molA_apfd

I=	1	J=	2	B=	1.399900
I=	1	J=	6	B=	1.399900
I=	1	J=	9	B=	1.416944
I=	2	J=	3	B=	1.379715
I=	2	J=	7	B=	1.326105
I=	3	J=	4	B=	1.399840
I=	3	J=	11	B=	1.340549
I=	4	J=	5	B=	1.399840
I=	4	J=	13	B=	1.359589
I=	5	J=	6	B=	1.379715
I=	5	J=	8	B=	1.340549
I=	6	J=	12	B=	1.326105
I=	9	J=	10	B=	1.155051
I=	13	J=	14	B=	1.006155
I=	13	J=	15	B=	1.006155

I=	1	J=	2	K=	3	A=	120.985
I=	1	J=	2	K=	7	A=	119.838
I=	1	J=	6	K=	12	A=	119.838
I=	1	J=	9	K=	10	A=	179.977
I=	2	J=	3	K=	4	A=	121.612
I=	2	J=	3	K=	11	A=	120.298
I=	3	J=	4	K=	5	A=	117.100
I=	3	J=	4	K=	13	A=	121.436
I=	4	J=	5	K=	6	A=	121.612
I=	4	J=	5	K=	8	A=	118.089
I=	4	J=	13	K=	14	A=	118.458
I=	4	J=	13	K=	15	A=	118.458
I=	5	J=	6	K=	12	A=	119.176

I=	1	J=	2	K=	3	L=	4	D=	0.035
I=	1	J=	2	K=	3	L=	11	D=	179.686
I=	2	J=	3	K=	4	L=	5	D=	0.273
I=	2	J=	3	K=	4	L=	13	D=	177.824
I=	3	J=	4	K=	5	L=	6	D=	0.273
I=	3	J=	4	K=	5	L=	8	D=	179.455
I=	3	J=	4	K=	13	L=	14	D=	15.084
I=	3	J=	4	K=	13	L=	15	D=	166.903
I=	4	J=	5	K=	6	L=	12	D=	179.954

molA_b3lypd

I=	1	J=	2	B=	1.402247
I=	1	J=	6	B=	1.402249
I=	1	J=	9	B=	1.418578
I=	2	J=	3	B=	1.379480
I=	2	J=	7	B=	1.333397
I=	3	J=	4	B=	1.401510
I=	3	J=	11	B=	1.348097
I=	4	J=	5	B=	1.401511
I=	4	J=	13	B=	1.364471

I=	5	J=	6	B=	1.379479
I=	5	J=	8	B=	1.348096
I=	6	J=	12	B=	1.333397
I=	9	J=	10	B=	1.154914
I=	13	J=	14	B=	1.006964
I=	13	J=	15	B=	1.006964

I=	1	J=	2	K=	3	A=	121.191
I=	1	J=	2	K=	7	A=	119.676
I=	1	J=	6	K=	12	A=	119.676
I=	1	J=	9	K=	10	A=	179.975
I=	2	J=	3	K=	4	A=	121.765
I=	2	J=	3	K=	11	A=	120.308
I=	3	J=	4	K=	5	A=	116.790
I=	3	J=	4	K=	13	A=	121.591
I=	4	J=	5	K=	6	A=	121.765
I=	4	J=	5	K=	8	A=	117.926
I=	4	J=	13	K=	14	A=	118.375
I=	4	J=	13	K=	15	A=	118.375
I=	5	J=	6	K=	12	A=	119.133

I=	1	J=	2	K=	3	L=	4	D=	0.070
I=	1	J=	2	K=	3	L=	11	D=	179.667
I=	2	J=	3	K=	4	L=	5	D=	0.327
I=	2	J=	3	K=	4	L=	13	D=	177.792
I=	3	J=	4	K=	5	L=	6	D=	0.327
I=	3	J=	4	K=	5	L=	8	D=	179.416
I=	3	J=	4	K=	13	L=	14	D=	15.097
I=	3	J=	4	K=	13	L=	15	D=	166.874
I=	4	J=	5	K=	6	L=	12	D=	179.968

molA_blyp

I=	1	J=	2	B=	1.415783
I=	1	J=	6	B=	1.415783
I=	1	J=	9	B=	1.423836
I=	2	J=	3	B=	1.390810
I=	2	J=	7	B=	1.352090
I=	3	J=	4	B=	1.413483
I=	3	J=	11	B=	1.366963
I=	4	J=	5	B=	1.413483
I=	4	J=	13	B=	1.376699
I=	5	J=	6	B=	1.390810
I=	5	J=	8	B=	1.366963
I=	6	J=	12	B=	1.352090
I=	9	J=	10	B=	1.168259
I=	13	J=	14	B=	1.014927
I=	13	J=	15	B=	1.014927

I=	1	J=	2	K=	3	A=	121.367
I=	1	J=	2	K=	7	A=	119.605
I=	1	J=	6	K=	12	A=	119.605
I=	1	J=	9	K=	10	A=	179.970
I=	2	J=	3	K=	4	A=	121.931
I=	2	J=	3	K=	11	A=	120.209
I=	3	J=	4	K=	5	A=	116.506

I=	3	J=	4	K=	13	A=	121.729
I=	4	J=	5	K=	6	A=	121.931
I=	4	J=	5	K=	8	A=	117.859
I=	4	J=	13	K=	14	A=	118.093
I=	4	J=	13	K=	15	A=	118.093
I=	5	J=	6	K=	12	A=	119.028

I=	1	J=	2	K=	3	L=	4	D=	0.089
I=	1	J=	2	K=	3	L=	11	D=	179.628
I=	2	J=	3	K=	4	L=	5	D=	0.387
I=	2	J=	3	K=	4	L=	13	D=	177.426
I=	3	J=	4	K=	5	L=	6	D=	0.387
I=	3	J=	4	K=	5	L=	8	D=	179.336
I=	3	J=	4	K=	13	L=	14	D=	16.409
I=	3	J=	4	K=	13	L=	15	D=	165.893
I=	4	J=	5	K=	6	L=	12	D=	179.962

molA_camb3lypd

I=	1	J=	2	B=	1.394848
I=	1	J=	6	B=	1.394848
I=	1	J=	9	B=	1.420991
I=	2	J=	3	B=	1.374357
I=	2	J=	7	B=	1.326970
I=	3	J=	4	B=	1.395306
I=	3	J=	11	B=	1.341921
I=	4	J=	5	B=	1.395306
I=	4	J=	13	B=	1.358644
I=	5	J=	6	B=	1.374357
I=	5	J=	8	B=	1.341921
I=	6	J=	12	B=	1.326970
I=	9	J=	10	B=	1.148090
I=	13	J=	14	B=	1.005790
I=	13	J=	15	B=	1.005790

I=	1	J=	2	K=	3	A=	121.181
I=	1	J=	2	K=	7	A=	119.758
I=	1	J=	6	K=	12	A=	119.758
I=	1	J=	9	K=	10	A=	179.981
I=	2	J=	3	K=	4	A=	121.741
I=	2	J=	3	K=	11	A=	120.313
I=	3	J=	4	K=	5	A=	116.790
I=	3	J=	4	K=	13	A=	121.597
I=	4	J=	5	K=	6	A=	121.741
I=	4	J=	5	K=	8	A=	117.946
I=	4	J=	13	K=	14	A=	119.028
I=	4	J=	13	K=	15	A=	119.028
I=	5	J=	6	K=	12	A=	119.061

I=	1	J=	2	K=	3	L=	4	D=	0.056
I=	1	J=	2	K=	3	L=	11	D=	179.731
I=	2	J=	3	K=	4	L=	5	D=	0.259
I=	2	J=	3	K=	4	L=	13	D=	178.323
I=	3	J=	4	K=	5	L=	6	D=	0.259
I=	3	J=	4	K=	5	L=	8	D=	179.534
I=	3	J=	4	K=	13	L=	14	D=	12.095

I=	3	J=	4	K=	13	L=	15	D=	169.392
I=	4	J=	5	K=	6	L=	12	D=	179.986

molA_m062x

I=	1	J=	2	B=	1.396454
I=	1	J=	6	B=	1.396454
I=	1	J=	9	B=	1.425184
I=	2	J=	3	B=	1.377340
I=	2	J=	7	B=	1.323777
I=	3	J=	4	B=	1.397286
I=	3	J=	11	B=	1.337422
I=	4	J=	5	B=	1.397286
I=	4	J=	13	B=	1.363441
I=	5	J=	6	B=	1.377340
I=	5	J=	8	B=	1.337422
I=	6	J=	12	B=	1.323777
I=	9	J=	10	B=	1.149601
I=	13	J=	14	B=	1.007458
I=	13	J=	15	B=	1.007457

I=	1	J=	2	K=	3	A=	121.028
I=	1	J=	2	K=	7	A=	119.853
I=	1	J=	6	K=	12	A=	119.853
I=	1	J=	9	K=	10	A=	179.977
I=	2	J=	3	K=	4	A=	121.637
I=	2	J=	3	K=	11	A=	120.352
I=	3	J=	4	K=	5	A=	117.010
I=	3	J=	4	K=	13	A=	121.477
I=	4	J=	5	K=	6	A=	121.637
I=	4	J=	5	K=	8	A=	118.010
I=	4	J=	13	K=	14	A=	117.926
I=	4	J=	13	K=	15	A=	117.926
I=	5	J=	6	K=	12	A=	119.119

I=	1	J=	2	K=	3	L=	4	D=	0.016
I=	1	J=	2	K=	3	L=	11	D=	179.669
I=	2	J=	3	K=	4	L=	5	D=	0.193
I=	2	J=	3	K=	4	L=	13	D=	177.683
I=	3	J=	4	K=	5	L=	6	D=	0.193
I=	3	J=	4	K=	5	L=	8	D=	179.468
I=	3	J=	4	K=	13	L=	14	D=	16.491
I=	3	J=	4	K=	13	L=	15	D=	165.728
I=	4	J=	5	K=	6	L=	12	D=	179.920

molA_mp2

I=	1	J=	2	B=	1.402330
I=	1	J=	6	B=	1.402270
I=	1	J=	9	B=	1.426422
I=	2	J=	3	B=	1.387617
I=	2	J=	7	B=	1.333924
I=	3	J=	4	B=	1.401589
I=	3	J=	11	B=	1.341702
I=	4	J=	5	B=	1.401571
I=	4	J=	13	B=	1.381505

I=	5	J=	6	B=	1.387804
I=	5	J=	8	B=	1.341658
I=	6	J=	12	B=	1.333860
I=	9	J=	10	B=	1.177799
I=	13	J=	14	B=	1.010799
I=	13	J=	15	B=	1.010798

I=	1	J=	2	K=	3	A=	120.785
I=	1	J=	2	K=	7	A=	119.894
I=	1	J=	6	K=	12	A=	119.911
I=	1	J=	9	K=	10	A=	179.816
I=	2	J=	3	K=	4	A=	121.682
I=	2	J=	3	K=	11	A=	120.040
I=	3	J=	4	K=	5	A=	116.965
I=	3	J=	4	K=	13	A=	121.332
I=	4	J=	5	K=	6	A=	121.682
I=	4	J=	5	K=	8	A=	118.156
I=	4	J=	13	K=	14	A=	115.227
I=	4	J=	13	K=	15	A=	115.231
I=	5	J=	6	K=	12	A=	119.240

I=	1	J=	2	K=	3	L=	4	D=	4.756
I=	1	J=	2	K=	3	L=	11	D=	179.376
I=	2	J=	3	K=	4	L=	5	D=	4.448
I=	2	J=	3	K=	4	L=	13	D=	177.731
I=	3	J=	4	K=	5	L=	6	D=	4.432
I=	3	J=	4	K=	5	L=	8	D=	179.598
I=	3	J=	4	K=	13	L=	14	D=	25.686
I=	3	J=	4	K=	13	L=	15	D=	161.363
I=	4	J=	5	K=	6	L=	12	D=	178.327

molA_pbe0d

I=	1	J=	2	B=	1.398326
I=	1	J=	6	B=	1.398326
I=	1	J=	9	B=	1.416012
I=	2	J=	3	B=	1.377018
I=	2	J=	7	B=	1.323009
I=	3	J=	4	B=	1.397974
I=	3	J=	11	B=	1.337348
I=	4	J=	5	B=	1.397974
I=	4	J=	13	B=	1.359074
I=	5	J=	6	B=	1.377018
I=	5	J=	8	B=	1.337348
I=	6	J=	12	B=	1.323009
I=	9	J=	10	B=	1.154211
I=	13	J=	14	B=	1.005904
I=	13	J=	15	B=	1.005904

I=	1	J=	2	K=	3	A=	121.062
I=	1	J=	2	K=	7	A=	119.775
I=	1	J=	6	K=	12	A=	119.775
I=	1	J=	9	K=	10	A=	179.976
I=	2	J=	3	K=	4	A=	121.677
I=	2	J=	3	K=	11	A=	120.335
I=	3	J=	4	K=	5	A=	116.973

I=	3	J=	4	K=	13	A=	121.498
I=	4	J=	5	K=	6	A=	121.677
I=	4	J=	5	K=	8	A=	117.987
I=	4	J=	13	K=	14	A=	118.191
I=	4	J=	13	K=	15	A=	118.191
I=	5	J=	6	K=	12	A=	119.163

I=	1	J=	2	K=	3	L=	4	D=	0.030
I=	1	J=	2	K=	3	L=	11	D=	179.659
I=	2	J=	3	K=	4	L=	5	D=	0.277
I=	2	J=	3	K=	4	L=	13	D=	177.767
I=	3	J=	4	K=	5	L=	6	D=	0.277
I=	3	J=	4	K=	5	L=	8	D=	179.419
I=	3	J=	4	K=	13	L=	14	D=	15.625
I=	3	J=	4	K=	13	L=	15	D=	166.420
I=	4	J=	5	K=	6	L=	12	D=	179.947

molA_pbe

I=	1	J=	2	B=	1.411479
I=	1	J=	6	B=	1.411479
I=	1	J=	9	B=	1.418617
I=	2	J=	3	B=	1.388120
I=	2	J=	7	B=	1.341194
I=	3	J=	4	B=	1.409503
I=	3	J=	11	B=	1.355630
I=	4	J=	5	B=	1.409503
I=	4	J=	13	B=	1.369615
I=	5	J=	6	B=	1.388120
I=	5	J=	8	B=	1.355630
I=	6	J=	12	B=	1.341194
I=	9	J=	10	B=	1.169090
I=	13	J=	14	B=	1.014788
I=	13	J=	15	B=	1.014788

I=	1	J=	2	K=	3	A=	121.199
I=	1	J=	2	K=	7	A=	119.699
I=	1	J=	6	K=	12	A=	119.699
I=	1	J=	9	K=	10	A=	179.970
I=	2	J=	3	K=	4	A=	121.818
I=	2	J=	3	K=	11	A=	120.291
I=	3	J=	4	K=	5	A=	116.750
I=	3	J=	4	K=	13	A=	121.607
I=	4	J=	5	K=	6	A=	121.818
I=	4	J=	5	K=	8	A=	117.891
I=	4	J=	13	K=	14	A=	117.954
I=	4	J=	13	K=	15	A=	117.954
I=	5	J=	6	K=	12	A=	119.102

I=	1	J=	2	K=	3	L=	4	D=	0.062
I=	1	J=	2	K=	3	L=	11	D=	179.612
I=	2	J=	3	K=	4	L=	5	D=	0.363
I=	2	J=	3	K=	4	L=	13	D=	177.464
I=	3	J=	4	K=	5	L=	6	D=	0.363
I=	3	J=	4	K=	5	L=	8	D=	179.318
I=	3	J=	4	K=	13	L=	14	D=	16.561

I=	3	J=	4	K=	13	L=	15	D=	165.718
I=	4	J=	5	K=	6	L=	12	D=	179.948

molA_rtpss

I=	1	J=	2	B=	1.408821
I=	1	J=	6	B=	1.408821
I=	1	J=	9	B=	1.419023
I=	2	J=	3	B=	1.385077
I=	2	J=	7	B=	1.342073
I=	3	J=	4	B=	1.405691
I=	3	J=	11	B=	1.356615
I=	4	J=	5	B=	1.405691
I=	4	J=	13	B=	1.374953
I=	5	J=	6	B=	1.385077
I=	5	J=	8	B=	1.356615
I=	6	J=	12	B=	1.342073
I=	9	J=	10	B=	1.166905
I=	13	J=	14	B=	1.014832
I=	13	J=	15	B=	1.014832

I=	1	J=	2	K=	3	A=	121.249
I=	1	J=	2	K=	7	A=	119.632
I=	1	J=	6	K=	12	A=	119.632
I=	1	J=	9	K=	10	A=	179.967
I=	2	J=	3	K=	4	A=	121.869
I=	2	J=	3	K=	11	A=	120.274
I=	3	J=	4	K=	5	A=	116.688
I=	3	J=	4	K=	13	A=	121.619
I=	4	J=	5	K=	6	A=	121.869
I=	4	J=	5	K=	8	A=	117.855
I=	4	J=	13	K=	14	A=	116.396
I=	4	J=	13	K=	15	A=	116.396
I=	5	J=	6	K=	12	A=	119.119

I=	1	J=	2	K=	3	L=	4	D=	0.059
I=	1	J=	2	K=	3	L=	11	D=	179.520
I=	2	J=	3	K=	4	L=	5	D=	0.255
I=	2	J=	3	K=	4	L=	13	D=	176.668
I=	3	J=	4	K=	5	L=	6	D=	0.255
I=	3	J=	4	K=	5	L=	8	D=	179.219
I=	3	J=	4	K=	13	L=	14	D=	21.051
I=	3	J=	4	K=	13	L=	15	D=	162.178
I=	4	J=	5	K=	6	L=	12	D=	179.841

molA_wb97xd

I=	1	J=	2	B=	1.396920
I=	1	J=	6	B=	1.396920
I=	1	J=	9	B=	1.422831
I=	2	J=	3	B=	1.377760
I=	2	J=	7	B=	1.324233
I=	3	J=	4	B=	1.397621
I=	3	J=	11	B=	1.339169
I=	4	J=	5	B=	1.397621
I=	4	J=	13	B=	1.362499

I=	5	J=	6	B=	1.377760
I=	5	J=	8	B=	1.339169
I=	6	J=	12	B=	1.324233
I=	9	J=	10	B=	1.150989
I=	13	J=	14	B=	1.005563
I=	13	J=	15	B=	1.005563

I=	1	J=	2	K=	3	A=	121.067
I=	1	J=	2	K=	7	A=	119.785
I=	1	J=	6	K=	12	A=	119.785
I=	1	J=	9	K=	10	A=	179.979
I=	2	J=	3	K=	4	A=	121.684
I=	2	J=	3	K=	11	A=	120.242
I=	3	J=	4	K=	5	A=	116.924
I=	3	J=	4	K=	13	A=	121.523
I=	4	J=	5	K=	6	A=	121.684
I=	4	J=	5	K=	8	A=	118.073
I=	4	J=	13	K=	14	A=	118.319
I=	4	J=	13	K=	15	A=	118.319
I=	5	J=	6	K=	12	A=	119.148

I=	1	J=	2	K=	3	L=	4	D=	0.001
I=	1	J=	2	K=	3	L=	11	D=	179.689
I=	2	J=	3	K=	4	L=	5	D=	0.215
I=	2	J=	3	K=	4	L=	13	D=	177.806
I=	3	J=	4	K=	5	L=	6	D=	0.215
I=	3	J=	4	K=	5	L=	8	D=	179.480
I=	3	J=	4	K=	13	L=	14	D=	15.446
I=	3	J=	4	K=	13	L=	15	D=	166.624
I=	4	J=	5	K=	6	L=	12	D=	179.950

molA_x31yp

I=	1	J=	2	B=	1.402033
I=	1	J=	6	B=	1.402033
I=	1	J=	9	B=	1.419688
I=	2	J=	3	B=	1.379244
I=	2	J=	7	B=	1.332334
I=	3	J=	4	B=	1.401214
I=	3	J=	11	B=	1.347037
I=	4	J=	5	B=	1.401214
I=	4	J=	13	B=	1.363931
I=	5	J=	6	B=	1.379244
I=	5	J=	8	B=	1.347037
I=	6	J=	12	B=	1.332334
I=	9	J=	10	B=	1.154260
I=	13	J=	14	B=	1.006793
I=	13	J=	15	B=	1.006793

I=	1	J=	2	K=	3	A=	121.246
I=	1	J=	2	K=	7	A=	119.708
I=	1	J=	6	K=	12	A=	119.708
I=	1	J=	9	K=	10	A=	179.977
I=	2	J=	3	K=	4	A=	121.811
I=	2	J=	3	K=	11	A=	120.257
I=	3	J=	4	K=	5	A=	116.697

I=	3	J=	4	K=	13	A=	121.639
I=	4	J=	5	K=	6	A=	121.811
I=	4	J=	5	K=	8	A=	117.932
I=	4	J=	13	K=	14	A=	118.568
I=	4	J=	13	K=	15	A=	118.568
I=	5	J=	6	K=	12	A=	119.046

I=	1	J=	2	K=	3	L=	4	D=	0.072
I=	1	J=	2	K=	3	L=	11	D=	179.688
I=	2	J=	3	K=	4	L=	5	D=	0.315
I=	2	J=	3	K=	4	L=	13	D=	177.864
I=	3	J=	4	K=	5	L=	6	D=	0.315
I=	3	J=	4	K=	5	L=	8	D=	179.450
I=	3	J=	4	K=	13	L=	14	D=	14.519
I=	3	J=	4	K=	13	L=	15	D=	167.392
I=	4	J=	5	K=	6	L=	12	D=	179.973

molB_apfd

I=	1	J=	2	B=	1.399149
I=	1	J=	6	B=	1.401156
I=	1	J=	9	B=	1.416687
I=	2	J=	3	B=	1.377423
I=	2	J=	7	B=	1.333569
I=	3	J=	4	B=	1.401744
I=	3	J=	15	B=	1.083782
I=	4	J=	5	B=	1.401708
I=	4	J=	12	B=	1.363641
I=	5	J=	6	B=	1.378373
I=	5	J=	8	B=	1.343312
I=	6	J=	11	B=	1.326061
I=	9	J=	10	B=	1.155278
I=	12	J=	13	B=	1.005401
I=	12	J=	14	B=	1.006517

I=	1	J=	2	K=	3	A=	122.947
I=	1	J=	2	K=	7	A=	118.200
I=	1	J=	6	K=	11	A=	119.712
I=	1	J=	9	K=	10	A=	179.967
I=	2	J=	3	K=	4	A=	119.710
I=	2	J=	3	K=	15	A=	119.278
I=	3	J=	4	K=	5	A=	118.091
I=	3	J=	4	K=	12	A=	122.512
I=	4	J=	5	K=	6	A=	121.354
I=	4	J=	5	K=	8	A=	118.641
I=	4	J=	12	K=	13	A=	118.809
I=	4	J=	12	K=	14	A=	118.416
I=	5	J=	6	K=	11	A=	119.094

I=	1	J=	2	K=	3	L=	4	D=	0.024
I=	1	J=	2	K=	3	L=	15	D=	179.597
I=	2	J=	3	K=	4	L=	5	D=	0.089
I=	2	J=	3	K=	4	L=	12	D=	177.945
I=	3	J=	4	K=	5	L=	6	D=	0.110
I=	3	J=	4	K=	5	L=	8	D=	179.527
I=	3	J=	4	K=	12	L=	13	D=	17.285

I=	3	J=	4	K=	12	L=	14	D=	167.700
I=	4	J=	5	K=	6	L=	11	D=	179.830

molB_b3lypd

I=	1	J=	2	B=	1.401102
I=	1	J=	6	B=	1.403390
I=	1	J=	9	B=	1.418337
I=	2	J=	3	B=	1.377752
I=	2	J=	7	B=	1.341459
I=	3	J=	4	B=	1.404330
I=	3	J=	15	B=	1.081938
I=	4	J=	5	B=	1.402863
I=	4	J=	12	B=	1.369088
I=	5	J=	6	B=	1.378125
I=	5	J=	8	B=	1.351081
I=	6	J=	11	B=	1.333339
I=	9	J=	10	B=	1.155134
I=	12	J=	13	B=	1.006374
I=	12	J=	14	B=	1.007413

I=	1	J=	2	K=	3	A=	123.271
I=	1	J=	2	K=	7	A=	118.108
I=	1	J=	6	K=	11	A=	119.592
I=	1	J=	9	K=	10	A=	179.972
I=	2	J=	3	K=	4	A=	119.645
I=	2	J=	3	K=	15	A=	119.380
I=	3	J=	4	K=	5	A=	117.886
I=	3	J=	4	K=	12	A=	122.532
I=	4	J=	5	K=	6	A=	121.549
I=	4	J=	5	K=	8	A=	118.422
I=	4	J=	12	K=	13	A=	118.676
I=	4	J=	12	K=	14	A=	118.184
I=	5	J=	6	K=	11	A=	119.098

I=	1	J=	2	K=	3	L=	4	D=	0.030
I=	1	J=	2	K=	3	L=	15	D=	179.580
I=	2	J=	3	K=	4	L=	5	D=	0.101
I=	2	J=	3	K=	4	L=	12	D=	177.891
I=	3	J=	4	K=	5	L=	6	D=	0.134
I=	3	J=	4	K=	5	L=	8	D=	179.484
I=	3	J=	4	K=	12	L=	13	D=	17.877
I=	3	J=	4	K=	12	L=	14	D=	167.540
I=	4	J=	5	K=	6	L=	11	D=	179.825

molB_blyp

I=	1	J=	2	B=	1.414689
I=	1	J=	6	B=	1.416632
I=	1	J=	9	B=	1.423606
I=	2	J=	3	B=	1.387876
I=	2	J=	7	B=	1.361227
I=	3	J=	4	B=	1.415850
I=	3	J=	15	B=	1.088768
I=	4	J=	5	B=	1.414399
I=	4	J=	12	B=	1.381616

I=	5	J=	6	B=	1.389666
I=	5	J=	8	B=	1.369991
I=	6	J=	11	B=	1.352186
I=	9	J=	10	B=	1.168441
I=	12	J=	13	B=	1.014473
I=	12	J=	14	B=	1.015425

I=	1	J=	2	K=	3	A=	123.557
I=	1	J=	2	K=	7	A=	118.025
I=	1	J=	6	K=	11	A=	119.535
I=	1	J=	9	K=	10	A=	179.967
I=	2	J=	3	K=	4	A=	119.718
I=	2	J=	3	K=	15	A=	119.342
I=	3	J=	4	K=	5	A=	117.678
I=	3	J=	4	K=	12	A=	122.530
I=	4	J=	5	K=	6	A=	121.684
I=	4	J=	5	K=	8	A=	118.398
I=	4	J=	12	K=	13	A=	118.419
I=	4	J=	12	K=	14	A=	117.928
I=	5	J=	6	K=	11	A=	118.990

I=	1	J=	2	K=	3	L=	4	D=	0.038
I=	1	J=	2	K=	3	L=	15	D=	179.553
I=	2	J=	3	K=	4	L=	5	D=	0.111
I=	2	J=	3	K=	4	L=	12	D=	177.546
I=	3	J=	4	K=	5	L=	6	D=	0.148
I=	3	J=	4	K=	5	L=	8	D=	179.425
I=	3	J=	4	K=	12	L=	13	D=	19.229
I=	3	J=	4	K=	12	L=	14	D=	166.789
I=	4	J=	5	K=	6	L=	11	D=	179.788

molB_camb3lypd

I=	1	J=	2	B=	1.393602
I=	1	J=	6	B=	1.396211
I=	1	J=	9	B=	1.420681
I=	2	J=	3	B=	1.373356
I=	2	J=	7	B=	1.334799
I=	3	J=	4	B=	1.398588
I=	3	J=	15	B=	1.081544
I=	4	J=	5	B=	1.397193
I=	4	J=	12	B=	1.363253
I=	5	J=	6	B=	1.372557
I=	5	J=	8	B=	1.344943
I=	6	J=	11	B=	1.326796
I=	9	J=	10	B=	1.148332
I=	12	J=	13	B=	1.004984
I=	12	J=	14	B=	1.006220

I=	1	J=	2	K=	3	A=	123.295
I=	1	J=	2	K=	7	A=	118.108
I=	1	J=	6	K=	11	A=	119.677
I=	1	J=	9	K=	10	A=	179.978
I=	2	J=	3	K=	4	A=	119.548
I=	2	J=	3	K=	15	A=	119.325
I=	3	J=	4	K=	5	A=	117.901

I=	3	J=	4	K=	12	A=	122.715
I=	4	J=	5	K=	6	A=	121.558
I=	4	J=	5	K=	8	A=	118.392
I=	4	J=	12	K=	13	A=	119.410
I=	4	J=	12	K=	14	A=	118.774
I=	5	J=	6	K=	11	A=	119.050

I=	1	J=	2	K=	3	L=	4	D=	0.025
I=	1	J=	2	K=	3	L=	15	D=	179.627
I=	2	J=	3	K=	4	L=	5	D=	0.082
I=	2	J=	3	K=	4	L=	12	D=	178.366
I=	3	J=	4	K=	5	L=	6	D=	0.112
I=	3	J=	4	K=	5	L=	8	D=	179.570
I=	3	J=	4	K=	12	L=	13	D=	14.881
I=	3	J=	4	K=	12	L=	14	D=	169.606
I=	4	J=	5	K=	6	L=	11	D=	179.873

molB_m062x

I=	1	J=	2	B=	1.395475
I=	1	J=	6	B=	1.397808
I=	1	J=	9	B=	1.424892
I=	2	J=	3	B=	1.376820
I=	2	J=	7	B=	1.330817
I=	3	J=	4	B=	1.400817
I=	3	J=	15	B=	1.082067
I=	4	J=	5	B=	1.399452
I=	4	J=	12	B=	1.367334
I=	5	J=	6	B=	1.375498
I=	5	J=	8	B=	1.340289
I=	6	J=	11	B=	1.323538
I=	9	J=	10	B=	1.149842
I=	12	J=	13	B=	1.006341
I=	12	J=	14	B=	1.007730

I=	1	J=	2	K=	3	A=	123.124
I=	1	J=	2	K=	7	A=	118.099
I=	1	J=	6	K=	11	A=	119.766
I=	1	J=	9	K=	10	A=	179.972
I=	2	J=	3	K=	4	A=	119.458
I=	2	J=	3	K=	15	A=	119.354
I=	3	J=	4	K=	5	A=	118.100
I=	3	J=	4	K=	12	A=	122.717
I=	4	J=	5	K=	6	A=	121.463
I=	4	J=	5	K=	8	A=	118.470
I=	4	J=	12	K=	13	A=	118.360
I=	4	J=	12	K=	14	A=	117.886
I=	5	J=	6	K=	11	A=	119.096

I=	1	J=	2	K=	3	L=	4	D=	0.062
I=	1	J=	2	K=	3	L=	15	D=	179.567
I=	2	J=	3	K=	4	L=	5	D=	0.021
I=	2	J=	3	K=	4	L=	12	D=	177.850
I=	3	J=	4	K=	5	L=	6	D=	0.039
I=	3	J=	4	K=	5	L=	8	D=	179.537
I=	3	J=	4	K=	12	L=	13	D=	18.692

I=	3	J=	4	K=	12	L=	14	D=	166.869
I=	4	J=	5	K=	6	L=	11	D=	179.800

molB_mp2

I=	1	J=	2	B=	1.401627
I=	1	J=	6	B=	1.402614
I=	1	J=	9	B=	1.426338
I=	2	J=	3	B=	1.385721
I=	2	J=	7	B=	1.341225
I=	3	J=	4	B=	1.404472
I=	3	J=	15	B=	1.085414
I=	4	J=	5	B=	1.402555
I=	4	J=	12	B=	1.385914
I=	5	J=	6	B=	1.387187
I=	5	J=	8	B=	1.344095
I=	6	J=	11	B=	1.333740
I=	9	J=	10	B=	1.177650
I=	12	J=	13	B=	1.010266
I=	12	J=	14	B=	1.011022

I=	1	J=	2	K=	3	A=	122.713
I=	1	J=	2	K=	7	A=	118.301
I=	1	J=	6	K=	11	A=	119.788
I=	1	J=	9	K=	10	A=	179.766
I=	2	J=	3	K=	4	A=	119.801
I=	2	J=	3	K=	15	A=	119.212
I=	3	J=	4	K=	5	A=	117.940
I=	3	J=	4	K=	12	A=	122.174
I=	4	J=	5	K=	6	A=	121.407
I=	4	J=	5	K=	8	A=	118.739
I=	4	J=	12	K=	13	A=	115.286
I=	4	J=	12	K=	14	A=	115.203
I=	5	J=	6	K=	11	A=	119.116

I=	1	J=	2	K=	3	L=	4	D=	4.425
I=	1	J=	2	K=	3	L=	15	D=	178.702
I=	2	J=	3	K=	4	L=	5	D=	4.283
I=	2	J=	3	K=	4	L=	12	D=	177.686
I=	3	J=	4	K=	5	L=	6	D=	4.536
I=	3	J=	4	K=	5	L=	8	D=	179.674
I=	3	J=	4	K=	12	L=	13	D=	28.900
I=	3	J=	4	K=	12	L=	14	D=	163.226
I=	4	J=	5	K=	6	L=	11	D=	178.042

molB_pbe0d

I=	1	J=	2	B=	1.397380
I=	1	J=	6	B=	1.399647
I=	1	J=	9	B=	1.415720
I=	2	J=	3	B=	1.375297
I=	2	J=	7	B=	1.330138
I=	3	J=	4	B=	1.400490
I=	3	J=	15	B=	1.083172
I=	4	J=	5	B=	1.399736
I=	4	J=	12	B=	1.362798

I=	5	J=	6	B=	1.375599
I=	5	J=	8	B=	1.340168
I=	6	J=	11	B=	1.322833
I=	9	J=	10	B=	1.154438
I=	12	J=	13	B=	1.005038
I=	12	J=	14	B=	1.006262

I=	1	J=	2	K=	3	A=	123.091
I=	1	J=	2	K=	7	A=	118.171
I=	1	J=	6	K=	11	A=	119.667
I=	1	J=	9	K=	10	A=	179.969
I=	2	J=	3	K=	4	A=	119.680
I=	2	J=	3	K=	15	A=	119.285
I=	3	J=	4	K=	5	A=	117.978
I=	3	J=	4	K=	12	A=	122.620
I=	4	J=	5	K=	6	A=	121.470
I=	4	J=	5	K=	8	A=	118.475
I=	4	J=	12	K=	13	A=	118.647
I=	4	J=	12	K=	14	A=	118.081
I=	5	J=	6	K=	11	A=	119.101

I=	1	J=	2	K=	3	L=	4	D=	0.032
I=	1	J=	2	K=	3	L=	15	D=	179.582
I=	2	J=	3	K=	4	L=	5	D=	0.085
I=	2	J=	3	K=	4	L=	12	D=	177.908
I=	3	J=	4	K=	5	L=	6	D=	0.108
I=	3	J=	4	K=	5	L=	8	D=	179.491
I=	3	J=	4	K=	12	L=	13	D=	17.925
I=	3	J=	4	K=	12	L=	14	D=	167.474
I=	4	J=	5	K=	6	L=	11	D=	179.815

molB_pbe

I=	1	J=	2	B=	1.410647
I=	1	J=	6	B=	1.412385
I=	1	J=	9	B=	1.418348
I=	2	J=	3	B=	1.384964
I=	2	J=	7	B=	1.349251
I=	3	J=	4	B=	1.411288
I=	3	J=	15	B=	1.090807
I=	4	J=	5	B=	1.410902
I=	4	J=	12	B=	1.373578
I=	5	J=	6	B=	1.386891
I=	5	J=	8	B=	1.358430
I=	6	J=	11	B=	1.341175
I=	9	J=	10	B=	1.169267
I=	12	J=	13	B=	1.013961
I=	12	J=	14	B=	1.015214

I=	1	J=	2	K=	3	A=	123.341
I=	1	J=	2	K=	7	A=	118.044
I=	1	J=	6	K=	11	A=	119.610
I=	1	J=	9	K=	10	A=	179.963
I=	2	J=	3	K=	4	A=	119.749
I=	2	J=	3	K=	15	A=	119.271
I=	3	J=	4	K=	5	A=	117.808

I=	3	J=	4	K=	12	A=	122.661
I=	4	J=	5	K=	6	A=	121.593
I=	4	J=	5	K=	8	A=	118.419
I=	4	J=	12	K=	13	A=	118.472
I=	4	J=	12	K=	14	A=	117.855
I=	5	J=	6	K=	11	A=	119.035

I=	1	J=	2	K=	3	L=	4	D=	0.031
I=	1	J=	2	K=	3	L=	15	D=	179.564
I=	2	J=	3	K=	4	L=	5	D=	0.114
I=	2	J=	3	K=	4	L=	12	D=	177.612
I=	3	J=	4	K=	5	L=	6	D=	0.139
I=	3	J=	4	K=	5	L=	8	D=	179.413
I=	3	J=	4	K=	12	L=	13	D=	18.937
I=	3	J=	4	K=	12	L=	14	D=	166.971
I=	4	J=	5	K=	6	L=	11	D=	179.777

molB_rtpss

I=	1	J=	2	B=	1.407849
I=	1	J=	6	B=	1.409414
I=	1	J=	9	B=	1.418782
I=	2	J=	3	B=	1.383389
I=	2	J=	7	B=	1.350665
I=	3	J=	4	B=	1.409158
I=	3	J=	15	B=	1.086990
I=	4	J=	5	B=	1.406835
I=	4	J=	12	B=	1.379330
I=	5	J=	6	B=	1.383660
I=	5	J=	8	B=	1.359609
I=	6	J=	11	B=	1.342036
I=	9	J=	10	B=	1.167087
I=	12	J=	13	B=	1.014032
I=	12	J=	14	B=	1.015235

I=	1	J=	2	K=	3	A=	123.612
I=	1	J=	2	K=	7	A=	117.859
I=	1	J=	6	K=	11	A=	119.592
I=	1	J=	9	K=	10	A=	179.971
I=	2	J=	3	K=	4	A=	119.417
I=	2	J=	3	K=	15	A=	119.511
I=	3	J=	4	K=	5	A=	117.931
I=	3	J=	4	K=	12	A=	122.625
I=	4	J=	5	K=	6	A=	121.683
I=	4	J=	5	K=	8	A=	118.350
I=	4	J=	12	K=	13	A=	116.968
I=	4	J=	12	K=	14	A=	116.278
I=	5	J=	6	K=	11	A=	119.079

I=	1	J=	2	K=	3	L=	4	D=	0.104
I=	1	J=	2	K=	3	L=	15	D=	179.523
I=	2	J=	3	K=	4	L=	5	D=	0.035
I=	2	J=	3	K=	4	L=	12	D=	176.862
I=	3	J=	4	K=	5	L=	6	D=	0.060
I=	3	J=	4	K=	5	L=	8	D=	179.317
I=	3	J=	4	K=	12	L=	13	D=	23.815

I=	3	J=	4	K=	12	L=	14	D=	164.057
I=	4	J=	5	K=	6	L=	11	D=	179.664

molB_wb97xd

I=	1	J=	2	B=	1.395932
I=	1	J=	6	B=	1.398525
I=	1	J=	9	B=	1.422513
I=	2	J=	3	B=	1.376026
I=	2	J=	7	B=	1.331698
I=	3	J=	4	B=	1.400133
I=	3	J=	15	B=	1.082317
I=	4	J=	5	B=	1.399405
I=	4	J=	12	B=	1.366412
I=	5	J=	6	B=	1.376242
I=	5	J=	8	B=	1.342100
I=	6	J=	11	B=	1.324037
I=	9	J=	10	B=	1.151236
I=	12	J=	13	B=	1.004831
I=	12	J=	14	B=	1.005957

I=	1	J=	2	K=	3	A=	123.088
I=	1	J=	2	K=	7	A=	118.254
I=	1	J=	6	K=	11	A=	119.673
I=	1	J=	9	K=	10	A=	179.971
I=	2	J=	3	K=	4	A=	119.634
I=	2	J=	3	K=	15	A=	119.359
I=	3	J=	4	K=	5	A=	118.015
I=	3	J=	4	K=	12	A=	122.404
I=	4	J=	5	K=	6	A=	121.430
I=	4	J=	5	K=	8	A=	118.564
I=	4	J=	12	K=	13	A=	118.575
I=	4	J=	12	K=	14	A=	118.266
I=	5	J=	6	K=	11	A=	119.108

I=	1	J=	2	K=	3	L=	4	D=	0.047
I=	1	J=	2	K=	3	L=	15	D=	179.561
I=	2	J=	3	K=	4	L=	5	D=	0.059
I=	2	J=	3	K=	4	L=	12	D=	177.970
I=	3	J=	4	K=	5	L=	6	D=	0.088
I=	3	J=	4	K=	5	L=	8	D=	179.531
I=	3	J=	4	K=	12	L=	13	D=	17.751
I=	3	J=	4	K=	12	L=	14	D=	167.434
I=	4	J=	5	K=	6	L=	11	D=	179.846

molB_x31yp

I=	1	J=	2	B=	1.400914
I=	1	J=	6	B=	1.403197
I=	1	J=	9	B=	1.419449
I=	2	J=	3	B=	1.377691
I=	2	J=	7	B=	1.340340
I=	3	J=	4	B=	1.404242
I=	3	J=	15	B=	1.082165
I=	4	J=	5	B=	1.402614
I=	4	J=	12	B=	1.368524

I=	5	J=	6	B=	1.377859
I=	5	J=	8	B=	1.350026
I=	6	J=	11	B=	1.332257
I=	9	J=	10	B=	1.154482
I=	12	J=	13	B=	1.006169
I=	12	J=	14	B=	1.007232

I=	1	J=	2	K=	3	A=	123.331
I=	1	J=	2	K=	7	A=	118.121
I=	1	J=	6	K=	11	A=	119.625
I=	1	J=	9	K=	10	A=	179.974
I=	2	J=	3	K=	4	A=	119.676
I=	2	J=	3	K=	15	A=	119.303
I=	3	J=	4	K=	5	A=	117.796
I=	3	J=	4	K=	12	A=	122.615
I=	4	J=	5	K=	6	A=	121.600
I=	4	J=	5	K=	8	A=	118.421
I=	4	J=	12	K=	13	A=	118.893
I=	4	J=	12	K=	14	A=	118.367
I=	5	J=	6	K=	11	A=	119.013

I=	1	J=	2	K=	3	L=	4	D=	0.028
I=	1	J=	2	K=	3	L=	15	D=	179.591
I=	2	J=	3	K=	4	L=	5	D=	0.096
I=	2	J=	3	K=	4	L=	12	D=	177.950
I=	3	J=	4	K=	5	L=	6	D=	0.128
I=	3	J=	4	K=	5	L=	8	D=	179.513
I=	3	J=	4	K=	12	L=	13	D=	17.267
I=	3	J=	4	K=	12	L=	14	D=	167.983
I=	4	J=	5	K=	6	L=	11	D=	179.835

molC_apfd

I=	1	J=	2	B=	1.402557
I=	1	J=	6	B=	1.396111
I=	1	J=	8	B=	1.420346
I=	2	J=	3	B=	1.372204
I=	2	J=	15	B=	1.082974
I=	3	J=	4	B=	1.402612
I=	3	J=	14	B=	1.348222
I=	4	J=	5	B=	1.397234
I=	4	J=	11	B=	1.362205
I=	5	J=	6	B=	1.383352
I=	5	J=	7	B=	1.340490
I=	6	J=	10	B=	1.328328
I=	8	J=	9	B=	1.155485
I=	11	J=	12	B=	1.006339
I=	11	J=	13	B=	1.006353

I=	1	J=	2	K=	3	A=	119.542
I=	1	J=	2	K=	15	A=	120.530
I=	1	J=	6	K=	10	A=	120.658
I=	1	J=	8	K=	9	A=	179.146
I=	2	J=	3	K=	4	A=	123.104
I=	2	J=	3	K=	14	A=	120.358
I=	3	J=	4	K=	5	A=	116.235

I=	3	J=	4	K=	11	A=	122.078
I=	4	J=	5	K=	6	A=	121.935
I=	4	J=	5	K=	7	A=	118.087
I=	4	J=	11	K=	12	A=	117.887
I=	4	J=	11	K=	13	A=	118.201
I=	5	J=	6	K=	10	A=	118.884

I=	1	J=	2	K=	3	L=	4	D=	0.066
I=	1	J=	2	K=	3	L=	14	D=	179.651
I=	2	J=	3	K=	4	L=	5	D=	0.309
I=	2	J=	3	K=	4	L=	11	D=	177.597
I=	3	J=	4	K=	5	L=	6	D=	0.307
I=	3	J=	4	K=	5	L=	7	D=	179.425
I=	3	J=	4	K=	11	L=	12	D=	16.452
I=	3	J=	4	K=	11	L=	13	D=	165.659
I=	4	J=	5	K=	6	L=	10	D=	179.961

molC_b3lypd

I=	1	J=	2	B=	1.406088
I=	1	J=	6	B=	1.398111
I=	1	J=	8	B=	1.421855
I=	2	J=	3	B=	1.372590
I=	2	J=	15	B=	1.081105
I=	3	J=	4	B=	1.403691
I=	3	J=	14	B=	1.356430
I=	4	J=	5	B=	1.398897
I=	4	J=	11	B=	1.367266
I=	5	J=	6	B=	1.382955
I=	5	J=	7	B=	1.348043
I=	6	J=	10	B=	1.335877
I=	8	J=	9	B=	1.155380
I=	11	J=	12	B=	1.007156
I=	11	J=	13	B=	1.007165

I=	1	J=	2	K=	3	A=	119.536
I=	1	J=	2	K=	15	A=	120.533
I=	1	J=	6	K=	10	A=	120.449
I=	1	J=	8	K=	9	A=	178.981
I=	2	J=	3	K=	4	A=	123.387
I=	2	J=	3	K=	14	A=	120.162
I=	3	J=	4	K=	5	A=	115.953
I=	3	J=	4	K=	11	A=	122.196
I=	4	J=	5	K=	6	A=	122.018
I=	4	J=	5	K=	7	A=	117.954
I=	4	J=	11	K=	12	A=	117.787
I=	4	J=	11	K=	13	A=	118.116
I=	5	J=	6	K=	10	A=	118.843

I=	1	J=	2	K=	3	L=	4	D=	0.094
I=	1	J=	2	K=	3	L=	14	D=	179.630
I=	2	J=	3	K=	4	L=	5	D=	0.360
I=	2	J=	3	K=	4	L=	11	D=	177.565
I=	3	J=	4	K=	5	L=	6	D=	0.357
I=	3	J=	4	K=	5	L=	7	D=	179.384
I=	3	J=	4	K=	11	L=	12	D=	16.464

I=	3	J=	4	K=	11	L=	13	D=	165.587
I=	4	J=	5	K=	6	L=	10	D=	179.971

molC_blyp

I=	1	J=	2	B=	1.419311
I=	1	J=	6	B=	1.411655
I=	1	J=	8	B=	1.427113
I=	2	J=	3	B=	1.382781
I=	2	J=	15	B=	1.087675
I=	3	J=	4	B=	1.415579
I=	3	J=	14	B=	1.376559
I=	4	J=	5	B=	1.411203
I=	4	J=	11	B=	1.378725
I=	5	J=	6	B=	1.393980
I=	5	J=	7	B=	1.367085
I=	6	J=	10	B=	1.354578
I=	8	J=	9	B=	1.168675
I=	11	J=	12	B=	1.015072
I=	11	J=	13	B=	1.015064

I=	1	J=	2	K=	3	A=	119.616
I=	1	J=	2	K=	15	A=	120.470
I=	1	J=	6	K=	10	A=	120.387
I=	1	J=	8	K=	9	A=	178.952
I=	2	J=	3	K=	4	A=	123.670
I=	2	J=	3	K=	14	A=	119.953
I=	3	J=	4	K=	5	A=	115.623
I=	3	J=	4	K=	11	A=	122.361
I=	4	J=	5	K=	6	A=	122.158
I=	4	J=	5	K=	7	A=	117.877
I=	4	J=	11	K=	12	A=	117.603
I=	4	J=	11	K=	13	A=	117.964
I=	5	J=	6	K=	10	A=	118.740

I=	1	J=	2	K=	3	L=	4	D=	0.105
I=	1	J=	2	K=	3	L=	14	D=	179.607
I=	2	J=	3	K=	4	L=	5	D=	0.401
I=	2	J=	3	K=	4	L=	11	D=	177.252
I=	3	J=	4	K=	5	L=	6	D=	0.403
I=	3	J=	4	K=	5	L=	7	D=	179.328
I=	3	J=	4	K=	11	L=	12	D=	17.310
I=	3	J=	4	K=	11	L=	13	D=	165.036
I=	4	J=	5	K=	6	L=	10	D=	179.965

molC_camb3lypd

I=	1	J=	2	B=	1.399218
I=	1	J=	6	B=	1.390375
I=	1	J=	8	B=	1.424492
I=	2	J=	3	B=	1.367652
I=	2	J=	15	B=	1.081013
I=	3	J=	4	B=	1.397799
I=	3	J=	14	B=	1.349898
I=	4	J=	5	B=	1.391941
I=	4	J=	11	B=	1.362216

I=	5	J=	6	B=	1.378250
I=	5	J=	7	B=	1.341725
I=	6	J=	10	B=	1.329506
I=	8	J=	9	B=	1.148553
I=	11	J=	12	B=	1.006030
I=	11	J=	13	B=	1.006042

I=	1	J=	2	K=	3	A=	119.474
I=	1	J=	2	K=	15	A=	120.698
I=	1	J=	6	K=	10	A=	120.532
I=	1	J=	8	K=	9	A=	178.983
I=	2	J=	3	K=	4	A=	123.371
I=	2	J=	3	K=	14	A=	120.247
I=	3	J=	4	K=	5	A=	115.976
I=	3	J=	4	K=	11	A=	122.165
I=	4	J=	5	K=	6	A=	121.983
I=	4	J=	5	K=	7	A=	118.007
I=	4	J=	11	K=	12	A=	118.308
I=	4	J=	11	K=	13	A=	118.626
I=	5	J=	6	K=	10	A=	118.766

I=	1	J=	2	K=	3	L=	4	D=	0.082
I=	1	J=	2	K=	3	L=	14	D=	179.672
I=	2	J=	3	K=	4	L=	5	D=	0.309
I=	2	J=	3	K=	4	L=	11	D=	177.988
I=	3	J=	4	K=	5	L=	6	D=	0.305
I=	3	J=	4	K=	5	L=	7	D=	179.470
I=	3	J=	4	K=	11	L=	12	D=	14.325
I=	3	J=	4	K=	11	L=	13	D=	167.326
I=	4	J=	5	K=	6	L=	10	D=	179.988

molC_m062x

I=	1	J=	2	B=	1.401186
I=	1	J=	6	B=	1.392032
I=	1	J=	8	B=	1.428974
I=	2	J=	3	B=	1.371124
I=	2	J=	15	B=	1.081664
I=	3	J=	4	B=	1.400377
I=	3	J=	14	B=	1.344596
I=	4	J=	5	B=	1.393697
I=	4	J=	11	B=	1.366914
I=	5	J=	6	B=	1.381425
I=	5	J=	7	B=	1.337158
I=	6	J=	10	B=	1.326132
I=	8	J=	9	B=	1.150046
I=	11	J=	12	B=	1.007686
I=	11	J=	13	B=	1.007699

I=	1	J=	2	K=	3	A=	119.291
I=	1	J=	2	K=	15	A=	120.806
I=	1	J=	6	K=	10	A=	120.650
I=	1	J=	8	K=	9	A=	179.074
I=	2	J=	3	K=	4	A=	123.271
I=	2	J=	3	K=	14	A=	120.412
I=	3	J=	4	K=	5	A=	116.195

I=	3	J=	4	K=	11	A=	122.047
I=	4	J=	5	K=	6	A=	121.880
I=	4	J=	5	K=	7	A=	118.085
I=	4	J=	11	K=	12	A=	117.245
I=	4	J=	11	K=	13	A=	117.554
I=	5	J=	6	K=	10	A=	118.787

I=	1	J=	2	K=	3	L=	4	D=	0.030
I=	1	J=	2	K=	3	L=	14	D=	179.628
I=	2	J=	3	K=	4	L=	5	D=	0.245
I=	2	J=	3	K=	4	L=	11	D=	177.439
I=	3	J=	4	K=	5	L=	6	D=	0.238
I=	3	J=	4	K=	5	L=	7	D=	179.434
I=	3	J=	4	K=	11	L=	12	D=	18.051
I=	3	J=	4	K=	11	L=	13	D=	164.292
I=	4	J=	5	K=	6	L=	10	D=	179.928

molC_mp2

I=	1	J=	2	B=	1.407935
I=	1	J=	6	B=	1.399014
I=	1	J=	8	B=	1.429808
I=	2	J=	3	B=	1.382873
I=	2	J=	15	B=	1.084391
I=	3	J=	4	B=	1.404284
I=	3	J=	14	B=	1.348905
I=	4	J=	5	B=	1.399610
I=	4	J=	11	B=	1.383501
I=	5	J=	6	B=	1.391195
I=	5	J=	7	B=	1.341581
I=	6	J=	10	B=	1.335796
I=	8	J=	9	B=	1.177886
I=	11	J=	12	B=	1.010883
I=	11	J=	13	B=	1.010936

I=	1	J=	2	K=	3	A=	119.104
I=	1	J=	2	K=	15	A=	120.850
I=	1	J=	6	K=	10	A=	120.737
I=	1	J=	8	K=	9	A=	179.189
I=	2	J=	3	K=	4	A=	123.339
I=	2	J=	3	K=	14	A=	119.943
I=	3	J=	4	K=	5	A=	116.083
I=	3	J=	4	K=	11	A=	122.029
I=	4	J=	5	K=	6	A=	122.057
I=	4	J=	5	K=	7	A=	118.120
I=	4	J=	11	K=	12	A=	114.834
I=	4	J=	11	K=	13	A=	115.101
I=	5	J=	6	K=	10	A=	118.918

I=	1	J=	2	K=	3	L=	4	D=	3.704
I=	1	J=	2	K=	3	L=	14	D=	179.565
I=	2	J=	3	K=	4	L=	5	D=	3.699
I=	2	J=	3	K=	4	L=	11	D=	177.122
I=	3	J=	4	K=	5	L=	6	D=	3.917
I=	3	J=	4	K=	5	L=	7	D=	179.710
I=	3	J=	4	K=	11	L=	12	D=	26.009

I=	3	J=	4	K=	11	L=	13	D=	160.640
I=	4	J=	5	K=	6	L=	10	D=	178.491

molC_pbe0d

I=	1	J=	2	B=	1.401664
I=	1	J=	6	B=	1.394281
I=	1	J=	8	B=	1.419394
I=	2	J=	3	B=	1.370019
I=	2	J=	15	B=	1.082452
I=	3	J=	4	B=	1.400567
I=	3	J=	14	B=	1.344697
I=	4	J=	5	B=	1.395276
I=	4	J=	11	B=	1.361758
I=	5	J=	6	B=	1.380714
I=	5	J=	7	B=	1.337164
I=	6	J=	10	B=	1.325285
I=	8	J=	9	B=	1.154641
I=	11	J=	12	B=	1.006109
I=	11	J=	13	B=	1.006102

I=	1	J=	2	K=	3	A=	119.534
I=	1	J=	2	K=	15	A=	120.566
I=	1	J=	6	K=	10	A=	120.580
I=	1	J=	8	K=	9	A=	179.061
I=	2	J=	3	K=	4	A=	123.231
I=	2	J=	3	K=	14	A=	120.305
I=	3	J=	4	K=	5	A=	116.103
I=	3	J=	4	K=	11	A=	122.114
I=	4	J=	5	K=	6	A=	121.982
I=	4	J=	5	K=	7	A=	118.007
I=	4	J=	11	K=	12	A=	117.595
I=	4	J=	11	K=	13	A=	117.939
I=	5	J=	6	K=	10	A=	118.850

I=	1	J=	2	K=	3	L=	4	D=	0.065
I=	1	J=	2	K=	3	L=	14	D=	179.623
I=	2	J=	3	K=	4	L=	5	D=	0.318
I=	2	J=	3	K=	4	L=	11	D=	177.544
I=	3	J=	4	K=	5	L=	6	D=	0.315
I=	3	J=	4	K=	5	L=	7	D=	179.390
I=	3	J=	4	K=	11	L=	12	D=	16.935
I=	3	J=	4	K=	11	L=	13	D=	165.161
I=	4	J=	5	K=	6	L=	10	D=	179.955

molC_pbe

I=	1	J=	2	B=	1.414261
I=	1	J=	6	B=	1.407631
I=	1	J=	8	B=	1.421967
I=	2	J=	3	B=	1.379772
I=	2	J=	15	B=	1.089778
I=	3	J=	4	B=	1.412052
I=	3	J=	14	B=	1.364133
I=	4	J=	5	B=	1.407195
I=	4	J=	11	B=	1.371293

I=	5	J=	6	B=	1.391359
I=	5	J=	7	B=	1.355618
I=	6	J=	10	B=	1.343406
I=	8	J=	9	B=	1.169449
I=	11	J=	12	B=	1.014927
I=	11	J=	13	B=	1.014889

I=	1	J=	2	K=	3	A=	119.596
I=	1	J=	2	K=	15	A=	120.464
I=	1	J=	6	K=	10	A=	120.504
I=	1	J=	8	K=	9	A=	179.088
I=	2	J=	3	K=	4	A=	123.487
I=	2	J=	3	K=	14	A=	120.190
I=	3	J=	4	K=	5	A=	115.829
I=	3	J=	4	K=	11	A=	122.248
I=	4	J=	5	K=	6	A=	122.089
I=	4	J=	5	K=	7	A=	117.903
I=	4	J=	11	K=	12	A=	117.480
I=	4	J=	11	K=	13	A=	117.874
I=	5	J=	6	K=	10	A=	118.786

I=	1	J=	2	K=	3	L=	4	D=	0.089
I=	1	J=	2	K=	3	L=	14	D=	179.592
I=	2	J=	3	K=	4	L=	5	D=	0.388
I=	2	J=	3	K=	4	L=	11	D=	177.301
I=	3	J=	4	K=	5	L=	6	D=	0.388
I=	3	J=	4	K=	5	L=	7	D=	179.312
I=	3	J=	4	K=	11	L=	12	D=	17.329
I=	3	J=	4	K=	11	L=	13	D=	164.946
I=	4	J=	5	K=	6	L=	10	D=	179.957

molC_rtpss

I=	1	J=	2	B=	1.413016
I=	1	J=	6	B=	1.404810
I=	1	J=	8	B=	1.422646
I=	2	J=	3	B=	1.378511
I=	2	J=	15	B=	1.085667
I=	3	J=	4	B=	1.408006
I=	3	J=	14	B=	1.365658
I=	4	J=	5	B=	1.403121
I=	4	J=	11	B=	1.376762
I=	5	J=	6	B=	1.388043
I=	5	J=	7	B=	1.356583
I=	6	J=	10	B=	1.344403
I=	8	J=	9	B=	1.167309
I=	11	J=	12	B=	1.014985
I=	11	J=	13	B=	1.014951

I=	1	J=	2	K=	3	A=	119.280
I=	1	J=	2	K=	15	A=	120.546
I=	1	J=	6	K=	10	A=	120.428
I=	1	J=	8	K=	9	A=	179.043
I=	2	J=	3	K=	4	A=	123.730
I=	2	J=	3	K=	14	A=	120.104
I=	3	J=	4	K=	5	A=	115.790

I=	3	J=	4	K=	11	A=	122.229
I=	4	J=	5	K=	6	A=	122.078
I=	4	J=	5	K=	7	A=	117.911
I=	4	J=	11	K=	12	A=	115.941
I=	4	J=	11	K=	13	A=	116.313
I=	5	J=	6	K=	10	A=	118.795

I=	1	J=	2	K=	3	L=	4	D=	0.000
I=	1	J=	2	K=	3	L=	14	D=	179.513
I=	2	J=	3	K=	4	L=	5	D=	0.304
I=	2	J=	3	K=	4	L=	11	D=	176.525
I=	3	J=	4	K=	5	L=	6	D=	0.306
I=	3	J=	4	K=	5	L=	7	D=	179.222
I=	3	J=	4	K=	11	L=	12	D=	21.587
I=	3	J=	4	K=	11	L=	13	D=	161.579
I=	4	J=	5	K=	6	L=	10	D=	179.862

molC_wb97xd

I=	1	J=	2	B=	1.400386
I=	1	J=	6	B=	1.392496
I=	1	J=	8	B=	1.426466
I=	2	J=	3	B=	1.370505
I=	2	J=	15	B=	1.081755
I=	3	J=	4	B=	1.400305
I=	3	J=	14	B=	1.346731
I=	4	J=	5	B=	1.394535
I=	4	J=	11	B=	1.365788
I=	5	J=	6	B=	1.381860
I=	5	J=	7	B=	1.338944
I=	6	J=	10	B=	1.326667
I=	8	J=	9	B=	1.151458
I=	11	J=	12	B=	1.005830
I=	11	J=	13	B=	1.005827

I=	1	J=	2	K=	3	A=	119.478
I=	1	J=	2	K=	15	A=	120.653
I=	1	J=	6	K=	10	A=	120.588
I=	1	J=	8	K=	9	A=	178.960
I=	2	J=	3	K=	4	A=	123.264
I=	2	J=	3	K=	14	A=	120.123
I=	3	J=	4	K=	5	A=	116.072
I=	3	J=	4	K=	11	A=	122.123
I=	4	J=	5	K=	6	A=	121.966
I=	4	J=	5	K=	7	A=	118.109
I=	4	J=	11	K=	12	A=	117.655
I=	4	J=	11	K=	13	A=	117.974
I=	5	J=	6	K=	10	A=	118.857

I=	1	J=	2	K=	3	L=	4	D=	0.036
I=	1	J=	2	K=	3	L=	14	D=	179.647
I=	2	J=	3	K=	4	L=	5	D=	0.260
I=	2	J=	3	K=	4	L=	11	D=	177.549
I=	3	J=	4	K=	5	L=	6	D=	0.256
I=	3	J=	4	K=	5	L=	7	D=	179.445
I=	3	J=	4	K=	11	L=	12	D=	17.029

I=	3	J=	4	K=	11	L=	13	D=	165.109
I=	4	J=	5	K=	6	L=	10	D=	179.959

molC_x31yp

I=	1	J=	2	B=	1.406021
I=	1	J=	6	B=	1.397831
I=	1	J=	8	B=	1.422987
I=	2	J=	3	B=	1.372466
I=	2	J=	15	B=	1.081357
I=	3	J=	4	B=	1.403454
I=	3	J=	14	B=	1.355301
I=	4	J=	5	B=	1.398535
I=	4	J=	11	B=	1.366836
I=	5	J=	6	B=	1.382788
I=	5	J=	7	B=	1.346962
I=	6	J=	10	B=	1.334818
I=	8	J=	9	B=	1.154720
I=	11	J=	12	B=	1.006992
I=	11	J=	13	B=	1.007003

I=	1	J=	2	K=	3	A=	119.582
I=	1	J=	2	K=	15	A=	120.589
I=	1	J=	6	K=	10	A=	120.487
I=	1	J=	8	K=	9	A=	178.981
I=	2	J=	3	K=	4	A=	123.429
I=	2	J=	3	K=	14	A=	120.131
I=	3	J=	4	K=	5	A=	115.866
I=	3	J=	4	K=	11	A=	122.238
I=	4	J=	5	K=	6	A=	122.066
I=	4	J=	5	K=	7	A=	117.961
I=	4	J=	11	K=	12	A=	117.965
I=	4	J=	11	K=	13	A=	118.292
I=	5	J=	6	K=	10	A=	118.753

I=	1	J=	2	K=	3	L=	4	D=	0.093
I=	1	J=	2	K=	3	L=	14	D=	179.649
I=	2	J=	3	K=	4	L=	5	D=	0.347
I=	2	J=	3	K=	4	L=	11	D=	177.620
I=	3	J=	4	K=	5	L=	6	D=	0.344
I=	3	J=	4	K=	5	L=	7	D=	179.415
I=	3	J=	4	K=	11	L=	12	D=	16.005
I=	3	J=	4	K=	11	L=	13	D=	166.007
I=	4	J=	5	K=	6	L=	10	D=	179.975

molD_apfd

I=	1	J=	2	B=	1.398281
I=	1	J=	6	B=	1.410742
I=	1	J=	11	B=	1.417375
I=	2	J=	3	B=	1.380610
I=	2	J=	8	B=	1.327690
I=	3	J=	4	B=	1.397469
I=	3	J=	15	B=	1.329980
I=	4	J=	5	B=	1.384199
I=	4	J=	10	B=	1.711002

I=	5	J=	6	B=	1.398805
I=	5	J=	9	B=	1.340636
I=	6	J=	7	B=	1.360604
I=	7	J=	13	B=	1.005800
I=	7	J=	14	B=	1.007586
I=	11	J=	12	B=	1.156266

I=	1	J=	2	K=	3	A=	121.134
I=	1	J=	2	K=	8	A=	119.491
I=	1	J=	6	K=	7	A=	122.416
I=	1	J=	11	K=	12	A=	175.906
I=	2	J=	3	K=	4	A=	119.305
I=	2	J=	3	K=	15	A=	120.151
I=	3	J=	4	K=	5	A=	119.562
I=	3	J=	4	K=	10	A=	119.991
I=	4	J=	5	K=	6	A=	122.483
I=	4	J=	5	K=	9	A=	119.991
I=	5	J=	6	K=	7	A=	120.393
I=	6	J=	7	K=	13	A=	118.579
I=	6	J=	7	K=	14	A=	118.936

I=	1	J=	2	K=	3	L=	4	D=	0.186
I=	1	J=	2	K=	3	L=	15	D=	179.970
I=	1	J=	6	K=	7	L=	13	D=	167.061
I=	1	J=	6	K=	7	L=	14	D=	13.930
I=	2	J=	3	K=	4	L=	5	D=	0.261
I=	2	J=	3	K=	4	L=	10	D=	179.701
I=	3	J=	4	K=	5	L=	6	D=	0.032
I=	3	J=	4	K=	5	L=	9	D=	179.800
I=	4	J=	5	K=	6	L=	7	D=	177.822
I=	5	J=	6	K=	7	L=	13	D=	14.826
I=	5	J=	6	K=	7	L=	14	D=	167.957

molD_b3lypd

I=	1	J=	2	B=	1.399966
I=	1	J=	6	B=	1.414644
I=	1	J=	11	B=	1.418726
I=	2	J=	3	B=	1.380648
I=	2	J=	8	B=	1.335224
I=	3	J=	4	B=	1.399112
I=	3	J=	15	B=	1.337213
I=	4	J=	5	B=	1.385309
I=	4	J=	10	B=	1.725973
I=	5	J=	6	B=	1.400232
I=	5	J=	9	B=	1.348652
I=	6	J=	7	B=	1.365754
I=	7	J=	13	B=	1.006588
I=	7	J=	14	B=	1.008125
I=	11	J=	12	B=	1.156071

I=	1	J=	2	K=	3	A=	121.414
I=	1	J=	2	K=	8	A=	119.298
I=	1	J=	6	K=	7	A=	122.339
I=	1	J=	11	K=	12	A=	175.728
I=	2	J=	3	K=	4	A=	119.437

I=	2	J=	3	K=	15	A=	120.034
I=	3	J=	4	K=	5	A=	119.230
I=	3	J=	4	K=	10	A=	120.150
I=	4	J=	5	K=	6	A=	122.753
I=	4	J=	5	K=	9	A=	120.010
I=	5	J=	6	K=	7	A=	120.428
I=	6	J=	7	K=	13	A=	118.403
I=	6	J=	7	K=	14	A=	118.975

I=	1	J=	2	K=	3	L=	4	D=	0.189
I=	1	J=	2	K=	3	L=	15	D=	179.963
I=	1	J=	6	K=	7	L=	13	D=	167.258
I=	1	J=	6	K=	7	L=	14	D=	14.321
I=	2	J=	3	K=	4	L=	5	D=	0.249
I=	2	J=	3	K=	4	L=	10	D=	179.686
I=	3	J=	4	K=	5	L=	6	D=	0.060
I=	3	J=	4	K=	5	L=	9	D=	179.762
I=	4	J=	5	K=	6	L=	7	D=	177.788
I=	5	J=	6	K=	7	L=	13	D=	14.636
I=	5	J=	6	K=	7	L=	14	D=	167.573

molD_blyp

I=	1	J=	2	B=	1.412647
I=	1	J=	6	B=	1.429932
I=	1	J=	11	B=	1.424099
I=	2	J=	3	B=	1.392719
I=	2	J=	8	B=	1.353923
I=	3	J=	4	B=	1.410278
I=	3	J=	15	B=	1.354994
I=	4	J=	5	B=	1.397118
I=	4	J=	10	B=	1.744802
I=	5	J=	6	B=	1.411801
I=	5	J=	9	B=	1.368116
I=	6	J=	7	B=	1.377694
I=	7	J=	13	B=	1.014552
I=	7	J=	14	B=	1.015991
I=	11	J=	12	B=	1.169504

I=	1	J=	2	K=	3	A=	121.657
I=	1	J=	2	K=	8	A=	119.243
I=	1	J=	6	K=	7	A=	122.321
I=	1	J=	11	K=	12	A=	176.048
I=	2	J=	3	K=	4	A=	119.520
I=	2	J=	3	K=	15	A=	119.927
I=	3	J=	4	K=	5	A=	118.993
I=	3	J=	4	K=	10	A=	120.267
I=	4	J=	5	K=	6	A=	123.003
I=	4	J=	5	K=	9	A=	119.896
I=	5	J=	6	K=	7	A=	120.402
I=	6	J=	7	K=	13	A=	118.176
I=	6	J=	7	K=	14	A=	118.759

I=	1	J=	2	K=	3	L=	4	D=	0.203
I=	1	J=	2	K=	3	L=	15	D=	179.934
I=	1	J=	6	K=	7	L=	13	D=	166.438

I=	1	J=	6	K=	7	L=	14	D=	15.562
I=	2	J=	3	K=	4	L=	5	D=	0.276
I=	2	J=	3	K=	4	L=	10	D=	179.639
I=	3	J=	4	K=	5	L=	6	D=	0.077
I=	3	J=	4	K=	5	L=	9	D=	179.735
I=	4	J=	5	K=	6	L=	7	D=	177.438
I=	5	J=	6	K=	7	L=	13	D=	15.744
I=	5	J=	6	K=	7	L=	14	D=	166.620

molD_camb3lypd

I=	1	J=	2	B=	1.393874
I=	1	J=	6	B=	1.405779
I=	1	J=	11	B=	1.421308
I=	2	J=	3	B=	1.374411
I=	2	J=	8	B=	1.328792
I=	3	J=	4	B=	1.393336
I=	3	J=	15	B=	1.331612
I=	4	J=	5	B=	1.378463
I=	4	J=	10	B=	1.717084
I=	5	J=	6	B=	1.395682
I=	5	J=	9	B=	1.342503
I=	6	J=	7	B=	1.360464
I=	7	J=	13	B=	1.005471
I=	7	J=	14	B=	1.006851
I=	11	J=	12	B=	1.149207

I=	1	J=	2	K=	3	A=	121.391
I=	1	J=	2	K=	8	A=	119.323
I=	1	J=	6	K=	7	A=	122.618
I=	1	J=	11	K=	12	A=	175.870
I=	2	J=	3	K=	4	A=	119.430
I=	2	J=	3	K=	15	A=	120.030
I=	3	J=	4	K=	5	A=	119.174
I=	3	J=	4	K=	10	A=	120.191
I=	4	J=	5	K=	6	A=	122.815
I=	4	J=	5	K=	9	A=	120.054
I=	5	J=	6	K=	7	A=	120.244
I=	6	J=	7	K=	13	A=	118.964
I=	6	J=	7	K=	14	A=	119.748

I=	1	J=	2	K=	3	L=	4	D=	0.148
I=	1	J=	2	K=	3	L=	15	D=	179.978
I=	1	J=	6	K=	7	L=	13	D=	170.027
I=	1	J=	6	K=	7	L=	14	D=	11.404
I=	2	J=	3	K=	4	L=	5	D=	0.183
I=	2	J=	3	K=	4	L=	10	D=	179.765
I=	3	J=	4	K=	5	L=	6	D=	0.050
I=	3	J=	4	K=	5	L=	9	D=	179.797
I=	4	J=	5	K=	6	L=	7	D=	178.359
I=	5	J=	6	K=	7	L=	13	D=	11.382
I=	5	J=	6	K=	7	L=	14	D=	170.006

molD_m062x

I=	1	J=	2	B=	1.395510
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I=	1	J=	6	B=	1.406771
I=	1	J=	11	B=	1.425732
I=	2	J=	3	B=	1.377631
I=	2	J=	8	B=	1.325379
I=	3	J=	4	B=	1.395609
I=	3	J=	15	B=	1.327829
I=	4	J=	5	B=	1.381463
I=	4	J=	10	B=	1.714501
I=	5	J=	6	B=	1.397804
I=	5	J=	9	B=	1.337644
I=	6	J=	7	B=	1.364867
I=	7	J=	13	B=	1.007165
I=	7	J=	14	B=	1.008750
I=	11	J=	12	B=	1.150758

I=	1	J=	2	K=	3	A=	121.184
I=	1	J=	2	K=	8	A=	119.469
I=	1	J=	6	K=	7	A=	122.614
I=	1	J=	11	K=	12	A=	175.779
I=	2	J=	3	K=	4	A=	119.378
I=	2	J=	3	K=	15	A=	120.084
I=	3	J=	4	K=	5	A=	119.361
I=	3	J=	4	K=	10	A=	120.096
I=	4	J=	5	K=	6	A=	122.634
I=	4	J=	5	K=	9	A=	120.077
I=	5	J=	6	K=	7	A=	120.259
I=	6	J=	7	K=	13	A=	117.931
I=	6	J=	7	K=	14	A=	118.557

I=	1	J=	2	K=	3	L=	4	D=	0.202
I=	1	J=	2	K=	3	L=	15	D=	179.978
I=	1	J=	6	K=	7	L=	13	D=	166.099
I=	1	J=	6	K=	7	L=	14	D=	15.833
I=	2	J=	3	K=	4	L=	5	D=	0.250
I=	2	J=	3	K=	4	L=	10	D=	179.702
I=	3	J=	4	K=	5	L=	6	D=	0.006
I=	3	J=	4	K=	5	L=	9	D=	179.764
I=	4	J=	5	K=	6	L=	7	D=	177.665
I=	5	J=	6	K=	7	L=	13	D=	16.052
I=	5	J=	6	K=	7	L=	14	D=	166.317

molD_mp2

I=	1	J=	2	B=	1.401058
I=	1	J=	6	B=	1.413117
I=	1	J=	11	B=	1.426673
I=	2	J=	3	B=	1.388184
I=	2	J=	8	B=	1.335069
I=	3	J=	4	B=	1.400992
I=	3	J=	15	B=	1.332398
I=	4	J=	5	B=	1.394354
I=	4	J=	10	B=	1.712615
I=	5	J=	6	B=	1.400162
I=	5	J=	9	B=	1.342511
I=	6	J=	7	B=	1.383364
I=	7	J=	13	B=	1.010824

I=	7	J=	14		B=	1.012154	
I=	11	J=	12		B=	1.178844	
I=	1	J=	2	K=	3	A=	120.879
I=	1	J=	2	K=	8	A=	119.593
I=	1	J=	6	K=	7	A=	122.004
I=	1	J=	11	K=	12	A=	175.824
I=	2	J=	3	K=	4	A=	119.723
I=	2	J=	3	K=	15	A=	119.722
I=	3	J=	4	K=	5	A=	118.760
I=	3	J=	4	K=	10	A=	120.409
I=	4	J=	5	K=	6	A=	122.798
I=	4	J=	5	K=	9	A=	119.665
I=	5	J=	6	K=	7	A=	120.483
I=	6	J=	7	K=	13	A=	115.215
I=	6	J=	7	K=	14	A=	115.663

I=	1	J=	2	K=	3	L=	4	D=	4.508
I=	1	J=	2	K=	3	L=	15	D=	178.892
I=	1	J=	6	K=	7	L=	13	D=	161.997
I=	1	J=	6	K=	7	L=	14	D=	26.223
I=	2	J=	3	K=	4	L=	5	D=	4.802
I=	2	J=	3	K=	4	L=	10	D=	179.560
I=	3	J=	4	K=	5	L=	6	D=	5.065
I=	3	J=	4	K=	5	L=	9	D=	178.951
I=	4	J=	5	K=	6	L=	7	D=	178.000
I=	5	J=	6	K=	7	L=	13	D=	25.050
I=	5	J=	6	K=	7	L=	14	D=	160.824

molD_pbe0d

I=	1	J=	2		B=	1.396500	
I=	1	J=	6		B=	1.409781	
I=	1	J=	11		B=	1.416172	
I=	2	J=	3		B=	1.377971	
I=	2	J=	8		B=	1.324625	
I=	3	J=	4		B=	1.396169	
I=	3	J=	15		B=	1.326860	
I=	4	J=	5		B=	1.382768	
I=	4	J=	10		B=	1.710138	
I=	5	J=	6		B=	1.396896	
I=	5	J=	9		B=	1.337389	
I=	6	J=	7		B=	1.359898	
I=	7	J=	13		B=	1.005545	
I=	7	J=	14		B=	1.007280	
I=	11	J=	12		B=	1.155435	
I=	1	J=	2	K=	3	A=	121.242
I=	1	J=	2	K=	8	A=	119.402
I=	1	J=	6	K=	7	A=	122.397
I=	1	J=	11	K=	12	A=	175.805
I=	2	J=	3	K=	4	A=	119.364
I=	2	J=	3	K=	15	A=	120.112
I=	3	J=	4	K=	5	A=	119.394
I=	3	J=	4	K=	10	A=	120.080
I=	4	J=	5	K=	6	A=	122.620

I=	4	J=	5	K=	9	A=	120.028		
I=	5	J=	6	K=	7	A=	120.430		
I=	6	J=	7	K=	13	A=	118.263		
I=	6	J=	7	K=	14	A=	118.769		
I=	1	J=	2	K=	3	L=	4	D=	0.203
I=	1	J=	2	K=	3	L=	15	D=	179.965
I=	1	J=	6	K=	7	L=	13	D=	166.738
I=	1	J=	6	K=	7	L=	14	D=	14.573
I=	2	J=	3	K=	4	L=	5	D=	0.274
I=	2	J=	3	K=	4	L=	10	D=	179.681
I=	3	J=	4	K=	5	L=	6	D=	0.031
I=	3	J=	4	K=	5	L=	9	D=	179.771
I=	4	J=	5	K=	6	L=	7	D=	177.763
I=	5	J=	6	K=	7	L=	13	D=	15.205
I=	5	J=	6	K=	7	L=	14	D=	167.369

molD_pbe

I=	1	J=	2	B=	1.408540
I=	1	J=	6	B=	1.424534
I=	1	J=	11	B=	1.418592
I=	2	J=	3	B=	1.389964
I=	2	J=	8	B=	1.342793
I=	3	J=	4	B=	1.407195
I=	3	J=	15	B=	1.344096
I=	4	J=	5	B=	1.394442
I=	4	J=	10	B=	1.724999
I=	5	J=	6	B=	1.407667
I=	5	J=	9	B=	1.356167
I=	6	J=	7	B=	1.369768
I=	7	J=	13	B=	1.014362
I=	7	J=	14	B=	1.016192
I=	11	J=	12	B=	1.170436

I=	1	J=	2	K=	3	A=	121.431
I=	1	J=	2	K=	8	A=	119.355
I=	1	J=	6	K=	7	A=	122.264
I=	1	J=	11	K=	12	A=	175.748
I=	2	J=	3	K=	4	A=	119.441
I=	2	J=	3	K=	15	A=	120.045
I=	3	J=	4	K=	5	A=	119.199
I=	3	J=	4	K=	10	A=	120.168
I=	4	J=	5	K=	6	A=	122.808
I=	4	J=	5	K=	9	A=	119.937
I=	5	J=	6	K=	7	A=	120.491
I=	6	J=	7	K=	13	A=	118.158
I=	6	J=	7	K=	14	A=	118.568

I=	1	J=	2	K=	3	L=	4	D=	0.217
I=	1	J=	2	K=	3	L=	15	D=	179.936
I=	1	J=	6	K=	7	L=	13	D=	166.233
I=	1	J=	6	K=	7	L=	14	D=	15.150
I=	2	J=	3	K=	4	L=	5	D=	0.309
I=	2	J=	3	K=	4	L=	10	D=	179.630
I=	3	J=	4	K=	5	L=	6	D=	0.052

I=	3	J=	4	K=	5	L=	9	D=	179.746
I=	4	J=	5	K=	6	L=	7	D=	177.500
I=	5	J=	6	K=	7	L=	13	D=	15.882
I=	5	J=	6	K=	7	L=	14	D=	166.965

molD_rtpss

I=	1	J=	2	B=	1.405992
I=	1	J=	6	B=	1.421123
I=	1	J=	11	B=	1.419561
I=	2	J=	3	B=	1.386729
I=	2	J=	8	B=	1.343714
I=	3	J=	4	B=	1.403907
I=	3	J=	15	B=	1.344802
I=	4	J=	5	B=	1.391717
I=	4	J=	10	B=	1.725176
I=	5	J=	6	B=	1.403482
I=	5	J=	9	B=	1.357132
I=	6	J=	7	B=	1.375708
I=	7	J=	13	B=	1.014539
I=	7	J=	14	B=	1.016187
I=	11	J=	12	B=	1.168208

I=	1	J=	2	K=	3	A=	121.482
I=	1	J=	2	K=	8	A=	119.292
I=	1	J=	6	K=	7	A=	122.268
I=	1	J=	11	K=	12	A=	175.927
I=	2	J=	3	K=	4	A=	119.453
I=	2	J=	3	K=	15	A=	120.085
I=	3	J=	4	K=	5	A=	119.098
I=	3	J=	4	K=	10	A=	120.227
I=	4	J=	5	K=	6	A=	122.916
I=	4	J=	5	K=	9	A=	119.842
I=	5	J=	6	K=	7	A=	120.445
I=	6	J=	7	K=	13	A=	116.496
I=	6	J=	7	K=	14	A=	116.982

I=	1	J=	2	K=	3	L=	4	D=	0.299
I=	1	J=	2	K=	3	L=	15	D=	179.934
I=	1	J=	6	K=	7	L=	13	D=	162.213
I=	1	J=	6	K=	7	L=	14	D=	20.106
I=	2	J=	3	K=	4	L=	5	D=	0.411
I=	2	J=	3	K=	4	L=	10	D=	179.512
I=	3	J=	4	K=	5	L=	6	D=	0.012
I=	3	J=	4	K=	5	L=	9	D=	179.689
I=	4	J=	5	K=	6	L=	7	D=	176.573
I=	5	J=	6	K=	7	L=	13	D=	20.881
I=	5	J=	6	K=	7	L=	14	D=	162.988

molD_wb97xd

I=	1	J=	2	B=	1.396109
I=	1	J=	6	B=	1.407428
I=	1	J=	11	B=	1.423216
I=	2	J=	3	B=	1.377824
I=	2	J=	8	B=	1.325906

I=	3	J=	4	B=	1.395638
I=	3	J=	15	B=	1.328681
I=	4	J=	5	B=	1.381796
I=	4	J=	10	B=	1.718811
I=	5	J=	6	B=	1.398074
I=	5	J=	9	B=	1.339380
I=	6	J=	7	B=	1.363514
I=	7	J=	13	B=	1.005233
I=	7	J=	14	B=	1.006884
I=	11	J=	12	B=	1.152199

I=	1	J=	2	K=	3	A=	121.251
I=	1	J=	2	K=	8	A=	119.385
I=	1	J=	6	K=	7	A=	122.497
I=	1	J=	11	K=	12	A=	175.976
I=	2	J=	3	K=	4	A=	119.380
I=	2	J=	3	K=	15	A=	120.024
I=	3	J=	4	K=	5	A=	119.328
I=	3	J=	4	K=	10	A=	120.126
I=	4	J=	5	K=	6	A=	122.666
I=	4	J=	5	K=	9	A=	120.050
I=	5	J=	6	K=	7	A=	120.357
I=	6	J=	7	K=	13	A=	118.413
I=	6	J=	7	K=	14	A=	119.027

I=	1	J=	2	K=	3	L=	4	D=	0.196
I=	1	J=	2	K=	3	L=	15	D=	179.965
I=	1	J=	6	K=	7	L=	13	D=	167.246
I=	1	J=	6	K=	7	L=	14	D=	14.426
I=	2	J=	3	K=	4	L=	5	D=	0.242
I=	2	J=	3	K=	4	L=	10	D=	179.720
I=	3	J=	4	K=	5	L=	6	D=	0.018
I=	3	J=	4	K=	5	L=	9	D=	179.779
I=	4	J=	5	K=	6	L=	7	D=	177.844
I=	5	J=	6	K=	7	L=	13	D=	14.698
I=	5	J=	6	K=	7	L=	14	D=	167.518

molD_x3lyp

I=	1	J=	2	B=	1.400058
I=	1	J=	6	B=	1.414605
I=	1	J=	11	B=	1.420077
I=	2	J=	3	B=	1.380260
I=	2	J=	8	B=	1.334106
I=	3	J=	4	B=	1.398551
I=	3	J=	15	B=	1.336199
I=	4	J=	5	B=	1.384834
I=	4	J=	10	B=	1.726042
I=	5	J=	6	B=	1.400478
I=	5	J=	9	B=	1.347714
I=	6	J=	7	B=	1.365509
I=	7	J=	13	B=	1.006484
I=	7	J=	14	B=	1.007890
I=	11	J=	12	B=	1.155426

I=	1	J=	2	K=	3	A=	121.490
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I=	1	J=	2	K=	8	A=	119.311
I=	1	J=	6	K=	7	A=	122.497
I=	1	J=	11	K=	12	A=	176.042
I=	2	J=	3	K=	4	A=	119.461
I=	2	J=	3	K=	15	A=	119.980
I=	3	J=	4	K=	5	A=	119.141
I=	3	J=	4	K=	10	A=	120.203
I=	4	J=	5	K=	6	A=	122.857
I=	4	J=	5	K=	9	A=	119.986
I=	5	J=	6	K=	7	A=	120.303
I=	6	J=	7	K=	13	A=	118.538
I=	6	J=	7	K=	14	A=	119.213

I=	1	J=	2	K=	3	L=	4	D=	0.178
I=	1	J=	2	K=	3	L=	15	D=	179.966
I=	1	J=	6	K=	7	L=	13	D=	167.830
I=	1	J=	6	K=	7	L=	14	D=	13.908
I=	2	J=	3	K=	4	L=	5	D=	0.231
I=	2	J=	3	K=	4	L=	10	D=	179.706
I=	3	J=	4	K=	5	L=	6	D=	0.058
I=	3	J=	4	K=	5	L=	9	D=	179.775
I=	4	J=	5	K=	6	L=	7	D=	177.859
I=	5	J=	6	K=	7	L=	13	D=	14.019
I=	5	J=	6	K=	7	L=	14	D=	167.941

molE_apfd

I=	1	J=	2	B=	1.398493
I=	1	J=	6	B=	1.412185
I=	1	J=	12	B=	1.417009
I=	2	J=	3	B=	1.376460
I=	2	J=	8	B=	1.334501
I=	3	J=	4	B=	1.396416
I=	3	J=	11	B=	1.081756
I=	4	J=	5	B=	1.381329
I=	4	J=	10	B=	1.721416
I=	5	J=	6	B=	1.401284
I=	5	J=	9	B=	1.343111
I=	6	J=	7	B=	1.355689
I=	7	J=	14	B=	1.005140
I=	7	J=	15	B=	1.007045
I=	12	J=	13	B=	1.156568

I=	1	J=	2	K=	3	A=	122.694
I=	1	J=	2	K=	8	A=	117.984
I=	1	J=	6	K=	7	A=	122.297
I=	1	J=	12	K=	13	A=	175.816
I=	2	J=	3	K=	4	A=	117.728
I=	2	J=	3	K=	11	A=	120.830
I=	3	J=	4	K=	5	A=	120.850
I=	3	J=	4	K=	10	A=	120.099
I=	4	J=	5	K=	6	A=	121.849
I=	4	J=	5	K=	9	A=	120.908
I=	5	J=	6	K=	7	A=	120.246
I=	6	J=	7	K=	14	A=	119.397
I=	6	J=	7	K=	15	A=	119.734

I=	1	J=	2	K=	3	L=	4	D=	0.124
I=	1	J=	2	K=	3	L=	11	D=	179.983
I=	1	J=	6	K=	7	L=	14	D=	170.555
I=	1	J=	6	K=	7	L=	15	D=	10.145
I=	2	J=	3	K=	4	L=	5	D=	0.183
I=	2	J=	3	K=	4	L=	10	D=	179.777
I=	3	J=	4	K=	5	L=	6	D=	0.038
I=	3	J=	4	K=	5	L=	9	D=	179.841
I=	4	J=	5	K=	6	L=	7	D=	178.435
I=	5	J=	6	K=	7	L=	14	D=	10.760
I=	5	J=	6	K=	7	L=	15	D=	171.170

molE_b3lypd

I=	1	J=	2	B=	1.399762
I=	1	J=	6	B=	1.416044
I=	1	J=	12	B=	1.418385
I=	2	J=	3	B=	1.376983
I=	2	J=	8	B=	1.342557
I=	3	J=	4	B=	1.398564
I=	3	J=	11	B=	1.079738
I=	4	J=	5	B=	1.382019
I=	4	J=	10	B=	1.736460
I=	5	J=	6	B=	1.402541
I=	5	J=	9	B=	1.351242
I=	6	J=	7	B=	1.361232
I=	7	J=	14	B=	1.006026
I=	7	J=	15	B=	1.007656
I=	12	J=	13	B=	1.156359

I=	1	J=	2	K=	3	A=	123.029
I=	1	J=	2	K=	8	A=	117.897
I=	1	J=	6	K=	7	A=	122.244
I=	1	J=	12	K=	13	A=	175.648
I=	2	J=	3	K=	4	A=	117.704
I=	2	J=	3	K=	11	A=	120.898
I=	3	J=	4	K=	5	A=	120.635
I=	3	J=	4	K=	10	A=	119.923
I=	4	J=	5	K=	6	A=	122.095
I=	4	J=	5	K=	9	A=	120.919
I=	5	J=	6	K=	7	A=	120.294
I=	6	J=	7	K=	14	A=	119.080
I=	6	J=	7	K=	15	A=	119.656

I=	1	J=	2	K=	3	L=	4	D=	0.135
I=	1	J=	2	K=	3	L=	11	D=	179.978
I=	1	J=	6	K=	7	L=	14	D=	170.031
I=	1	J=	6	K=	7	L=	15	D=	11.149
I=	2	J=	3	K=	4	L=	5	D=	0.187
I=	2	J=	3	K=	4	L=	10	D=	179.753
I=	3	J=	4	K=	5	L=	6	D=	0.056
I=	3	J=	4	K=	5	L=	9	D=	179.802
I=	4	J=	5	K=	6	L=	7	D=	178.299
I=	5	J=	6	K=	7	L=	14	D=	11.392
I=	5	J=	6	K=	7	L=	15	D=	170.274

molE_blyp

I=	1	J=	2	B=	1.412270
I=	1	J=	6	B=	1.431157
I=	1	J=	12	B=	1.423840
I=	2	J=	3	B=	1.388010
I=	2	J=	8	B=	1.362241
I=	3	J=	4	B=	1.408617
I=	3	J=	11	B=	1.086387
I=	4	J=	5	B=	1.393729
I=	4	J=	10	B=	1.756430
I=	5	J=	6	B=	1.413938
I=	5	J=	9	B=	1.370589
I=	6	J=	7	B=	1.373626
I=	7	J=	14	B=	1.014038
I=	7	J=	15	B=	1.015557
I=	12	J=	13	B=	1.169735

I=	1	J=	2	K=	3	A=	123.360
I=	1	J=	2	K=	8	A=	117.864
I=	1	J=	6	K=	7	A=	122.229
I=	1	J=	12	K=	13	A=	175.989
I=	2	J=	3	K=	4	A=	117.715
I=	2	J=	3	K=	11	A=	120.824
I=	3	J=	4	K=	5	A=	120.472
I=	3	J=	4	K=	10	A=	119.950
I=	4	J=	5	K=	6	A=	122.308
I=	4	J=	5	K=	9	A=	120.831
I=	5	J=	6	K=	7	A=	120.277
I=	6	J=	7	K=	14	A=	118.770
I=	6	J=	7	K=	15	A=	119.358

I=	1	J=	2	K=	3	L=	4	D=	0.153
I=	1	J=	2	K=	3	L=	11	D=	179.957
I=	1	J=	6	K=	7	L=	14	D=	168.593
I=	1	J=	6	K=	7	L=	15	D=	13.029
I=	2	J=	3	K=	4	L=	5	D=	0.222
I=	2	J=	3	K=	4	L=	10	D=	179.698
I=	3	J=	4	K=	5	L=	6	D=	0.071
I=	3	J=	4	K=	5	L=	9	D=	179.769
I=	4	J=	5	K=	6	L=	7	D=	177.884
I=	5	J=	6	K=	7	L=	14	D=	13.180
I=	5	J=	6	K=	7	L=	15	D=	168.744

molE_camb3lypd

I=	1	J=	2	B=	1.393954
I=	1	J=	6	B=	1.407231
I=	1	J=	12	B=	1.420816
I=	2	J=	3	B=	1.371094
I=	2	J=	8	B=	1.335920
I=	3	J=	4	B=	1.393831
I=	3	J=	11	B=	1.079516
I=	4	J=	5	B=	1.375112
I=	4	J=	10	B=	1.727106

I=	5	J=	6	B=	1.398239
I=	5	J=	9	B=	1.345253
I=	6	J=	7	B=	1.355191
I=	7	J=	14	B=	1.004828
I=	7	J=	15	B=	1.006312
I=	12	J=	13	B=	1.149536

I=	1	J=	2	K=	3	A=	123.034
I=	1	J=	2	K=	8	A=	117.814
I=	1	J=	6	K=	7	A=	122.544
I=	1	J=	12	K=	13	A=	175.760
I=	2	J=	3	K=	4	A=	117.634
I=	2	J=	3	K=	11	A=	120.886
I=	3	J=	4	K=	5	A=	120.599
I=	3	J=	4	K=	10	A=	120.042
I=	4	J=	5	K=	6	A=	122.178
I=	4	J=	5	K=	9	A=	120.958
I=	5	J=	6	K=	7	A=	120.111
I=	6	J=	7	K=	14	A=	119.797
I=	6	J=	7	K=	15	A=	120.585

I=	1	J=	2	K=	3	L=	4	D=	0.063
I=	1	J=	2	K=	3	L=	11	D=	179.990
I=	1	J=	6	K=	7	L=	14	D=	175.321
I=	1	J=	6	K=	7	L=	15	D=	5.298
I=	2	J=	3	K=	4	L=	5	D=	0.084
I=	2	J=	3	K=	4	L=	10	D=	179.887
I=	3	J=	4	K=	5	L=	6	D=	0.031
I=	3	J=	4	K=	5	L=	9	D=	179.895
I=	4	J=	5	K=	6	L=	7	D=	179.249
I=	5	J=	6	K=	7	L=	14	D=	5.299
I=	5	J=	6	K=	7	L=	15	D=	175.323

mo1E_m062x

I=	1	J=	2	B=	1.395964
I=	1	J=	6	B=	1.408085
I=	1	J=	12	B=	1.425243
I=	2	J=	3	B=	1.374712
I=	2	J=	8	B=	1.331794
I=	3	J=	4	B=	1.396563
I=	3	J=	11	B=	1.080248
I=	4	J=	5	B=	1.378158
I=	4	J=	10	B=	1.724601
I=	5	J=	6	B=	1.400541
I=	5	J=	9	B=	1.340176
I=	6	J=	7	B=	1.359039
I=	7	J=	14	B=	1.006421
I=	7	J=	15	B=	1.008124
I=	12	J=	13	B=	1.151087

I=	1	J=	2	K=	3	A=	122.828
I=	1	J=	2	K=	8	A=	117.835
I=	1	J=	6	K=	7	A=	122.540
I=	1	J=	12	K=	13	A=	175.654
I=	2	J=	3	K=	4	A=	117.560

I=	2	J=	3	K=	11	A=	120.935
I=	3	J=	4	K=	5	A=	120.793
I=	3	J=	4	K=	10	A=	120.124
I=	4	J=	5	K=	6	A=	122.002
I=	4	J=	5	K=	9	A=	121.010
I=	5	J=	6	K=	7	A=	120.122
I=	6	J=	7	K=	14	A=	118.852
I=	6	J=	7	K=	15	A=	119.471

I=	1	J=	2	K=	3	L=	4	D=	0.140
I=	1	J=	2	K=	3	L=	11	D=	179.983
I=	1	J=	6	K=	7	L=	14	D=	169.446
I=	1	J=	6	K=	7	L=	15	D=	11.926
I=	2	J=	3	K=	4	L=	5	D=	0.185
I=	2	J=	3	K=	4	L=	10	D=	179.765
I=	3	J=	4	K=	5	L=	6	D=	0.022
I=	3	J=	4	K=	5	L=	9	D=	179.803
I=	4	J=	5	K=	6	L=	7	D=	178.254
I=	5	J=	6	K=	7	L=	14	D=	12.109
I=	5	J=	6	K=	7	L=	15	D=	169.629

molE_mp2

I=	1	J=	2	B=	1.401360
I=	1	J=	6	B=	1.413293
I=	1	J=	12	B=	1.426817
I=	2	J=	3	B=	1.384418
I=	2	J=	8	B=	1.342023
I=	3	J=	4	B=	1.401004
I=	3	J=	11	B=	1.083733
I=	4	J=	5	B=	1.391464
I=	4	J=	10	B=	1.721301
I=	5	J=	6	B=	1.402471
I=	5	J=	9	B=	1.344462
I=	6	J=	7	B=	1.379823
I=	7	J=	14	B=	1.010434
I=	7	J=	15	B=	1.011835
I=	12	J=	13	B=	1.178719

I=	1	J=	2	K=	3	A=	122.393
I=	1	J=	2	K=	8	A=	118.168
I=	1	J=	6	K=	7	A=	121.915
I=	1	J=	12	K=	13	A=	175.791
I=	2	J=	3	K=	4	A=	118.154
I=	2	J=	3	K=	11	A=	120.566
I=	3	J=	4	K=	5	A=	120.010
I=	3	J=	4	K=	10	A=	120.398
I=	4	J=	5	K=	6	A=	122.151
I=	4	J=	5	K=	9	A=	120.586
I=	5	J=	6	K=	7	A=	120.272
I=	6	J=	7	K=	14	A=	115.666
I=	6	J=	7	K=	15	A=	116.109

I=	1	J=	2	K=	3	L=	4	D=	4.422
I=	1	J=	2	K=	3	L=	11	D=	179.479
I=	1	J=	6	K=	7	L=	14	D=	162.659

I=	1	J=	6	K=	7	L=	15	D=	24.831
I=	2	J=	3	K=	4	L=	5	D=	4.682
I=	2	J=	3	K=	4	L=	10	D=	179.460
I=	3	J=	4	K=	5	L=	6	D=	5.041
I=	3	J=	4	K=	5	L=	9	D=	179.165
I=	4	J=	5	K=	6	L=	7	D=	178.391
I=	5	J=	6	K=	7	L=	14	D=	23.975
I=	5	J=	6	K=	7	L=	15	D=	161.803

molE_pbe0d

I=	1	J=	2	B=	1.396576
I=	1	J=	6	B=	1.411244
I=	1	J=	12	B=	1.415758
I=	2	J=	3	B=	1.374216
I=	2	J=	8	B=	1.331059
I=	3	J=	4	B=	1.395503
I=	3	J=	11	B=	1.081111
I=	4	J=	5	B=	1.379593
I=	4	J=	10	B=	1.719879
I=	5	J=	6	B=	1.399411
I=	5	J=	9	B=	1.339862
I=	6	J=	7	B=	1.354828
I=	7	J=	14	B=	1.004879
I=	7	J=	15	B=	1.006728
I=	12	J=	13	B=	1.155738

I=	1	J=	2	K=	3	A=	122.803
I=	1	J=	2	K=	8	A=	117.949
I=	1	J=	6	K=	7	A=	122.278
I=	1	J=	12	K=	13	A=	175.711
I=	2	J=	3	K=	4	A=	117.755
I=	2	J=	3	K=	11	A=	120.894
I=	3	J=	4	K=	5	A=	120.711
I=	3	J=	4	K=	10	A=	120.017
I=	4	J=	5	K=	6	A=	121.966
I=	4	J=	5	K=	9	A=	120.965
I=	5	J=	6	K=	7	A=	120.266
I=	6	J=	7	K=	14	A=	119.081
I=	6	J=	7	K=	15	A=	119.585

I=	1	J=	2	K=	3	L=	4	D=	0.140
I=	1	J=	2	K=	3	L=	11	D=	179.982
I=	1	J=	6	K=	7	L=	14	D=	170.076
I=	1	J=	6	K=	7	L=	15	D=	10.867
I=	2	J=	3	K=	4	L=	5	D=	0.198
I=	2	J=	3	K=	4	L=	10	D=	179.756
I=	3	J=	4	K=	5	L=	6	D=	0.037
I=	3	J=	4	K=	5	L=	9	D=	179.814
I=	4	J=	5	K=	6	L=	7	D=	178.353
I=	5	J=	6	K=	7	L=	14	D=	11.312
I=	5	J=	6	K=	7	L=	15	D=	170.521

molE_pbe

I=	1	J=	2	B=	1.408444
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I=	1	J=	6	B=	1.425708
I=	1	J=	12	B=	1.418299
I=	2	J=	3	B=	1.384939
I=	2	J=	8	B=	1.350088
I=	3	J=	4	B=	1.405086
I=	3	J=	11	B=	1.088575
I=	4	J=	5	B=	1.391300
I=	4	J=	10	B=	1.735714
I=	5	J=	6	B=	1.409886
I=	5	J=	9	B=	1.358466
I=	6	J=	7	B=	1.365339
I=	7	J=	14	B=	1.013772
I=	7	J=	15	B=	1.015704
I=	12	J=	13	B=	1.170668

I=	1	J=	2	K=	3	A=	123.075
I=	1	J=	2	K=	8	A=	117.892
I=	1	J=	6	K=	7	A=	122.149
I=	1	J=	12	K=	13	A=	175.678
I=	2	J=	3	K=	4	A=	117.789
I=	2	J=	3	K=	11	A=	120.854
I=	3	J=	4	K=	5	A=	120.561
I=	3	J=	4	K=	10	A=	120.095
I=	4	J=	5	K=	6	A=	122.133
I=	4	J=	5	K=	9	A=	120.892
I=	5	J=	6	K=	7	A=	120.340
I=	6	J=	7	K=	14	A=	118.863
I=	6	J=	7	K=	15	A=	119.271

I=	1	J=	2	K=	3	L=	4	D=	0.159
I=	1	J=	2	K=	3	L=	11	D=	179.963
I=	1	J=	6	K=	7	L=	14	D=	168.921
I=	1	J=	6	K=	7	L=	15	D=	12.177
I=	2	J=	3	K=	4	L=	5	D=	0.238
I=	2	J=	3	K=	4	L=	10	D=	179.699
I=	3	J=	4	K=	5	L=	6	D=	0.052
I=	3	J=	4	K=	5	L=	9	D=	179.786
I=	4	J=	5	K=	6	L=	7	D=	178.020
I=	5	J=	6	K=	7	L=	14	D=	12.720
I=	5	J=	6	K=	7	L=	15	D=	169.464

molE_rtpss

I=	1	J=	2	B=	1.405772
I=	1	J=	6	B=	1.421991
I=	1	J=	12	B=	1.419302
I=	2	J=	3	B=	1.383336
I=	2	J=	8	B=	1.351538
I=	3	J=	4	B=	1.403624
I=	3	J=	11	B=	1.084531
I=	4	J=	5	B=	1.388544
I=	4	J=	10	B=	1.736442
I=	5	J=	6	B=	1.405373
I=	5	J=	9	B=	1.359500
I=	6	J=	7	B=	1.371173
I=	7	J=	14	B=	1.013922

I=	7	J=	15		B=	1.015659			
I=	12	J=	13		B=	1.168449			
I=	1	J=	2	K=	3	A=	123.327		
I=	1	J=	2	K=	8	A=	117.705		
I=	1	J=	6	K=	7	A=	122.192		
I=	1	J=	12	K=	13	A=	175.836		
I=	2	J=	3	K=	4	A=	117.416		
I=	2	J=	3	K=	11	A=	121.116		
I=	3	J=	4	K=	5	A=	120.665		
I=	3	J=	4	K=	10	A=	120.094		
I=	4	J=	5	K=	6	A=	122.254		
I=	4	J=	5	K=	9	A=	120.786		
I=	5	J=	6	K=	7	A=	120.323		
I=	6	J=	7	K=	14	A=	117.157		
I=	6	J=	7	K=	15	A=	117.646		
I=	1	J=	2	K=	3	L=	4	D=	0.245
I=	1	J=	2	K=	3	L=	11	D=	179.959
I=	1	J=	6	K=	7	L=	14	D=	163.914
I=	1	J=	6	K=	7	L=	15	D=	18.149
I=	2	J=	3	K=	4	L=	5	D=	0.354
I=	2	J=	3	K=	4	L=	10	D=	179.558
I=	3	J=	4	K=	5	L=	6	D=	0.006
I=	3	J=	4	K=	5	L=	9	D=	179.704
I=	4	J=	5	K=	6	L=	7	D=	176.944
I=	5	J=	6	K=	7	L=	14	D=	18.797
I=	5	J=	6	K=	7	L=	15	D=	164.561

molE_wb97xd

I=	1	J=	2		B=	1.396370	
I=	1	J=	6		B=	1.409084	
I=	1	J=	12		B=	1.422692	
I=	2	J=	3		B=	1.373886	
I=	2	J=	8		B=	1.332649	
I=	3	J=	4		B=	1.395320	
I=	3	J=	11		B=	1.080364	
I=	4	J=	5		B=	1.378402	
I=	4	J=	10		B=	1.728794	
I=	5	J=	6		B=	1.400887	
I=	5	J=	9		B=	1.342022	
I=	6	J=	7		B=	1.358091	
I=	7	J=	14		B=	1.004538	
I=	7	J=	15		B=	1.006284	
I=	12	J=	13		B=	1.152536	
I=	1	J=	2	K=	3	A=	122.834
I=	1	J=	2	K=	8	A=	117.987
I=	1	J=	6	K=	7	A=	122.404
I=	1	J=	12	K=	13	A=	175.877
I=	2	J=	3	K=	4	A=	117.710
I=	2	J=	3	K=	11	A=	120.856
I=	3	J=	4	K=	5	A=	120.715
I=	3	J=	4	K=	10	A=	119.885
I=	4	J=	5	K=	6	A=	121.987

I=	4	J=	5	K=	9	A=	120.988		
I=	5	J=	6	K=	7	A=	120.193		
I=	6	J=	7	K=	14	A=	119.274		
I=	6	J=	7	K=	15	A=	119.899		
I=	1	J=	2	K=	3	L=	4	D=	0.130
I=	1	J=	2	K=	3	L=	11	D=	179.978
I=	1	J=	6	K=	7	L=	14	D=	170.886
I=	1	J=	6	K=	7	L=	15	D=	10.253
I=	2	J=	3	K=	4	L=	5	D=	0.168
I=	2	J=	3	K=	4	L=	10	D=	179.795
I=	3	J=	4	K=	5	L=	6	D=	0.027
I=	3	J=	4	K=	5	L=	9	D=	179.824
I=	4	J=	5	K=	6	L=	7	D=	178.487
I=	5	J=	6	K=	7	L=	14	D=	10.437
I=	5	J=	6	K=	7	L=	15	D=	171.070

molE_x3lyp

I=	1	J=	2	B=	1.399910
I=	1	J=	6	B=	1.416013
I=	1	J=	12	B=	1.419730
I=	2	J=	3	B=	1.376746
I=	2	J=	8	B=	1.341386
I=	3	J=	4	B=	1.398239
I=	3	J=	11	B=	1.079958
I=	4	J=	5	B=	1.381518
I=	4	J=	10	B=	1.736520
I=	5	J=	6	B=	1.402837
I=	5	J=	9	B=	1.350313
I=	6	J=	7	B=	1.360881
I=	7	J=	14	B=	1.005910
I=	7	J=	15	B=	1.007407
I=	12	J=	13	B=	1.155718

I=	1	J=	2	K=	3	A=	123.107
I=	1	J=	2	K=	8	A=	117.889
I=	1	J=	6	K=	7	A=	122.403
I=	1	J=	12	K=	13	A=	175.960
I=	2	J=	3	K=	4	A=	117.713
I=	2	J=	3	K=	11	A=	120.821
I=	3	J=	4	K=	5	A=	120.554
I=	3	J=	4	K=	10	A=	119.994
I=	4	J=	5	K=	6	A=	122.199
I=	4	J=	5	K=	9	A=	120.900
I=	5	J=	6	K=	7	A=	120.167
I=	6	J=	7	K=	14	A=	119.234
I=	6	J=	7	K=	15	A=	119.914

I=	1	J=	2	K=	3	L=	4	D=	0.122
I=	1	J=	2	K=	3	L=	11	D=	179.979
I=	1	J=	6	K=	7	L=	14	D=	170.816
I=	1	J=	6	K=	7	L=	15	D=	10.426
I=	2	J=	3	K=	4	L=	5	D=	0.168
I=	2	J=	3	K=	4	L=	10	D=	179.777
I=	3	J=	4	K=	5	L=	6	D=	0.053

I=	3	J=	4	K=	5	L=	9	D=	179.819
I=	4	J=	5	K=	6	L=	7	D=	178.414
I=	5	J=	6	K=	7	L=	14	D=	10.521
I=	5	J=	6	K=	7	L=	15	D=	170.911

Performance of the different levels of theory. Standard deviations (std dev), intercepts (a_0), slopes (a_1) and correlation coefficients (R^2) as obtained upon least squares linear regression of the computed values of the internal coordinates (bond distances, B; bond angles, A; and dihedral angles, D) vs the experimental values.

		APF[D]	B3LYP[D]	BLYP	CAM-B3LYP[D]	M06-2X	PBE	PBE0[D]	RevTPSS	wB97-X[D]	X3LYP	MP2
B (N=49)	std dev / A	0.01198	0.01142	0.02132	0.00957	0.01163	0.01231	0.01716	0.01606	0.01141	0.01132	0.01767
	a_0 / A	0.02658	0.00968	0.02734	-0.00174	-0.00240	0.02556	0.05634	0.05421	-0.00041	0.00534	0.10309
	a_1	0.98166	0.99655	0.99350	1.00084	1.00199	0.98098	0.96782	0.96879	1.00074	0.99947	0.93122
	R^2	0.99036	0.99287	0.99280	0.99386	0.99097	0.98965	0.99077	0.99192	0.99129	0.99284	0.98543
A (N=41)	std dev / deg	1.0	1.0	0.9	0.9	1.0	1.0	1.0	0.9	1.0	0.9	1.1
	a_0 / deg	-0.8	-0.8	-1.0	-0.8	-0.7	-0.7	-0.8	-1.0	-0.8	-0.9	-0.7
	a_1	1.00697	1.00676	1.00883	1.00725	1.00656	1.00666	1.00722	1.00862	1.00707	1.00822	1.00592
	R^2	0.99841	0.99858	0.99878	0.99862	0.99848	0.99846	0.99858	0.99877	0.99855	0.99869	0.99823
D (N=26)	std dev / deg	1.0	1.0	1.0	0.9	1.0	1.0	1.0	1.1	1.0	0.9	2.5
	a_0 / deg	-0.7	-0.7	-0.7	-0.7	-0.8	-0.7	-0.7	-0.7	-0.8	-0.7	3.5
	a_1	1.00578	1.00543	1.00454	1.00691	1.00570	1.00557	1.00468	1.00311	1.00597	1.00568	0.97952
	R^2	0.99996	0.99996	0.99995	0.99997	0.99996	0.99996	0.99996	0.99994	0.99996	0.99996	0.99998

Vibrational (IR) Spectra

molA_apfd

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A'	89.0373	0.0467	0.2461
2	A''	127.9496	0.1374	2.5479
3	A''	133.9299	0.1922	0.0102
4	A'	163.9163	0.1796	3.1550
5	A'	202.9821	0.2135	0.7718
6	A'	280.9726	0.7905	0.6529
7	A''	293.7062	0.2248	4.4823
8	A''	306.3018	0.5713	0.0013
9	A'	315.5955	0.1478	114.7694
10	A'	324.4423	0.7329	6.9373
11	A'	337.9996	0.1411	189.2274
12	A''	385.1084	0.2080	2.6381
13	A'	426.8083	1.1194	0.3696
14	A''	444.7844	0.2005	5.8120
15	A''	448.4322	0.9515	0.3579
16	A''	494.0204	1.8566	1.7939
17	A'	505.5120	1.8118	1.2421
18	A'	543.4931	2.7341	0.3718
19	A'	608.9401	2.0985	3.7599
20	A''	669.8482	3.2222	0.0001
21	A'	676.0706	2.9465	0.7008
22	A'	700.0101	3.4719	1.6393
23	A''	776.6768	1.8814	0.2576
24	A''	962.4248	2.4266	132.6404
25	A'	982.2328	6.6677	67.6584
26	A''	1150.4743	2.7952	67.2069
27	A''	1197.7766	2.6697	63.8004
28	A'	1202.8079	7.1918	38.8230
29	A'	1339.7451	10.5260	79.5112
30	A''	1385.4865	9.2921	8.2854
31	A'	1485.4455	15.3661	16.4874
32	A''	1556.4372	16.4319	387.3387
33	A'	1567.8640	7.1522	189.7815
34	A'	1648.6248	2.2501	77.9052
35	A''	1653.0445	15.4376	0.0426
36	A'	1713.8843	12.7023	325.5442
37	A'	2363.1776	41.6665	62.2565
38	A'	3628.1344	8.1122	144.6137
39	A''	3746.8421	9.1358	72.1820

molA_b3lypd

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	88.6564	0.0465	0.2539
2	A	128.8469	0.1394	2.5656
3	A	133.4505	0.1908	0.0105
4	A	163.2186	0.1792	3.3601

5	A	200.9637	0.2104	0.7525
6	A	280.2386	0.7921	0.5163
7	A	283.6422	0.1878	4.7295
8	A	304.5029	0.6873	0.0410
9	A	314.1839	0.2290	59.0118
10	A	319.8985	0.7825	4.2013
11	A	342.3812	0.1099	249.1826
12	A	381.7140	0.2446	2.0031
13	A	424.6830	1.0997	0.5502
14	A	438.9393	0.7926	3.7628
15	A	444.4561	0.1862	2.8547
16	A	486.7427	1.7867	2.0337
17	A	496.9664	1.7539	1.4296
18	A	535.0774	2.6335	0.3435
19	A	604.7164	2.0457	4.4040
20	A	663.2339	3.1602	0.0002
21	A	676.4771	3.0114	0.8898
22	A	711.4183	3.5541	1.4619
23	A	770.2073	1.8383	0.4614
24	A	948.6366	2.5671	145.1274
25	A	964.1115	6.4216	70.1421
26	A	1129.0585	4.0109	40.8217
27	A	1178.5936	2.0077	92.0120
28	A	1180.4033	7.0640	39.6241
29	A	1321.1120	10.6082	80.1976
30	A	1359.4501	8.2896	9.5948
31	A	1454.7420	14.6639	18.0074
32	A	1533.4692	15.9393	359.5697
33	A	1545.4508	8.9165	203.8877
34	A	1624.6167	14.2483	0.6211
35	A	1640.0189	2.1372	44.1533
36	A	1692.4814	10.8090	329.1365
37	A	2343.7001	40.9850	59.7491
38	A	3602.6308	7.9948	138.4320
39	A	3718.0345	8.9947	68.7276

molA_blyp

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A'	84.8267	0.0426	0.1757
2	A''	125.8534	0.1330	2.2874
3	A''	126.9759	0.1729	0.0191
4	A'	156.1930	0.1593	3.7543
5	A'	192.4205	0.2007	0.5907
6	A'	271.5540	0.7560	0.1729
7	A''	274.5232	0.1723	4.7540
8	A''	293.7925	0.6638	0.0160
9	A'	301.6430	0.4458	11.0276
10	A'	307.7433	0.7750	2.5549
11	A''	360.7353	0.2633	1.5628
12	A'	362.6268	0.1025	292.1861
13	A'	409.9442	0.9382	2.6008
14	A''	422.7379	0.7427	3.5129
15	A''	429.5068	0.1599	3.5914

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16	A''	467.3433	1.6455	1.6864
17	A'	471.8807	1.5866	1.3042
18	A'	511.4122	2.3829	0.5782
19	A'	581.4722	1.8468	6.7300
20	A''	627.9576	2.8336	0.0016
21	A'	645.9730	2.7466	0.9705
22	A'	678.6818	3.2113	0.7502
23	A''	741.2770	1.7410	0.5421
24	A''	903.6965	2.6140	156.4382
25	A'	923.6113	5.8981	69.0385
26	A''	1069.3535	5.3768	20.6582
27	A'	1126.3884	6.5828	30.4440
28	A''	1133.7573	1.5443	107.3521
29	A'	1251.5620	9.8381	80.7113
30	A''	1319.7560	7.7093	21.9099
31	A'	1378.7630	13.2095	17.3092
32	A''	1456.4519	14.4225	309.2918
33	A'	1478.8336	9.9305	168.8447
34	A''	1540.4021	11.9330	1.9550
35	A'	1587.9700	2.3524	2.6948
36	A'	1622.6732	5.1306	318.8095
37	A'	2232.7305	37.1825	52.3689
38	A'	3497.7506	7.5345	118.3854
39	A''	3608.1205	8.4650	57.6247

molA_camb3lypd

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A'	90.7606	0.0496	0.4013
2	A''	129.7482	0.1415	2.7041
3	A''	136.7347	0.2001	0.0068
4	A'	165.1876	0.2310	1.5781
5	A'	204.0335	0.1738	2.1163
6	A'	264.0348	0.0515	283.1443
7	A'	280.9128	0.6487	5.4564
8	A''	282.9992	0.1898	4.6704
9	A''	306.3433	0.6738	0.0494
10	A'	324.0018	0.8511	1.7530
11	A'	326.9418	0.8138	7.6617
12	A''	393.3186	0.2571	1.4342
13	A'	428.8062	1.1631	0.1249
14	A''	444.5424	1.2690	2.6524
15	A''	455.2128	0.1788	2.7611
16	A''	492.9062	1.8282	2.4150
17	A'	510.3983	1.8334	1.3384
18	A'	542.8581	2.7339	0.1422
19	A'	612.0666	2.1703	2.3676
20	A''	681.2908	3.3351	0.0002
21	A'	692.8184	3.1247	0.8506
22	A'	734.4307	3.8030	2.2520
23	A''	777.9371	1.8004	0.3481
24	A''	964.1384	2.4024	129.4108
25	A'	977.6021	6.5901	66.7408
26	A''	1149.3776	2.8639	73.5353

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27	A''	1191.2281	2.8741	66.5226
28	A'	1202.2943	7.1493	49.0252
29	A'	1348.9081	10.6273	76.4404
30	A''	1353.8955	8.1574	3.5934
31	A'	1489.1173	14.9711	22.0232
32	A''	1569.2777	16.6697	380.2420
33	A'	1574.5344	6.6375	195.1765
34	A'	1649.9935	2.2476	135.4355
35	A''	1669.4923	15.9428	0.0058
36	A'	1728.6467	16.1073	328.5466
37	A'	2405.5800	43.1949	59.0562
38	A'	3632.5109	8.1267	162.2554
39	A''	3750.0497	9.1592	80.8429

molA_m062x

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	90.5377	0.0476	0.2444
2	A	126.2110	0.1339	2.5252
3	A	137.0145	0.2011	0.0109
4	A	167.1383	0.1772	4.0563
5	A	203.3404	0.2178	0.8841
6	A	278.2250	0.7815	0.4157
7	A	282.3160	0.1935	4.3039
8	A	305.3922	0.6581	0.0724
9	A	320.2109	0.2901	43.8386
10	A	324.3623	0.9134	1.3263
11	A	358.2431	0.1129	288.7644
12	A	386.0053	0.1611	4.6022
13	A	425.6732	1.0724	1.2985
14	A	439.0596	0.2420	5.4707
15	A	442.2154	1.0629	0.3821
16	A	492.2064	1.8256	1.9268
17	A	507.9871	1.8392	1.5601
18	A	544.7540	2.7120	0.5339
19	A	611.0904	2.0179	4.7413
20	A	664.5577	2.8652	0.0998
21	A	670.7617	3.2267	0.0019
22	A	689.9270	3.3802	2.3043
23	A	774.7464	1.9076	0.2028
24	A	974.8453	2.2681	120.7709
25	A	981.6074	6.6346	63.7236
26	A	1163.0808	2.2709	87.6981
27	A	1207.8718	7.0706	50.4334
28	A	1211.4179	4.0090	39.4252
29	A	1357.5759	8.0886	1.2837
30	A	1363.0869	10.4160	65.7276
31	A	1505.8171	15.4862	16.2187
32	A	1577.1824	6.4008	201.5722
33	A	1585.5227	17.1690	403.5406
34	A	1645.7227	2.2624	140.0882
35	A	1681.3699	16.3931	0.0072
36	A	1732.3040	16.4477	277.3790
37	A	2416.1546	43.5810	52.3296

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38	A	3621.2893	8.0815	156.4103
39	A	3740.7213	9.1047	81.6269

molA_mp2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	89.7758	0.0474	0.2532
2	A	120.9802	0.1231	2.2770
3	A	133.3524	0.1908	0.0390
4	A	165.4334	0.1461	5.2165
5	A	208.4203	0.2599	1.1618
6	A	279.7460	0.8007	0.0118
7	A	284.9275	0.1810	3.9491
8	A	304.6139	0.7805	0.1171
9	A	316.2237	0.6137	4.1794
10	A	322.3331	0.9253	1.7383
11	A	358.1390	0.0943	14.4201
12	A	422.3611	1.1719	0.2955
13	A	424.2165	0.5028	2.6138
14	A	431.6909	1.3160	1.8909
15	A	452.1426	1.2322	2.7210
16	A	476.1068	1.8238	1.2521
17	A	536.5690	2.6110	0.0860
18	A	577.9548	0.4287	209.0406
19	A	616.6105	0.5887	141.5299
20	A	656.4063	3.0992	0.0325
21	A	669.9307	2.1580	31.6416
22	A	763.7994	2.0803	0.2981
23	A	800.8817	4.5052	1.0838
24	A	961.4033	2.7861	146.7338
25	A	963.3792	6.3879	60.5910
26	A	1146.4657	4.4833	23.4861
27	A	1172.7805	6.6891	49.1859
28	A	1216.4914	1.7463	72.6141
29	A	1331.6355	10.4994	55.3858
30	A	1464.3250	11.2611	21.9391
31	A	1480.5339	15.6917	4.3072
32	A	1552.9034	15.8657	356.4172
33	A	1558.9592	10.5678	169.5720
34	A	1647.8989	2.0421	32.1507
35	A	1657.4056	15.0045	0.9343
36	A	1716.4169	11.8222	177.9475
37	A	2187.5213	35.5235	1.7993
38	A	3598.4596	7.9900	97.4071
39	A	3715.9248	8.9557	54.8658

molA_pbe0d

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A'	89.4767	0.0471	0.2474
2	A''	127.8537	0.1375	2.5639
3	A''	134.9206	0.1948	0.0111

4	A'	165.3275	0.1787	3.3967
5	A'	203.8072	0.2165	0.8055
6	A'	278.3603	0.7812	0.3199
7	A''	280.2936	0.1824	4.6448
8	A''	305.7471	0.6868	0.0435
9	A'	319.0228	0.2369	59.7168
10	A'	323.9912	0.8819	1.9181
11	A'	349.2035	0.1133	255.5868
12	A''	386.7164	0.2118	2.7496
13	A'	425.6523	1.1116	0.5208
14	A''	440.1417	0.9703	3.1439
15	A''	446.6256	0.2010	3.1679
16	A''	491.8229	1.8193	1.8056
17	A'	506.2827	1.8240	1.4594
18	A'	543.2156	2.7073	0.3801
19	A'	611.1138	2.0815	4.0418
20	A''	671.5864	3.2397	0.0001
21	A'	678.4831	2.9892	0.6017
22	A'	701.9168	3.4907	1.7038
23	A''	776.3878	1.8700	0.2889
24	A''	967.3225	2.3726	127.9228
25	A'	982.4270	6.6779	63.8137
26	A''	1155.2375	2.7953	69.1455
27	A''	1201.6892	2.7915	61.4152
28	A'	1205.9702	7.1807	41.2089
29	A'	1348.9587	10.4961	80.5324
30	A''	1395.5074	9.6446	9.2537
31	A'	1491.8604	15.3585	14.5721
32	A''	1570.9046	16.9053	394.9782
33	A'	1576.5183	6.3133	175.4584
34	A'	1646.5316	2.2857	110.8708
35	A''	1662.7860	15.6527	0.2155
36	A'	1725.7024	15.1609	311.2889
37	A'	2373.8663	42.0311	63.5534
38	A'	3637.2978	8.1522	143.1827
39	A''	3756.9182	9.1827	72.9413

molA_pbe

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A'	84.9495	0.0427	0.1830
2	A''	123.1825	0.1276	2.2722
3	A''	127.7494	0.1747	0.0127
4	A'	157.4074	0.1612	3.4828
5	A'	193.4227	0.1999	0.5680
6	A'	268.4021	0.7323	0.1372
7	A''	270.4228	0.1668	4.7144
8	A''	293.8780	0.6446	0.0084
9	A'	303.7880	0.4268	13.4214
10	A'	310.9351	0.7900	2.5636
11	A'	362.0800	0.1027	289.4682
12	A''	364.2722	0.2474	1.8090
13	A'	409.7172	0.9748	1.7515
14	A''	422.4947	0.9335	2.7345

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15	A''	432.2333	0.1609	4.1507
16	A''	470.4226	1.6629	1.3629
17	A'	476.8512	1.6237	1.3246
18	A'	520.1098	2.4665	0.5895
19	A'	587.0206	1.8983	5.6546
20	A''	633.1131	2.8817	0.0012
21	A'	646.3503	2.7365	0.9732
22	A'	666.1228	3.0986	0.6694
23	A''	744.3786	1.7533	0.2739
24	A''	920.5267	2.3615	136.0551
25	A'	942.4810	6.1578	61.9954
26	A''	1097.2063	3.7335	39.7034
27	A''	1147.4654	1.8437	85.5215
28	A'	1152.5504	6.7183	30.5859
29	A'	1275.9520	9.7126	83.6226
30	A''	1362.1939	9.3913	29.2239
31	A'	1413.7559	13.9282	13.0510
32	A''	1489.7251	15.3059	339.8830
33	A'	1510.3727	7.2720	147.9963
34	A''	1572.3097	13.3146	1.1421
35	A'	1584.9306	2.0244	50.9664
36	A'	1649.0223	11.5205	303.4848
37	A'	2251.6229	37.7869	56.5187
38	A'	3520.6820	7.6354	123.8321
39	A''	3635.3885	8.5928	62.0953

mola_rtpss

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A'	86.1679	0.0434	0.2171
2	A''	121.0607	0.1237	2.2646
3	A''	129.7010	0.1803	0.0178
4	A'	160.4220	0.1517	5.0735
5	A'	193.6839	0.2077	0.7006
6	A'	259.9492	0.6873	0.0764
7	A''	261.5662	0.1584	4.6061
8	A''	288.1779	0.5684	0.0038
9	A'	304.9509	0.5536	5.3108
10	A'	309.5152	0.8463	1.3082
11	A''	361.4914	0.1936	3.9563
12	A'	410.1499	1.1098	3.4977
13	A''	419.2258	0.3095	7.0159
14	A''	423.9257	0.2890	1.4339
15	A'	468.1260	0.2109	248.7644
16	A''	471.1947	1.6933	1.0693
17	A'	480.9672	0.6331	92.2636
18	A'	522.8810	2.1472	6.9625
19	A'	592.4678	1.4762	21.1413
20	A''	627.6036	2.8284	0.0004
21	A'	630.0603	2.7028	0.1860
22	A'	644.5331	2.9485	0.9605
23	A''	745.7079	1.8606	0.4625
24	A''	927.7064	2.6429	157.4001
25	A'	942.9322	6.1610	65.2259

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26	A''	1103.4620	5.5367	18.0903
27	A'	1150.4967	6.6088	30.3916
28	A''	1167.0517	1.5876	94.3308
29	A'	1279.3915	10.0682	76.5356
30	A''	1368.8512	8.8235	22.1196
31	A'	1420.6542	14.1404	16.0376
32	A''	1499.8699	15.2455	339.1303
33	A'	1516.2427	10.1166	166.2370
34	A''	1590.3231	12.9132	1.8289
35	A'	1621.7137	2.1842	9.3749
36	A'	1666.2392	7.3705	282.8626
37	A'	2265.8715	38.2743	54.5250
38	A'	3508.4579	7.5864	82.6338
39	A''	3618.7631	8.5023	45.2620

molA_wb97xd

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A'	89.7027	0.0471	0.2783
2	A''	129.8423	0.1416	2.6310
3	A''	135.0144	0.1955	0.0101
4	A'	164.9677	0.1779	3.3187
5	A'	205.4719	0.2226	0.8435
6	A'	283.0600	0.7983	0.7116
7	A''	284.8845	0.1872	4.4971
8	A''	308.7914	0.7344	0.0650
9	A'	317.5462	0.1559	111.5317
10	A'	324.6960	0.9018	1.0554
11	A'	341.1241	0.1354	206.0004
12	A''	386.5603	0.1704	3.6023
13	A'	427.3118	1.1171	0.4912
14	A''	440.8442	0.2740	5.4902
15	A''	443.7617	0.6265	0.0238
16	A''	491.7112	1.8308	2.0548
17	A'	507.6059	1.8283	1.3907
18	A'	540.2016	2.6823	0.3589
19	A'	610.2653	2.0791	4.0641
20	A''	672.5122	3.2458	0.0017
21	A'	677.6310	2.9634	0.3870
22	A'	709.8404	3.5815	1.9624
23	A''	778.7836	1.8752	0.3884
24	A''	965.0936	2.4610	137.7952
25	A'	974.6564	6.5852	66.4605
26	A''	1151.6401	3.0828	61.8229
27	A''	1194.9468	2.5799	69.3558
28	A'	1198.4346	7.1213	46.8420
29	A'	1344.7830	10.6224	76.0224
30	A''	1359.4183	8.1089	2.0420
31	A'	1486.3454	15.1102	18.6304
32	A''	1565.8380	16.4860	397.8319
33	A'	1572.0743	7.3870	202.3768
34	A'	1652.5800	2.2007	97.6407
35	A''	1667.9869	15.8141	0.0039
36	A'	1725.6446	14.5372	319.5865

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37	A'	2389.7028	42.6183	57.3586
38	A'	3643.5794	8.1815	132.8983
39	A''	3762.3613	9.2096	68.9535

molA_x3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A'	89.3650	0.0473	0.2540
2	A''	129.5162	0.1409	2.5667
3	A''	134.2326	0.1930	0.0097
4	A'	163.9244	0.1871	2.9544
5	A'	202.1919	0.2104	0.7468
6	A'	279.7884	0.7761	0.8770
7	A''	282.2059	0.1856	4.6893
8	A''	304.4015	0.6932	0.0486
9	A'	312.3510	0.1242	140.0943
10	A'	320.0104	0.8735	0.6057
11	A'	332.6697	0.1514	167.7815
12	A''	383.5979	0.2478	1.8656
13	A'	424.4112	1.1123	0.3732
14	A''	439.3572	0.9897	3.1639
15	A''	446.3182	0.1788	3.1913
16	A''	487.3462	1.7878	2.0799
17	A'	499.9268	1.7675	1.2702
18	A'	533.9064	2.6220	0.2519
19	A'	604.6469	2.0641	3.9733
20	A''	666.9944	3.1960	0.0003
21	A'	679.9785	3.0277	1.0409
22	A'	716.2800	3.5977	1.4702
23	A''	770.8121	1.8267	0.4333
24	A''	950.1273	2.5344	142.1285
25	A'	964.1685	6.4254	69.2015
26	A''	1130.8592	3.8858	43.6343
27	A''	1179.4805	2.0707	91.2318
28	A'	1181.3152	7.0665	41.1234
29	A'	1322.1872	10.6169	79.7437
30	A''	1358.5168	8.3142	8.9998
31	A'	1455.8889	14.6543	18.4145
32	A''	1536.1890	16.0086	363.7953
33	A'	1547.4636	8.8305	206.8804
34	A''	1627.9918	14.3994	0.5695
35	A'	1641.7867	2.1385	48.4161
36	A'	1695.2248	11.1412	333.9280
37	A'	2348.7960	41.1696	60.1163
38	A'	3606.7242	8.0131	143.5899
39	A''	3722.5031	9.0177	70.6619

molB_apfd

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	87.7936	0.0433	0.1275
2	A	130.5263	0.1373	2.2033

3	A	142.8679	0.1626	2.0068
4	A	203.7160	0.1974	1.1058
5	A	258.8573	0.2443	2.3868
6	A	290.8352	0.7289	2.5204
7	A	306.9786	0.2038	25.9783
8	A	321.6796	0.1186	122.7923
9	A	330.0418	0.2484	73.9297
10	A	369.5364	0.2613	75.1979
11	A	422.0083	0.1342	26.7762
12	A	423.6578	0.7916	2.2232
13	A	449.1691	1.4277	3.3978
14	A	490.1435	1.6434	1.0960
15	A	517.1020	1.7995	1.2352
16	A	598.8804	2.0929	3.5921
17	A	603.8412	0.7905	4.4318
18	A	686.5490	1.4971	8.5754
19	A	690.9255	3.1003	0.9162
20	A	696.9990	1.6627	3.9921
21	A	720.3986	2.9136	0.6545
22	A	829.5340	0.6126	30.7519
23	A	946.9549	4.0465	83.7525
24	A	1058.4082	1.4357	33.0046
25	A	1128.2414	2.3781	56.5036
26	A	1190.8235	4.4910	44.4112
27	A	1234.6391	1.3974	57.5526
28	A	1290.8113	8.7873	99.0467
29	A	1383.6985	9.4716	14.7170
30	A	1450.3711	7.9678	22.7179
31	A	1523.7952	12.2033	100.7055
32	A	1573.3477	7.3838	280.7452
33	A	1638.0959	14.1701	41.6330
34	A	1657.4039	2.1443	45.9247
35	A	1709.0908	11.6916	486.3857
36	A	2361.0315	41.5913	70.3131
37	A	3218.5482	6.6678	0.2516
38	A	3629.4419	8.1226	119.6942
39	A	3745.8925	9.1238	55.8920

molB_b31ypd

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	87.4233	0.0431	0.1365
2	A	131.4656	0.1393	2.2135
3	A	142.5642	0.1616	2.1298
4	A	202.0377	0.1966	0.8653
5	A	258.4998	0.2441	2.7676
6	A	288.2695	0.5567	2.2154
7	A	301.5456	0.2416	4.0132
8	A	321.6972	0.3319	22.6611
9	A	331.4659	0.1186	139.9476
10	A	372.2895	0.2335	118.6660
11	A	421.7688	0.1347	41.7378
12	A	424.3536	0.6273	5.9784
13	A	448.9863	1.3924	4.0414

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14	A	485.9215	1.6484	0.8932
15	A	508.2891	1.7325	1.4409
16	A	592.9562	2.0509	4.2998
17	A	597.5997	0.7825	3.7890
18	A	680.0232	1.3469	8.1123
19	A	687.5582	3.0242	1.2529
20	A	692.4485	1.8119	5.6713
21	A	725.5717	2.6776	0.3546
22	A	829.8971	0.6194	30.3828
23	A	932.0831	4.1352	89.2836
24	A	1048.5544	1.6962	46.1956
25	A	1113.5607	2.0859	44.1660
26	A	1172.9870	3.9262	49.0955
27	A	1226.6410	1.3997	65.7106
28	A	1273.7133	8.5787	98.2518
29	A	1357.4233	8.3488	13.5247
30	A	1429.0658	7.9023	26.1032
31	A	1502.5598	12.3147	100.0655
32	A	1552.5342	7.3532	272.0948
33	A	1614.2758	13.3067	34.6509
34	A	1651.0248	2.1131	21.2269
35	A	1688.8523	9.5581	478.1850
36	A	2341.6179	40.9125	67.8817
37	A	3204.7052	6.6082	0.1940
38	A	3602.1010	7.9972	111.4219
39	A	3714.5226	8.9697	51.8141

molB_blyp

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	83.7051	0.0398	0.1055
2	A	128.4060	0.1329	1.9584
3	A	136.1280	0.1474	2.1073
4	A	193.7461	0.1871	0.5827
5	A	248.9135	0.2286	2.4238
6	A	278.9474	0.5278	1.3308
7	A	291.2627	0.2249	2.0591
8	A	310.2761	0.6202	1.7925
9	A	326.7324	0.1475	58.6321
10	A	373.5730	0.1550	167.0062
11	A	409.0176	0.5650	5.8078
12	A	414.8605	0.1287	95.0375
13	A	432.4361	1.1742	5.7398
14	A	466.9815	1.5402	0.8248
15	A	484.1874	1.5679	1.0622
16	A	567.2402	1.7799	5.3059
17	A	567.6090	0.7310	3.6123
18	A	654.6176	1.2461	8.5820
19	A	655.7744	2.7995	1.1611
20	A	668.6132	1.6897	6.3337
21	A	690.0342	2.4278	0.0959
22	A	792.6009	0.5571	26.9036
23	A	891.2851	3.9743	93.7216
24	A	1005.2232	2.2137	64.2187

25	A	1065.8435	1.7243	21.2395
26	A	1122.0277	2.8267	47.6570
27	A	1183.5761	1.3717	89.2975
28	A	1213.8436	6.6871	68.6440
29	A	1318.8221	7.5095	23.8630
30	A	1360.5859	6.7722	24.9998
31	A	1434.3764	11.5926	102.1989
32	A	1483.7734	6.7181	210.9343
33	A	1534.6898	11.2408	21.1729
34	A	1599.4042	2.7681	27.8098
35	A	1622.0936	3.6973	410.9224
36	A	2231.1401	37.1293	58.9684
37	A	3123.6954	6.2724	0.2555
38	A	3495.9639	7.5309	93.1633
39	A	3603.2426	8.4347	42.0950

molB_camb3lypd

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	89.4895	0.0451	0.1424
2	A	132.4652	0.1415	2.3399
3	A	145.7143	0.1755	1.6403
4	A	205.4215	0.1774	2.2683
5	A	263.3740	0.2702	0.7705
6	A	275.4544	0.0610	251.2965
7	A	290.0298	0.4461	11.9076
8	A	304.8313	0.2095	10.4756
9	A	327.1320	0.8262	5.5971
10	A	367.3684	0.3433	17.0136
11	A	428.2342	1.0333	0.4400
12	A	428.8112	0.1305	19.3457
13	A	454.4503	1.4501	3.8964
14	A	491.7543	1.6702	0.9982
15	A	521.0428	1.7913	1.4602
16	A	602.3939	2.1659	2.9492
17	A	613.1231	0.8013	4.4576
18	A	686.7128	1.3704	7.7456
19	A	698.6497	1.7754	5.8624
20	A	705.5852	3.2563	0.9129
21	A	747.6310	2.6917	0.5026
22	A	850.6549	0.6693	33.2516
23	A	946.7363	4.1247	84.0458
24	A	1058.5618	1.3755	28.3783
25	A	1129.9773	2.5683	64.1074
26	A	1192.5607	4.7963	50.9981
27	A	1236.8644	1.4024	57.3958
28	A	1295.6386	9.5737	109.9869
29	A	1352.3837	8.2739	6.0795
30	A	1456.7214	8.1045	29.7227
31	A	1534.9033	12.2084	96.1228
32	A	1583.3097	7.1166	296.7325
33	A	1656.7625	12.7629	39.1299
34	A	1659.5822	2.1526	102.7162
35	A	1724.4843	14.7751	482.6404

36	A	2403.1469	43.1084	68.0165
37	A	3225.8906	6.7014	0.4196
38	A	3633.5782	8.1371	133.9310
39	A	3748.3895	9.1423	62.4502

molB_m062x

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	89.0821	0.0440	0.1482
2	A	128.7147	0.1336	2.1770
3	A	145.7918	0.1659	2.2488
4	A	204.4885	0.2009	1.1874
5	A	260.4790	0.2385	3.6949
6	A	288.1094	0.6266	2.9524
7	A	303.3700	0.2321	9.2413
8	A	324.3699	0.2229	42.6878
9	A	334.2195	0.1339	125.6752
10	A	377.7007	0.2463	117.7205
11	A	415.1536	0.1279	52.2933
12	A	425.0951	0.9468	2.0049
13	A	452.1033	1.4362	3.9177
14	A	490.8115	1.6563	0.9337
15	A	518.4801	1.8236	1.6542
16	A	603.0276	2.0789	4.3158
17	A	608.7628	0.8381	3.7314
18	A	686.2825	1.3733	6.3643
19	A	689.3260	3.0019	1.0390
20	A	693.8365	1.8405	5.0584
21	A	712.0050	3.0644	1.4912
22	A	839.2626	0.6127	33.1391
23	A	950.6577	3.8547	75.7080
24	A	1063.2462	1.2971	25.9092
25	A	1141.9812	2.6030	64.7002
26	A	1200.1683	5.0685	47.4526
27	A	1232.3753	1.4071	51.3405
28	A	1307.2117	9.2932	101.8777
29	A	1355.7379	8.2047	3.4268
30	A	1468.7780	8.4113	29.6083
31	A	1542.7596	11.4972	72.5879
32	A	1589.1769	7.7359	340.9415
33	A	1654.5077	2.1104	93.9298
34	A	1665.7810	14.9837	56.9174
35	A	1726.2251	15.1693	429.6680
36	A	2413.6305	43.4909	60.6513
37	A	3236.4030	6.7449	1.0545
38	A	3625.2130	8.1044	131.0635
39	A	3742.9475	9.1076	64.3869

molB_mp2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	88.3639	0.0441	0.1901

2	A	123.4826	0.1232	1.9794
3	A	142.0279	0.1523	2.2441
4	A	206.6204	0.2169	0.8651
5	A	255.4759	0.2439	3.5329
6	A	288.2996	0.6032	0.6354
7	A	299.3233	0.2349	0.9874
8	A	320.6544	0.3929	0.8727
9	A	330.9888	0.0954	21.3278
10	A	382.6418	0.2976	5.1378
11	A	421.1249	1.0870	0.4836
12	A	437.2046	1.3072	3.3994
13	A	464.1912	1.1977	2.2901
14	A	480.1021	1.7226	0.2596
15	A	572.9705	0.5714	123.1453
16	A	584.1413	1.3583	0.8813
17	A	613.0733	0.4133	222.2547
18	A	666.0442	2.0848	34.8959
19	A	677.3451	1.2139	5.8284
20	A	691.0256	1.8850	18.3091
21	A	756.1413	2.1533	0.3859
22	A	843.3096	0.6252	32.3564
23	A	931.8807	3.9246	80.2731
24	A	1060.1354	2.3591	72.1353
25	A	1132.8758	1.9797	17.4609
26	A	1176.1622	2.5367	54.4983
27	A	1230.5991	1.4558	33.2436
28	A	1287.0283	6.1097	80.0295
29	A	1445.7480	7.9906	17.6564
30	A	1454.1443	11.6551	27.5526
31	A	1518.7496	12.5225	82.9887
32	A	1566.4804	8.5520	262.7151
33	A	1647.3945	14.0829	22.2728
34	A	1656.1579	2.0334	21.7895
35	A	1710.9561	10.7983	286.1891
36	A	2190.5880	35.6228	3.2642
37	A	3235.8935	6.7431	0.2605
38	A	3599.7727	7.9999	77.4061
39	A	3714.5582	8.9423	41.8329

molB_pbe0d

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	88.1957	0.0436	0.1360
2	A	130.4335	0.1373	2.2126
3	A	143.9939	0.1642	2.0304
4	A	204.5258	0.1992	1.1748
5	A	260.2673	0.2458	2.7153
6	A	286.7995	0.5060	2.5868
7	A	301.3042	0.2445	4.7384
8	A	324.1077	0.2084	56.2950
9	A	332.2810	0.1364	135.4294
10	A	374.9737	0.2597	97.0779
11	A	424.7403	0.6298	2.8457
12	A	425.7936	0.1400	36.9491

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13	A	450.5796	1.3959	3.6740
14	A	490.4242	1.6559	0.7960
15	A	517.8440	1.8081	1.3963
16	A	601.5585	2.1108	3.7502
17	A	605.7509	0.7952	4.2153
18	A	686.0181	1.3629	6.6797
19	A	692.8116	2.9406	1.5265
20	A	695.7316	1.8810	4.6613
21	A	722.3266	2.9238	0.7025
22	A	830.3938	0.6140	31.1049
23	A	948.6690	3.9467	79.4026
24	A	1060.2056	1.3694	30.5929
25	A	1134.6669	2.4553	59.6805
26	A	1197.8952	4.8259	43.0346
27	A	1230.9652	1.3967	54.1532
28	A	1298.7108	8.6858	100.1502
29	A	1393.5079	9.7413	15.8712
30	A	1462.2230	8.2260	20.9469
31	A	1533.8611	11.6490	88.6101
32	A	1582.9406	7.4635	299.5565
33	A	1649.7209	13.6226	39.8989
34	A	1655.8676	2.1546	78.2393
35	A	1721.2495	13.9633	465.9766
36	A	2371.7199	41.9554	71.8695
37	A	3227.9829	6.7083	0.2778
38	A	3639.1152	8.1652	119.0018
39	A	3756.7020	9.1743	56.8140

molB_pbe

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	83.8187	0.0398	0.1050
2	A	125.6899	0.1275	1.9368
3	A	136.8397	0.1489	1.9403
4	A	194.6720	0.1870	0.8468
5	A	248.6947	0.2278	2.1548
6	A	276.5285	0.4956	1.4447
7	A	290.5627	0.2231	2.2111
8	A	312.8878	0.5619	3.9481
9	A	326.8746	0.1319	86.1333
10	A	369.6686	0.1678	167.9380
11	A	409.1557	0.9159	0.1362
12	A	416.8876	0.1212	64.9879
13	A	432.4389	1.1532	4.6621
14	A	470.0712	1.5409	0.6124
15	A	489.7769	1.6054	0.9100
16	A	571.6676	0.7138	3.7768
17	A	575.9274	1.9158	4.4761
18	A	657.9132	2.5335	0.8670
19	A	659.0016	1.2836	6.2499
20	A	670.3099	1.7709	6.3289
21	A	683.4315	2.5738	0.1731
22	A	786.1938	0.5464	27.1853
23	A	907.3397	3.7416	82.6918

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24	A	1018.1655	1.5355	42.5848
25	A	1082.3619	1.9393	43.6860
26	A	1144.6841	3.8437	39.8227
27	A	1183.7225	1.2993	61.9579
28	A	1234.4440	7.6562	84.4690
29	A	1360.6890	8.8724	34.7587
30	A	1392.1310	7.5109	14.7168
31	A	1463.4647	11.2651	96.6367
32	A	1510.8919	7.2202	233.5114
33	A	1564.3048	12.5126	28.3813
34	A	1596.8594	1.9615	30.2323
35	A	1646.4130	10.6196	437.2569
36	A	2250.0813	37.7348	62.8109
37	A	3137.9408	6.3328	0.1680
38	A	3521.5856	7.6440	101.2617
39	A	3634.3033	8.5805	47.0476

molB_rtpss

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	85.0900	0.0408	0.1674
2	A	123.5829	0.1238	1.9324
3	A	139.1127	0.1502	2.2842
4	A	195.4411	0.1956	0.7723
5	A	250.5420	0.2263	3.1835
6	A	269.1075	0.5048	1.0091
7	A	285.3794	0.2072	1.4829
8	A	310.0992	0.6987	0.5256
9	A	334.4836	0.1820	17.2457
10	A	393.5491	0.1402	24.9756
11	A	409.2884	0.9246	1.0584
12	A	429.2713	1.2291	4.1785
13	A	470.3328	1.2557	6.4504
14	A	479.8578	0.1970	278.9350
15	A	492.5435	0.9367	56.5706
16	A	574.0409	0.8113	2.1257
17	A	579.1409	1.5644	14.9528
18	A	652.2831	2.8397	0.7159
19	A	659.7131	1.1564	5.1541
20	A	663.7440	2.7670	1.0262
21	A	673.1098	1.9865	9.4250
22	A	801.4796	0.5340	26.9675
23	A	908.9045	3.8730	87.4133
24	A	1027.8546	2.0977	65.7262
25	A	1095.8209	1.9077	20.0639
26	A	1148.3201	2.7754	45.8098
27	A	1205.0339	1.3935	64.6453
28	A	1239.9244	7.1376	82.5882
29	A	1367.5309	8.6174	24.8591
30	A	1396.5220	7.4825	21.5039
31	A	1473.6472	12.2334	99.4158
32	A	1520.7576	7.2731	236.8502
33	A	1583.3264	12.1634	21.1032
34	A	1634.0690	2.3552	8.6792

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35	A	1663.7542	5.6406	403.1800
36	A	2264.2519	38.2194	61.1554
37	A	3164.9835	6.4425	0.7667
38	A	3509.3168	7.5942	64.2561
39	A	3616.9699	8.4873	32.4122

molB_wb97xd

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	88.4889	0.0438	0.1568
2	A	132.5278	0.1415	2.2889
3	A	144.0109	0.1644	2.0605
4	A	205.8186	0.2013	1.1512
5	A	261.2799	0.2446	3.3176
6	A	289.8518	0.4443	4.0229
7	A	303.6740	0.2685	6.7977
8	A	322.8611	0.1152	130.4781
9	A	330.8482	0.2345	78.2196
10	A	373.4063	0.2583	82.9295
11	A	417.6053	0.1298	34.5196
12	A	426.9269	1.0087	0.8531
13	A	452.7792	1.4467	3.8190
14	A	490.7115	1.6846	0.9352
15	A	518.2907	1.8077	1.5578
16	A	599.9436	2.1070	4.0282
17	A	610.7345	0.8243	4.1614
18	A	686.7983	1.5656	10.0963
19	A	695.5732	2.6355	0.9610
20	A	697.9925	1.7386	2.6602
21	A	730.0231	2.8988	0.7542
22	A	841.1767	0.6319	32.6917
23	A	944.6947	4.1531	84.4787
24	A	1060.7696	1.4777	36.2794
25	A	1131.5337	2.3709	56.9899
26	A	1191.1980	4.5644	49.3616
27	A	1238.6141	1.4084	51.1339
28	A	1292.4182	8.7965	111.4247
29	A	1358.3518	8.3431	5.3958
30	A	1454.9436	8.1113	26.1227
31	A	1530.5350	12.1708	100.7333
32	A	1580.9753	7.3314	300.4392
33	A	1655.2523	14.5494	46.5848
34	A	1661.6107	2.1030	68.7059
35	A	1721.5499	13.4911	476.7428
36	A	2387.3066	42.5339	66.0548
37	A	3224.6654	6.6967	0.2085
38	A	3644.3001	8.1891	109.6857
39	A	3760.9296	9.1955	53.1837

molB_x31yp

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A	88.0914	0.0438	0.1266
2	A	132.1598	0.1408	2.2120
3	A	143.3571	0.1646	2.0394
4	A	203.2147	0.1973	0.8737
5	A	260.2445	0.2496	2.3434
6	A	287.7452	0.5194	3.1353
7	A	300.6785	0.2411	7.0764
8	A	319.5952	0.1446	92.9984
9	A	327.1344	0.1682	109.0437
10	A	368.8563	0.2715	81.6790
11	A	422.6332	0.1419	30.5074
12	A	424.0208	0.5360	6.1430
13	A	449.3290	1.4094	3.8630
14	A	486.1290	1.6442	0.8970
15	A	511.0859	1.7406	1.2920
16	A	592.3135	2.0565	4.0733
17	A	600.3048	0.7857	4.0137
18	A	680.0189	1.3698	8.3225
19	A	690.4251	2.5155	2.5730
20	A	692.4054	2.0061	3.9423
21	A	729.3277	2.6916	0.3463
22	A	833.2778	0.6264	30.5937
23	A	932.8065	4.1363	87.8825
24	A	1048.5963	1.6453	43.7300
25	A	1114.4735	2.1455	46.4004
26	A	1173.9394	3.9997	49.9394
27	A	1227.4453	1.4024	63.4331
28	A	1274.2007	8.5625	101.8742
29	A	1356.3218	8.3857	13.0469
30	A	1429.7895	7.9119	26.8114
31	A	1504.3485	12.2836	99.6052
32	A	1554.6751	7.3619	277.4269
33	A	1617.0957	13.4249	35.9246
34	A	1652.7435	2.1116	24.0319
35	A	1691.3234	9.8239	485.1014
36	A	2346.6685	41.0954	68.4108
37	A	3206.3927	6.6153	0.2042
38	A	3606.4839	8.0168	116.0413
39	A	3719.3118	8.9941	53.4890

molC_apfd

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	95.7747	0.0469	0.2914
2	A	132.5802	0.1343	3.3811
3	A	156.1881	0.1370	0.3464
4	A	166.8666	0.2182	3.9680
5	A	290.4136	0.8143	1.0863
6	A	294.2608	0.1969	5.8232
7	A	296.8793	0.2556	15.9722
8	A	326.5467	0.7946	4.6363
9	A	366.0266	0.1299	220.3078
10	A	372.9924	0.2449	78.6267
11	A	416.1195	0.7269	2.2725

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12	A	420.8861	0.1266	6.9353
13	A	473.2897	1.2998	1.1233
14	A	493.3375	1.6626	2.6033
15	A	499.7418	1.3212	0.6615
16	A	550.8708	2.4681	3.1186
17	A	576.8350	0.9760	4.9117
18	A	685.2247	3.1530	0.9803
19	A	703.9033	1.3522	0.8603
20	A	721.0095	3.1720	1.2701
21	A	743.7162	2.4630	17.2879
22	A	881.5829	0.6300	22.4984
23	A	925.6169	1.9200	68.4770
24	A	1014.7642	2.7855	44.4827
25	A	1156.8609	2.8836	18.8285
26	A	1183.6728	1.8276	150.1392
27	A	1237.3240	1.6837	8.7027
28	A	1313.3730	6.4553	19.2752
29	A	1378.0503	7.9467	54.3566
30	A	1425.3687	12.0698	58.1367
31	A	1539.6399	12.1645	229.7058
32	A	1570.1544	6.4818	207.8757
33	A	1644.1518	3.0969	60.4869
34	A	1645.9233	5.3857	28.7430
35	A	1703.4710	9.3849	240.5687
36	A	2357.9828	41.4942	72.0955
37	A	3233.8878	6.7381	3.0365
38	A	3625.8050	8.1025	129.5230
39	A	3743.2240	9.1136	66.8954

molC_b3lypd

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	95.4274	0.0466	0.3210
2	A	133.2723	0.1360	3.4415
3	A	155.5697	0.1362	0.2820
4	A	166.1951	0.2178	4.3862
5	A	283.8646	0.1797	5.3447
6	A	289.6473	0.7314	1.0211
7	A	293.0818	0.2657	13.2868
8	A	321.4383	0.8208	3.0410
9	A	366.1014	0.2863	45.8937
10	A	376.1424	0.1276	257.5801
11	A	416.2425	0.7691	3.5463
12	A	422.0183	0.1236	7.1270
13	A	468.4391	1.2611	1.3375
14	A	487.9402	1.6135	2.5759
15	A	492.5804	1.2877	1.0402
16	A	545.3069	2.3958	3.6044
17	A	570.9905	0.9445	4.6564
18	A	681.9587	3.1378	1.0479
19	A	699.5827	1.3393	0.9525
20	A	725.8417	3.0620	1.5818
21	A	736.8376	2.4258	19.0755
22	A	881.1607	0.6323	21.4720

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23	A	911.9942	2.0188	72.9331
24	A	998.9804	2.8439	50.5071
25	A	1138.0012	3.3924	20.1695
26	A	1170.8222	1.7809	153.2883
27	A	1228.5151	1.6150	9.1678
28	A	1298.8066	5.8643	20.9775
29	A	1352.6968	6.6736	49.4846
30	A	1401.1966	11.2299	64.2467
31	A	1518.3067	11.7197	206.0300
32	A	1549.7335	7.2874	224.2263
33	A	1619.8882	13.0775	20.5609
34	A	1636.1880	2.2185	37.2411
35	A	1683.4860	7.7224	241.4072
36	A	2338.2479	40.8042	70.7849
37	A	3220.3976	6.6787	2.3529
38	A	3599.9657	7.9837	123.1228
39	A	3714.0186	8.9709	63.4598

molC_blyp

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	91.4464	0.0430	0.2316
2	A	130.0648	0.1297	3.0911
3	A	148.4597	0.1238	0.3556
4	A	159.3822	0.1998	4.2885
5	A	274.3968	0.1650	5.4242
6	A	279.7693	0.3012	7.2365
7	A	280.2861	0.5742	1.0972
8	A	308.9463	0.8074	1.7618
9	A	350.3797	0.4126	4.7052
10	A	384.8418	0.1235	279.3314
11	A	403.1618	0.5822	21.0079
12	A	412.9787	0.1156	7.6190
13	A	450.6223	1.1537	1.1366
14	A	469.1778	1.3262	1.2574
15	A	469.6569	1.2513	2.4409
16	A	522.9285	2.1233	5.5326
17	A	544.6631	0.8594	4.0140
18	A	650.3717	2.8290	1.1282
19	A	674.4379	1.2633	0.7863
20	A	692.0261	2.7751	0.9758
21	A	707.4363	2.2400	21.5189
22	A	838.2209	0.5682	20.6265
23	A	873.5697	1.9835	75.3384
24	A	955.3086	2.9796	56.7943
25	A	1083.4720	3.5130	15.0776
26	A	1126.2606	1.6006	152.3423
27	A	1183.4188	1.6034	11.1119
28	A	1238.6199	4.0506	27.0666
29	A	1303.7034	5.8532	63.0792
30	A	1347.9769	9.6485	48.5515
31	A	1446.2278	10.5460	168.4151
32	A	1484.6383	7.1119	191.8405
33	A	1537.6975	10.8630	21.9752

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34	A	1583.1540	2.5779	3.7297
35	A	1618.2542	4.0075	236.0955
36	A	2227.7047	37.0246	63.9418
37	A	3141.1696	6.3479	1.7534
38	A	3495.5525	7.5253	106.3378
39	A	3605.1594	8.4481	53.7130

molC_camb3lypd

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	97.7939	0.0493	0.4065
2	A	134.6578	0.1388	3.6434
3	A	159.0001	0.1478	0.1129
4	A	169.1489	0.2319	3.3452
5	A	283.7323	0.1844	5.4258
6	A	290.2632	0.5059	8.7511
7	A	296.0909	0.1475	67.9235
8	A	320.2358	0.2080	92.1208
9	A	331.6366	0.1760	144.9860
10	A	376.3518	0.4477	1.1115
11	A	419.9729	0.9405	0.5081
12	A	429.1309	0.1246	6.0805
13	A	474.7554	1.2927	1.4588
14	A	493.8823	1.6748	2.7268
15	A	504.8973	1.3244	0.6032
16	A	551.8871	2.5606	1.7496
17	A	584.2480	0.9844	5.1689
18	A	699.6336	3.2690	1.0602
19	A	706.8580	1.3442	1.1073
20	A	746.7093	2.8530	5.8699
21	A	747.8531	2.7023	14.2264
22	A	906.9562	0.6797	21.7260
23	A	924.2978	1.9440	68.4033
24	A	1012.4685	2.6539	42.2055
25	A	1157.9980	3.0546	24.0353
26	A	1180.7267	1.9210	154.7432
27	A	1240.3680	1.7095	10.5652
28	A	1322.9336	6.4513	15.5360
29	A	1354.6010	6.6853	32.1719
30	A	1423.2329	11.7651	84.1371
31	A	1551.5693	12.2320	223.0786
32	A	1578.3824	6.0499	215.4077
33	A	1646.9903	2.2307	123.5200
34	A	1664.3363	14.7684	16.0561
35	A	1717.2893	12.1771	228.1315
36	A	2400.0456	43.0061	67.8489
37	A	3238.7933	6.7612	3.4293
38	A	3629.6255	8.1153	142.9856
39	A	3745.1845	9.1295	74.0367

molC_m062x

NM#	Symm	Wavenumber	Force Const	IR Intens
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1	A	97.1284	0.0475	0.3483
2	A	131.6197	0.1324	3.4116
3	A	159.1524	0.1401	0.3064
4	A	168.8394	0.2191	4.9191
5	A	283.4550	0.1935	4.9117
6	A	289.1194	0.6141	0.5700
7	A	298.6220	0.2757	13.4426
8	A	325.9620	0.8647	2.6639
9	A	370.9641	0.2385	16.3149
10	A	395.6008	0.1377	290.4761
11	A	406.8680	0.1270	18.9092
12	A	416.8309	0.7430	12.4757
13	A	472.6682	1.2957	1.2160
14	A	492.6544	1.6223	2.9913
15	A	502.2011	1.3957	1.5495
16	A	553.1338	2.3827	4.4583
17	A	579.2144	1.0139	4.7890
18	A	684.2428	3.1374	0.5507
19	A	703.0873	1.3494	0.7722
20	A	714.5662	3.1744	1.7089
21	A	745.1620	2.4212	15.8137
22	A	896.3876	0.6471	24.3268
23	A	930.1616	1.9783	63.9643
24	A	1019.7937	2.4273	39.0290
25	A	1164.8349	2.4608	18.5371
26	A	1192.0992	1.9431	148.1640
27	A	1241.5348	1.8618	10.3265
28	A	1330.7123	6.8810	6.8946
29	A	1359.6517	7.1521	31.1707
30	A	1430.3920	12.2551	72.6814
31	A	1565.3108	12.6220	239.7318
32	A	1579.4908	5.9637	220.7940
33	A	1641.9310	2.2443	128.9641
34	A	1674.0321	15.2488	17.7971
35	A	1718.7553	12.5242	188.2506
36	A	2410.5124	43.3876	59.4547
37	A	3247.5094	6.7975	4.9301
38	A	3618.4668	8.0704	137.9418
39	A	3736.0784	9.0765	75.2029

molC_mp2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	94.0670	0.0455	0.3693
2	A	126.0757	0.1217	3.0695
3	A	154.7363	0.1285	0.3966
4	A	164.7976	0.1931	5.3990
5	A	284.3827	0.1767	4.0093
6	A	290.8238	0.7968	0.8549
7	A	294.6790	0.3391	4.5990
8	A	323.1111	0.9149	2.0881
9	A	349.4035	0.1307	9.9972
10	A	376.2866	0.1698	7.8179

11	A	411.7341	1.0062	0.0447
12	A	448.6103	1.1779	2.2875
13	A	454.3537	1.2588	1.5537
14	A	482.5692	1.6700	1.6357
15	A	547.9722	2.2089	3.1930
16	A	555.5728	0.9937	7.4360
17	A	603.7465	0.3264	302.6161
18	A	632.3164	1.8958	32.8129
19	A	690.1685	1.3512	0.4794
20	A	703.3923	2.0135	29.7688
21	A	740.0720	2.2267	17.1618
22	A	846.1050	0.5476	27.8669
23	A	917.5906	2.3320	62.8362
24	A	1011.8112	2.8044	53.4960
25	A	1142.2917	3.5677	18.5849
26	A	1203.0410	1.5691	131.5141
27	A	1240.1964	1.5252	6.6163
28	A	1303.7707	6.5984	9.6248
29	A	1389.3347	9.5022	77.1779
30	A	1481.0658	12.0317	27.9904
31	A	1537.2532	12.5525	204.6454
32	A	1561.0982	8.1603	196.9353
33	A	1643.8107	2.1042	35.4468
34	A	1646.9909	12.6833	27.0208
35	A	1705.4882	9.2293	115.1684
36	A	2184.4065	35.4304	3.0867
37	A	3248.8717	6.8020	2.8310
38	A	3597.0050	7.9842	85.9180
39	A	3713.8052	8.9423	51.2918

molC_pbe0d

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	96.2417	0.0472	0.3019
2	A	132.5891	0.1345	3.3985
3	A	157.2804	0.1381	0.3522
4	A	168.0290	0.2207	4.0882
5	A	280.7925	0.1764	5.1987
6	A	288.9782	0.7236	0.4680
7	A	297.7283	0.2645	15.4791
8	A	325.2698	0.8498	2.7457
9	A	371.3872	0.2828	40.5607
10	A	382.6862	0.1302	266.4207
11	A	416.1382	0.7397	3.7636
12	A	421.3661	0.1274	7.3372
13	A	471.4712	1.2682	1.0357
14	A	492.6294	1.6423	2.6130
15	A	500.8083	1.3396	0.9804
16	A	552.1157	2.4740	3.3032
17	A	578.2568	0.9789	4.9763
18	A	687.1982	3.1836	0.9363
19	A	703.9219	1.3417	0.7739
20	A	723.3968	3.1945	1.3188
21	A	744.1917	2.4462	16.1130

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22	A	882.6897	0.6314	22.7017
23	A	927.7257	1.9161	65.5096
24	A	1015.6928	2.6750	42.9564
25	A	1159.8686	2.6122	18.5677
26	A	1187.8571	1.8592	151.0673
27	A	1239.1849	1.7651	8.2898
28	A	1322.0655	6.8871	19.3962
29	A	1384.9578	8.2113	59.9763
30	A	1433.4431	12.1225	49.3862
31	A	1552.4503	12.4680	236.0490
32	A	1578.4902	5.9244	194.4325
33	A	1642.8537	2.2749	103.8489
34	A	1656.3931	14.4035	19.8656
35	A	1714.4086	11.7102	224.4106
36	A	2368.6572	41.8561	72.9824
37	A	3242.4956	6.7745	3.1805
38	A	3634.7172	8.1415	128.0604
39	A	3753.0279	9.1591	67.5848

molC_pbe

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	91.4941	0.0431	0.2166
2	A	127.8667	0.1252	3.0087
3	A	149.4658	0.1254	0.3711
4	A	159.8903	0.2010	3.6605
5	A	270.7806	0.1617	5.3154
6	A	278.2867	0.6799	0.3965
7	A	281.7563	0.2629	9.9624
8	A	312.1420	0.8181	1.7767
9	A	353.8471	0.3970	6.4938
10	A	382.1700	0.1187	284.1320
11	A	401.7135	0.6875	11.4567
12	A	415.1278	0.1176	7.6342
13	A	452.4031	1.1365	0.8336
14	A	472.4257	1.4954	2.2723
15	A	474.2247	1.1682	1.0332
16	A	529.6474	2.2519	4.3669
17	A	548.4657	0.8674	4.3308
18	A	652.3513	2.8635	1.0867
19	A	676.2473	1.2543	0.5299
20	A	687.6408	2.8730	0.6381
21	A	713.8626	2.2586	17.7892
22	A	831.1877	0.5565	21.6897
23	A	888.6366	1.8247	66.4558
24	A	971.6000	2.7607	47.2471
25	A	1105.9895	2.7120	19.3697
26	A	1138.6265	1.6854	143.7471
27	A	1189.0564	1.5400	8.2990
28	A	1256.5361	5.4216	28.7943
29	A	1334.3786	7.7490	76.3583
30	A	1386.1235	10.5554	37.9506
31	A	1476.4236	11.3144	195.3548
32	A	1512.3068	6.4066	167.1475

33	A	1567.9856	12.4122	21.4948
34	A	1581.3249	2.0355	50.3675
35	A	1641.7338	9.2156	227.4107
36	A	2246.9163	37.6386	66.6890
37	A	3154.6717	6.4056	2.6693
38	A	3518.8341	7.6276	112.5857
39	A	3632.9633	8.5786	58.3501

molC_rtpss

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	92.7545	0.0439	0.3014
2	A	126.0916	0.1221	3.0642
3	A	151.7843	0.1257	0.3919
4	A	161.8906	0.1980	5.0616
5	A	262.5845	0.1588	5.1142
6	A	270.9310	0.5430	0.1748
7	A	281.8196	0.2886	6.1949
8	A	309.5078	0.8334	1.3611
9	A	354.3118	0.3360	2.7167
10	A	399.8446	0.3621	3.1268
11	A	403.2601	0.1474	7.5225
12	A	451.0702	1.1488	0.6772
13	A	470.4822	0.5634	63.4892
14	A	474.0378	1.2514	1.8197
15	A	490.7905	0.2531	260.9698
16	A	536.0339	1.1636	44.7513
17	A	548.2459	0.9283	3.8091
18	A	647.8864	2.8945	0.4591
19	A	669.4645	2.8758	0.8319
20	A	675.9704	1.2736	0.4638
21	A	717.8330	2.1669	21.2925
22	A	850.4446	0.5686	21.5472
23	A	892.8592	2.0763	72.4864
24	A	978.9534	2.9537	59.9434
25	A	1108.3614	3.4161	14.5600
26	A	1158.6243	1.6110	140.2818
27	A	1207.7556	1.6072	9.8458
28	A	1262.4267	4.7019	23.4156
29	A	1341.2225	6.8357	74.1218
30	A	1391.5184	10.5782	33.5037
31	A	1487.2732	11.1828	191.5723
32	A	1521.1555	7.5875	182.8899
33	A	1587.1698	11.9170	21.9075
34	A	1617.0108	2.3307	9.4361
35	A	1659.7546	5.5605	209.2346
36	A	2260.5700	38.1057	64.7850
37	A	3184.6115	6.5279	0.9170
38	A	3506.4133	7.5777	73.3789
39	A	3616.0381	8.4868	42.0523

molC_wb97xd

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	96.7245	0.0476	0.3488
2	A	134.0924	0.1375	3.5264
3	A	157.2150	0.1379	0.3877
4	A	168.5666	0.2210	4.3895
5	A	285.8238	0.1811	5.0225
6	A	293.0933	0.8003	0.7650
7	A	300.3373	0.2675	16.1538
8	A	326.4005	0.8443	3.1756
9	A	371.0524	0.2181	62.0685
10	A	380.4353	0.1358	246.1286
11	A	411.6201	0.1267	7.7100
12	A	418.4743	0.8423	3.1557
13	A	472.6653	1.3101	1.3158
14	A	492.8697	1.6512	2.7285
15	A	502.5509	1.3840	0.9625
16	A	550.0243	2.4166	3.5410
17	A	580.2695	0.9971	4.8351
18	A	690.0647	3.1918	0.6819
19	A	707.1188	1.3652	0.9824
20	A	727.2742	3.1230	1.9134
21	A	744.4103	2.4578	17.5217
22	A	897.7695	0.6563	23.0728
23	A	924.4837	2.0579	70.0877
24	A	1011.8995	2.6621	46.9778
25	A	1156.5180	3.1030	21.2337
26	A	1185.3271	1.8419	151.3633
27	A	1241.2153	1.6829	9.8173
28	A	1318.9153	6.6332	16.8278
29	A	1360.0090	6.5832	33.5446
30	A	1419.5071	11.8017	74.6696
31	A	1548.0516	12.2647	234.8838
32	A	1576.2092	6.5967	226.6399
33	A	1650.3316	2.2167	89.9965
34	A	1662.5044	14.2059	16.7243
35	A	1715.5037	10.8352	219.9974
36	A	2384.2672	42.4338	64.8913
37	A	3237.2908	6.7553	2.3651
38	A	3640.5526	8.1691	117.0031
39	A	3757.6308	9.1811	63.2927

molC_x3lyp

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	96.1651	0.0474	0.3133
2	A	134.1032	0.1377	3.4429
3	A	156.3512	0.1388	0.2579
4	A	167.2314	0.2216	4.1695
5	A	282.5329	0.1786	5.2487
6	A	289.3623	0.7372	0.9261
7	A	294.9054	0.2551	15.9218
8	A	321.2388	0.7738	4.3541
9	A	362.7175	0.1194	245.0284

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10	A	370.8548	0.2959	53.2594
11	A	415.8758	0.8503	2.1024
12	A	423.5780	0.1230	6.9236
13	A	468.8717	1.2674	1.2848
14	A	488.1842	1.6239	2.6424
15	A	495.0670	1.2872	0.7327
16	A	544.5573	2.4103	3.0621
17	A	573.7517	0.9536	4.7369
18	A	685.1992	3.1548	1.1547
19	A	699.9416	1.3365	1.0011
20	A	729.8948	3.0774	1.6201
21	A	736.6741	2.4349	18.4410
22	A	884.8203	0.6385	21.5215
23	A	912.2392	2.0085	71.7057
24	A	999.2440	2.7965	49.2250
25	A	1139.3689	3.4147	20.4952
26	A	1171.5114	1.7937	155.0997
27	A	1229.4752	1.6229	9.2205
28	A	1299.5298	5.9306	20.5236
29	A	1351.9135	6.6190	49.2364
30	A	1401.0202	11.2410	64.9294
31	A	1520.4690	11.7898	208.4125
32	A	1551.6819	7.2416	227.9699
33	A	1623.0799	13.2127	20.6259
34	A	1637.9669	2.2160	40.4757
35	A	1685.8833	7.9185	244.6866
36	A	2343.3828	40.9897	70.9926
37	A	3221.8293	6.6848	2.4640
38	A	3603.9925	8.0018	127.5993
39	A	3718.3548	8.9930	65.1702

mold_apfd

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	78.9232	0.0572	1.6842
2	A	126.5108	0.1192	4.9343
3	A	127.9376	0.1086	0.4375
4	A	141.4082	0.1765	1.8197
5	A	195.3909	0.1938	0.3913
6	A	207.7249	0.4825	0.6007
7	A	283.5809	0.6963	0.9774
8	A	311.7151	0.0933	186.8651
9	A	315.1428	0.3031	14.1389
10	A	316.1455	0.4228	11.2280
11	A	322.9050	0.2381	55.3190
12	A	376.5829	1.1996	2.7992
13	A	381.7936	0.3337	1.3756
14	A	425.4348	0.1451	4.3877
15	A	447.0388	1.3721	0.6502
16	A	502.3130	1.2123	1.1777
17	A	508.2763	1.6114	1.2022
18	A	538.5030	1.6193	5.6764
19	A	550.6024	2.6367	1.8861
20	A	642.4739	2.9276	1.8962

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21	A	687.2045	3.2080	0.2536
22	A	741.6253	3.7595	0.9128
23	A	757.1116	1.9137	0.9470
24	A	873.7031	3.6154	81.4475
25	A	996.3554	3.5997	113.3888
26	A	1048.0256	5.0820	55.3484
27	A	1165.0966	1.9097	28.1062
28	A	1197.0406	4.4703	15.0665
29	A	1326.2280	10.2233	51.2941
30	A	1357.3785	8.9689	54.8492
31	A	1467.1443	13.0237	58.8653
32	A	1506.8784	10.8471	32.8133
33	A	1544.6985	10.3804	461.0059
34	A	1631.1034	5.3861	26.9222
35	A	1658.2643	3.0098	125.4927
36	A	1698.6362	10.5020	114.4059
37	A	2349.3172	41.1592	58.7876
38	A	3616.4483	8.0676	95.6703
39	A	3738.5303	9.0891	67.9643

molD_b3lypd

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	78.3352	0.0564	1.7408
2	A	126.4168	0.1185	4.9988
3	A	127.5870	0.1082	0.4416
4	A	140.0103	0.1693	2.0531
5	A	193.4313	0.1904	0.4969
6	A	206.8268	0.4742	0.6344
7	A	284.1519	0.6464	0.9597
8	A	310.6408	0.3894	4.5334
9	A	312.4897	0.5442	1.2562
10	A	313.6847	0.2374	40.1837
11	A	325.3447	0.0885	221.2238
12	A	373.3933	1.1963	3.4939
13	A	376.1825	0.4095	1.6944
14	A	423.6906	0.1356	4.5246
15	A	443.1515	1.3688	0.5709
16	A	495.3161	1.1274	1.1346
17	A	501.2684	1.5668	1.2155
18	A	531.9327	1.5694	6.5708
19	A	545.8605	2.5458	1.8708
20	A	638.3434	2.8900	1.8738
21	A	680.0941	3.1428	0.1851
22	A	743.6636	3.7895	1.0999
23	A	752.9944	1.8969	0.9835
24	A	856.7454	3.6449	86.5390
25	A	980.7924	3.6475	122.0956
26	A	1029.0045	5.2712	54.8237
27	A	1150.8294	2.4409	20.9023
28	A	1175.3146	2.8162	24.6113
29	A	1308.6879	10.2923	52.3305
30	A	1332.2398	7.9003	41.8033
31	A	1439.1977	12.5307	46.8268

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32	A	1484.6369	11.1167	35.5116
33	A	1519.5530	11.4103	472.3314
34	A	1605.7456	9.6119	10.6148
35	A	1647.8843	2.5098	97.8518
36	A	1677.3364	7.1787	127.5832
37	A	2330.3220	40.5022	57.4965
38	A	3593.1870	7.9598	91.1445
39	A	3710.7655	8.9540	63.6258

molD_blyp

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	74.6614	0.0505	1.8244
2	A	121.3281	0.0955	0.7534
3	A	122.7130	0.1131	4.5526
4	A	133.6926	0.1502	2.3136
5	A	185.8135	0.1835	0.4489
6	A	198.6123	0.4352	0.6252
7	A	274.9357	0.6267	0.6921
8	A	297.3904	0.4600	1.3967
9	A	298.9721	0.4369	0.8834
10	A	304.5084	0.3637	4.5738
11	A	342.0798	0.0960	202.2356
12	A	353.8883	0.3087	41.9546
13	A	359.0523	0.8809	12.1030
14	A	411.4451	0.1238	4.9499
15	A	426.6450	1.2128	1.1852
16	A	472.2355	0.9618	0.9807
17	A	481.2625	1.4354	1.2278
18	A	507.3235	1.4452	7.7813
19	A	524.5008	2.2050	2.2989
20	A	606.5046	2.6064	1.3120
21	A	644.0070	2.8079	0.2649
22	A	706.4128	3.3966	0.6866
23	A	724.8713	1.7972	0.5734
24	A	816.1890	3.4218	89.6850
25	A	934.1099	3.5870	124.2163
26	A	981.3704	4.7991	48.2561
27	A	1096.3633	4.6302	4.9871
28	A	1127.9016	1.6052	36.8965
29	A	1244.3064	9.4911	46.9824
30	A	1299.6088	7.7005	37.6973
31	A	1365.8501	11.2869	47.2433
32	A	1415.9016	10.5085	29.3374
33	A	1446.9099	10.5887	433.1631
34	A	1524.4243	11.0561	11.6160
35	A	1584.8322	5.0333	39.8939
36	A	1612.3673	2.4149	153.0039
37	A	2219.0873	36.7084	51.5702
38	A	3488.9836	7.5029	76.3073
39	A	3601.4212	8.4288	53.1750

molD_camb3lypd

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	80.0367	0.0607	1.1341
2	A	127.4514	0.1216	4.8584
3	A	130.4383	0.1256	0.3892
4	A	143.0361	0.1982	0.8682
5	A	197.0129	0.1711	0.6644
6	A	207.7023	0.4780	0.6599
7	A	249.9609	0.0448	257.8639
8	A	285.2594	0.6442	1.4594
9	A	313.6001	0.2940	2.7726
10	A	318.5863	0.7239	4.3338
11	A	319.5148	0.5834	0.3391
12	A	377.9662	1.2644	2.3729
13	A	389.5915	0.3848	0.7300
14	A	432.0421	0.1436	3.6483
15	A	448.5059	1.4319	0.2716
16	A	507.0153	1.4849	1.4155
17	A	508.4099	1.2705	1.1534
18	A	541.2145	1.6367	5.0513
19	A	551.7863	2.7166	1.7053
20	A	658.2523	3.0707	2.1290
21	A	700.2404	3.3158	0.1732
22	A	761.0457	1.8594	1.5218
23	A	771.0091	4.0873	1.4502
24	A	872.2737	3.6305	78.5008
25	A	999.2865	3.5026	118.5772
26	A	1048.2066	5.4141	63.4267
27	A	1161.7168	1.8544	41.3260
28	A	1195.9236	5.4704	11.5306
29	A	1316.2980	7.9345	87.0390
30	A	1335.3612	9.7003	24.0663
31	A	1473.8645	12.2995	37.0226
32	A	1517.4933	11.2386	48.9105
33	A	1553.2711	10.9702	461.6373
34	A	1642.8778	3.6119	57.1691
35	A	1666.6654	3.7909	133.1243
36	A	1717.5712	14.9676	99.6758
37	A	2392.2509	42.7090	55.9559
38	A	3624.1599	8.0959	111.2940
39	A	3743.0137	9.1199	74.6701

molD_m062x

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	80.3888	0.0588	1.8489
2	A	124.7762	0.1168	4.5604
3	A	131.5596	0.1101	0.6611
4	A	143.8510	0.1738	2.3957
5	A	195.4728	0.1903	0.5877
6	A	206.1057	0.4762	0.6073
7	A	283.1960	0.6587	0.9897
8	A	314.6612	0.3075	2.5131

9	A	317.1308	0.5376	8.3930
10	A	317.5730	0.5459	4.4005
11	A	342.5914	0.0897	263.9357
12	A	376.8473	1.1332	5.2394
13	A	386.3115	0.1914	7.0212
14	A	416.5891	0.1888	4.1653
15	A	445.4903	1.3772	0.7977
16	A	502.5097	1.3241	0.9189
17	A	507.3657	1.6271	1.3096
18	A	540.8223	1.5510	6.4005
19	A	551.9115	2.6725	2.1543
20	A	642.6910	2.9361	2.3362
21	A	688.9985	3.2275	0.1471
22	A	731.8401	3.6821	1.0243
23	A	756.8804	1.9382	1.2371
24	A	875.8039	3.6399	78.8676
25	A	1007.6936	3.3590	103.9125
26	A	1054.8313	5.7599	60.0502
27	A	1168.2863	1.7445	38.4731
28	A	1214.9838	6.2186	10.8771
29	A	1320.1797	7.7885	77.3841
30	A	1340.6541	9.5736	24.1150
31	A	1487.7497	12.0837	32.6666
32	A	1523.4686	10.7468	64.2840
33	A	1565.5893	11.3340	456.6828
34	A	1644.3047	2.5924	113.8278
35	A	1671.6130	6.4929	80.5941
36	A	1719.3907	15.7843	79.1490
37	A	2402.7874	43.0919	47.9548
38	A	3611.7955	8.0461	107.8113
39	A	3733.0048	9.0617	75.8335

molD_mp2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	78.2976	0.0550	1.7921
2	A	118.2606	0.1038	4.2426
3	A	128.2172	0.1017	0.8862
4	A	135.9671	0.1355	3.3093
5	A	194.6986	0.2017	0.7900
6	A	206.6873	0.4686	0.6617
7	A	282.7064	0.5351	1.1902
8	A	305.9995	0.4160	1.1298
9	A	309.6071	0.3376	0.8398
10	A	316.4971	0.7302	1.7901
11	A	348.3419	0.0884	13.4984
12	A	375.1195	1.1053	1.9755
13	A	394.9780	0.5626	6.4630
14	A	436.6063	1.2951	0.1616
15	A	447.7837	0.9885	2.2242
16	A	486.1185	1.5369	0.3938
17	A	527.2766	1.6054	4.2095
18	A	547.7315	1.7326	24.6188
19	A	586.9582	0.5931	91.3699

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20	A	603.4644	0.4638	189.5975
21	A	666.8002	2.6781	11.4641
22	A	743.2898	2.0298	0.4545
23	A	797.5865	4.3950	1.9218
24	A	871.3989	3.6018	78.9242
25	A	989.3437	4.2959	117.0855
26	A	1041.3860	5.6925	28.7619
27	A	1166.8168	4.0188	5.1540
28	A	1203.1155	1.7139	23.8483
29	A	1313.2230	9.8313	39.4182
30	A	1447.1983	12.7002	44.6642
31	A	1472.7478	11.9853	8.4768
32	A	1507.4277	11.4261	41.5043
33	A	1535.2533	12.2570	467.6261
34	A	1630.7581	5.4781	9.3871
35	A	1660.4566	2.8657	68.0373
36	A	1691.9686	8.7784	54.6275
37	A	2175.5768	35.1441	1.3774
38	A	3586.4026	7.9418	64.4204
39	A	3705.1324	8.8986	48.6968

molD_pbe0d

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	79.3839	0.0577	1.7610
2	A	125.0786	0.1155	4.9850
3	A	129.0179	0.1094	0.4927
4	A	142.2866	0.1755	1.9793
5	A	196.2641	0.1939	0.4351
6	A	206.6025	0.4745	0.5945
7	A	281.7925	0.5747	1.1847
8	A	311.1011	0.2417	8.5140
9	A	315.4622	0.4749	23.7696
10	A	317.3272	0.5595	0.6120
11	A	329.0164	0.0870	237.5800
12	A	377.1766	1.2147	3.0986
13	A	383.3987	0.3452	1.5293
14	A	426.1574	0.1458	4.4046
15	A	443.4207	1.3418	0.6274
16	A	503.0615	1.2356	1.1162
17	A	505.7558	1.5909	0.9858
18	A	540.0459	1.6229	6.1143
19	A	552.4992	2.6210	1.9137
20	A	643.6479	2.9387	1.9938
21	A	688.8107	3.2326	0.2245
22	A	742.9266	3.7741	0.9302
23	A	757.8079	1.9035	0.9508
24	A	876.7448	3.6054	79.4740
25	A	1002.2728	3.5326	109.3212
26	A	1051.9142	5.4011	57.4814
27	A	1167.3521	1.8215	29.0037
28	A	1203.7668	5.1576	12.5352
29	A	1333.3013	10.2464	51.5329
30	A	1366.3890	9.2341	55.2782

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31	A	1477.7727	12.6400	53.4707
32	A	1515.6134	10.6905	37.1467
33	A	1556.3283	10.0700	458.4816
34	A	1636.2062	3.8184	57.2148
35	A	1661.3781	3.7181	124.5167
36	A	1710.2029	13.8456	97.5398
37	A	2360.0356	41.5208	59.7597
38	A	3625.8523	8.1086	94.9478
39	A	3748.6718	9.1364	68.5487

molD_pbe

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	75.3125	0.0516	1.7454
2	A	119.3257	0.1047	4.7567
3	A	122.0998	0.0988	0.5251
4	A	135.2735	0.1561	2.0930
5	A	186.5224	0.1823	0.3035
6	A	198.3879	0.4380	0.5682
7	A	271.4006	0.5414	0.9491
8	A	299.2031	0.2922	2.7174
9	A	300.5053	0.4156	1.3348
10	A	303.6921	0.7194	3.1991
11	A	337.5364	0.0834	241.5444
12	A	356.7594	0.4263	6.9870
13	A	362.5524	1.0864	4.5096
14	A	417.4552	0.1324	4.2721
15	A	425.9329	0.9981	1.3703
16	A	476.5211	0.9536	1.0475
17	A	484.0056	1.4522	0.7779
18	A	516.1990	1.5083	7.1083
19	A	531.2039	2.3162	2.1315
20	A	606.5243	2.6025	1.3572
21	A	648.4533	2.8622	0.3219
22	A	700.9790	3.3256	0.5026
23	A	726.9874	1.7881	0.5861
24	A	837.0033	3.3427	81.2846
25	A	955.0118	3.4895	110.5934
26	A	1004.2118	4.7293	50.6337
27	A	1119.9742	2.2291	15.8737
28	A	1144.2170	2.7058	20.6242
29	A	1267.1225	9.3833	49.5316
30	A	1341.9243	9.3727	48.3324
31	A	1403.8324	11.7747	60.5065
32	A	1444.6374	10.7196	30.7989
33	A	1481.8559	9.1213	418.5132
34	A	1554.7745	7.3783	13.5648
35	A	1592.4472	2.3894	107.7241
36	A	1629.9169	8.4918	118.9641
37	A	2237.3765	37.2791	55.0397
38	A	3508.9585	7.5924	79.7366
39	A	3627.7121	8.5507	58.8001

molD_rtpss

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	76.4157	0.0520	2.1906
2	A	117.7133	0.1017	4.6250
3	A	124.8404	0.0975	0.9438
4	A	137.5627	0.1492	2.9850
5	A	186.9612	0.1841	0.5572
6	A	194.0248	0.4244	0.5122
7	A	263.7417	0.5015	0.9996
8	A	295.2027	0.2244	4.0485
9	A	300.1616	0.8573	0.6507
10	A	302.0229	0.5571	0.1530
11	A	355.9454	0.3158	3.9422
12	A	363.2951	1.1585	1.8294
13	A	401.6437	0.1247	13.6665
14	A	423.5555	1.1881	4.9473
15	A	457.0537	0.1736	254.0855
16	A	476.5026	1.1578	2.5875
17	A	484.1087	1.3548	6.5541
18	A	517.5225	1.3595	15.2032
19	A	537.0350	1.5102	14.7748
20	A	605.2121	2.5994	1.4580
21	A	644.4121	2.8974	0.0978
22	A	684.7025	3.2059	0.7098
23	A	727.9858	1.8876	0.2967
24	A	840.0063	3.4460	87.4712
25	A	959.1384	3.8715	121.7003
26	A	1007.3711	5.2160	39.8046
27	A	1127.7882	4.2475	4.7096
28	A	1158.9319	1.6740	32.3058
29	A	1269.8293	9.5899	45.9541
30	A	1348.7612	8.8697	43.7574
31	A	1409.4247	11.8626	46.4430
32	A	1455.4112	10.8221	32.6654
33	A	1489.1769	11.0162	446.2392
34	A	1572.4855	10.3688	8.8540
35	A	1625.7534	3.1959	50.7100
36	A	1649.8483	3.8345	126.6436
37	A	2251.8327	37.7714	51.5637
38	A	3496.9775	7.5441	51.9521
39	A	3610.3004	8.4568	42.1643

molD_wb97xd

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	79.5671	0.0580	1.7832
2	A	129.1630	0.1105	3.2450
3	A	129.2807	0.1243	2.0187
4	A	142.2084	0.1770	1.8964
5	A	197.9841	0.1953	0.4994
6	A	207.7905	0.4763	0.6359
7	A	286.2495	0.6044	1.3578

8	A	310.1435	0.0909	188.2270
9	A	313.8991	0.2843	11.2360
10	A	318.5269	0.5862	0.0453
11	A	321.4604	0.2267	75.3074
12	A	376.5913	1.2395	3.0313
13	A	386.7494	0.2143	2.4434
14	A	419.4079	0.1774	3.5230
15	A	446.2772	1.4038	0.4350
16	A	503.7972	1.2962	1.2233
17	A	506.1204	1.6157	1.2646
18	A	538.0994	1.6139	5.8347
19	A	549.8257	2.5752	1.8365
20	A	650.0993	3.0022	1.9132
21	A	692.7905	3.2516	0.1895
22	A	751.4460	3.8681	1.0390
23	A	760.1262	1.8987	1.0979
24	A	869.7967	3.6947	81.7297
25	A	997.4664	3.5172	114.7516
26	A	1043.9221	5.6809	61.7496
27	A	1163.3355	1.8503	37.1362
28	A	1196.4340	4.9498	14.9331
29	A	1321.2091	8.9352	106.5780
30	A	1331.2941	8.5323	4.2389
31	A	1470.5585	12.6340	43.3643
32	A	1513.6631	10.9894	43.9484
33	A	1551.7553	11.0580	472.1532
34	A	1642.2795	3.9075	46.1769
35	A	1667.6088	3.5442	125.2407
36	A	1713.7562	13.6362	96.7227
37	A	2375.9083	42.1159	54.5353
38	A	3633.6400	8.1441	91.6543
39	A	3754.8204	9.1675	65.3887

molD_x31yp

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	78.7418	0.0569	1.6894
2	A	126.8390	0.1195	4.9482
3	A	128.2416	0.1100	0.4302
4	A	140.8026	0.1739	1.8859
5	A	194.9239	0.1935	0.4815
6	A	205.4073	0.4654	0.6487
7	A	283.7438	0.6396	1.1012
8	A	307.9141	0.1017	169.3222
9	A	310.2459	0.2505	13.6593
10	A	314.4992	0.5585	0.7292
11	A	318.5280	0.1847	82.5258
12	A	372.9186	1.2191	3.2272
13	A	377.9293	0.3997	1.2288
14	A	424.3309	0.1363	4.5474
15	A	442.9110	1.3735	0.4756
16	A	497.9412	1.1689	1.1335
17	A	501.4049	1.5672	1.2394
18	A	530.3071	1.5783	6.2811

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19	A	544.9771	2.5155	1.7016
20	A	641.3280	2.9177	1.8665
21	A	683.5671	3.1640	0.2190
22	A	747.2504	3.8179	1.0744
23	A	753.1971	1.8811	0.9418
24	A	856.3468	3.6556	85.5675
25	A	981.7270	3.5573	118.3440
26	A	1028.6938	5.4051	58.1529
27	A	1150.8236	2.3192	23.2259
28	A	1175.8735	3.0282	23.4927
29	A	1308.2656	10.3679	55.1866
30	A	1330.0329	7.8315	39.8643
31	A	1440.1244	12.3867	43.9886
32	A	1486.1073	11.2164	38.2969
33	A	1521.1922	11.4221	477.6591
34	A	1608.8554	9.5407	11.0105
35	A	1649.6223	2.4978	103.5194
36	A	1679.7701	7.4634	125.2119
37	A	2335.2960	40.6842	57.2003
38	A	3597.7069	7.9795	95.1810
39	A	3715.0702	8.9765	64.8921

molE_apfd

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	78.4199	0.0574	0.8078
2	A	127.9433	0.1223	4.0234
3	A	130.8314	0.1364	2.0360
4	A	184.4420	0.1846	0.4670
5	A	218.6445	0.4202	0.7877
6	A	226.4175	0.0354	242.9535
7	A	245.5911	0.2306	0.0420
8	A	307.5770	0.2780	3.1309
9	A	322.8657	1.1044	2.2633
10	A	368.2270	0.7921	6.0742
11	A	372.1930	0.4862	0.8209
12	A	450.5835	0.9520	0.3251
13	A	454.2495	0.1557	2.8075
14	A	505.5870	1.3883	0.0997
15	A	518.7328	1.0024	1.0829
16	A	538.2265	1.5979	4.4572
17	A	599.1975	0.7752	4.0328
18	A	664.2171	2.2915	0.1856
19	A	678.1342	1.4462	4.3099
20	A	689.7092	2.1984	7.0503
21	A	757.8249	2.9479	0.0335
22	A	824.7586	0.6120	31.9941
23	A	844.1340	1.9448	63.8915
24	A	991.3428	2.6496	48.0152
25	A	1120.5902	4.7806	83.4187
26	A	1169.1204	1.5658	9.2507
27	A	1202.2485	1.2637	32.0841
28	A	1290.0853	9.0156	72.9007
29	A	1356.5040	9.1777	8.7148

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30	A	1394.1764	10.5428	40.6717
31	A	1511.5478	6.9155	17.3657
32	A	1538.0557	7.8482	310.9961
33	A	1625.1810	5.7912	8.2196
34	A	1654.4574	3.2475	109.4500
35	A	1687.2981	7.2010	350.1230
36	A	2346.5487	41.0611	66.4232
37	A	3244.3565	6.7814	7.2269
38	A	3622.7620	8.0932	107.1793
39	A	3748.8385	9.1465	74.4429

molE_b3lypd

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	78.3274	0.0569	1.1965
2	A	127.9221	0.1204	4.5950
3	A	131.4434	0.1249	1.4717
4	A	182.5562	0.1848	0.2800
5	A	216.7322	0.4219	0.3898
6	A	244.3956	0.2098	0.5794
7	A	253.2227	0.0455	244.9780
8	A	302.6020	0.2556	3.4603
9	A	318.3196	1.0328	3.2545
10	A	364.2704	0.8255	6.5738
11	A	367.4118	0.5156	0.3689
12	A	450.3957	0.1526	3.2185
13	A	453.6450	0.9692	0.5939
14	A	499.9684	1.3930	0.1686
15	A	511.2503	0.9242	1.0797
16	A	533.5900	1.5698	5.0534
17	A	594.2994	0.7566	3.9475
18	A	657.6648	2.3704	0.2710
19	A	673.5427	1.4112	5.3233
20	A	684.5312	2.1813	7.5541
21	A	755.9012	2.7422	0.0220
22	A	824.3173	0.6149	31.2119
23	A	831.6819	2.0027	70.7863
24	A	975.0482	2.6502	46.8300
25	A	1104.6043	5.0929	85.6762
26	A	1160.8816	1.6161	19.1097
27	A	1195.7291	1.2101	30.8047
28	A	1271.8342	8.9480	72.8932
29	A	1332.0786	8.4948	7.3731
30	A	1373.2942	9.7831	31.7400
31	A	1490.1294	7.3405	34.9388
32	A	1516.8071	7.4564	295.0114
33	A	1602.8177	9.0808	26.6283
34	A	1642.9932	3.0657	72.7999
35	A	1668.9481	4.6652	335.5987
36	A	2327.6745	40.4091	65.2079
37	A	3231.7782	6.7269	6.3177
38	A	3598.5698	7.9814	100.6776
39	A	3719.6328	9.0030	68.8457

molE_blyp

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	75.0726	0.0513	1.6195
2	A	124.2011	0.1123	4.6410
3	A	126.1523	0.1016	2.1115
4	A	174.8610	0.1777	0.1329
5	A	207.9250	0.3880	0.3798
6	A	236.2172	0.2164	0.0627
7	A	289.5351	0.0624	223.4701
8	A	292.6659	0.2340	4.0808
9	A	306.0317	0.5834	16.2644
10	A	348.8284	0.4762	0.9459
11	A	350.2248	0.7748	7.4641
12	A	434.9481	0.2139	2.5511
13	A	437.1991	0.3024	1.8124
14	A	479.1868	1.2801	0.2615
15	A	488.4987	0.7846	0.9259
16	A	510.8512	1.4036	6.4901
17	A	565.3226	0.6850	3.3727
18	A	624.9622	2.2018	0.1895
19	A	649.1511	1.3180	5.5544
20	A	657.9829	2.0721	7.1853
21	A	719.5732	2.6378	0.0111
22	A	784.0231	0.5444	28.5940
23	A	793.6350	1.9674	79.4608
24	A	929.1432	2.4929	43.4577
25	A	1050.8781	4.9539	76.5268
26	A	1122.1354	1.4850	28.7182
27	A	1157.5804	1.1419	34.2122
28	A	1213.2144	7.8310	60.7123
29	A	1274.6647	8.8321	13.5104
30	A	1329.6415	8.3626	19.9828
31	A	1427.8649	6.8349	25.0380
32	A	1446.8816	6.3981	266.5906
33	A	1524.8195	10.0946	39.9389
34	A	1578.7490	5.6378	107.7816
35	A	1610.3798	2.2809	239.3890
36	A	2217.1928	36.6444	57.3855
37	A	3152.5880	6.3951	4.9637
38	A	3493.9148	7.5223	83.2903
39	A	3609.2519	8.4704	57.2003

molE_camb3lypd

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	72.4366	0.0240	18.7776
2	A	105.2838	0.0210	96.4553
3	A	129.6156	0.1229	6.4101
4	A	153.8027	0.0242	123.3204
5	A	186.8040	0.2416	1.1197
6	A	218.5441	0.4291	0.3421

7	A	249.3099	0.2306	0.0280
8	A	304.2882	0.2578	3.6559
9	A	322.2109	1.1012	2.1013
10	A	368.7980	0.8565	5.6315
11	A	377.4948	0.5487	0.3431
12	A	458.9008	1.3690	0.4170
13	A	462.3167	0.1530	1.7668
14	A	505.8023	1.4297	0.0364
15	A	525.1222	0.9259	0.9270
16	A	542.0815	1.6625	3.4970
17	A	611.8683	0.7763	4.1908
18	A	677.4239	2.5405	0.3240
19	A	680.8179	1.4163	5.7883
20	A	692.8671	2.1969	7.2428
21	A	783.1819	2.5270	0.0048
22	A	844.1886	1.8892	59.0465
23	A	849.1648	0.6850	33.5170
24	A	994.5618	2.6688	49.0866
25	A	1126.0410	4.7110	101.0775
26	A	1165.3517	1.7480	12.4415
27	A	1203.3798	1.2302	31.0566
28	A	1290.9824	9.1677	88.9622
29	A	1336.2703	7.6013	5.0644
30	A	1393.2721	10.8348	31.0664
31	A	1518.3510	7.0102	41.1902
32	A	1549.3128	7.9391	295.5664
33	A	1638.7848	4.0445	8.1034
34	A	1663.2809	3.5890	165.2718
35	A	1703.5244	11.6716	326.7994
36	A	2388.9761	42.5917	64.9717
37	A	3251.1316	6.8136	8.4683
38	A	3630.1371	8.1194	124.5719
39	A	3753.2823	9.1780	82.0319

molE_m062x

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	80.1013	0.0592	1.2807
2	A	126.5462	0.1173	4.5247
3	A	135.5698	0.1284	1.3998
4	A	185.8563	0.1949	0.2211
5	A	218.4336	0.4310	0.2826
6	A	245.2240	0.1993	1.6535
7	A	260.6727	0.0492	256.4950
8	A	304.1185	0.2664	3.2662
9	A	323.2110	1.0325	4.4941
10	A	367.3370	0.8125	5.8530
11	A	376.3172	0.4834	0.6103
12	A	448.1006	0.1420	4.3429
13	A	456.6803	1.4709	0.2720
14	A	506.4357	1.4209	0.1633
15	A	518.5775	1.0870	1.1133
16	A	540.8565	1.6097	4.6949
17	A	603.6844	0.8288	3.9520

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18	A	664.6650	2.2754	0.2926
19	A	676.3413	1.4313	4.3471
20	A	691.1798	2.1541	6.8710
21	A	747.4031	2.9818	0.1744
22	A	837.1776	0.6167	33.7771
23	A	848.9623	1.9509	60.0167
24	A	998.2478	2.5914	48.5714
25	A	1134.7214	4.5562	91.4145
26	A	1170.4997	1.6285	5.2550
27	A	1197.3863	1.2584	27.2239
28	A	1298.8489	9.3814	84.1005
29	A	1339.7313	7.1112	6.5644
30	A	1400.4076	11.1262	26.0475
31	A	1519.8864	6.8431	35.2495
32	A	1557.1471	8.5429	321.9502
33	A	1639.7085	2.8885	29.0029
34	A	1666.5065	5.6329	130.2485
35	A	1701.7369	11.8716	305.6373
36	A	2399.3840	42.9700	56.1379
37	A	3259.3032	6.8474	11.0008
38	A	3618.8256	8.0739	122.8317
39	A	3744.5092	9.1264	83.3107

molE_mp2

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	78.3444	0.0551	1.8610
2	A	120.0836	0.1048	4.2315
3	A	131.9000	0.0883	4.4238
4	A	181.2208	0.1984	0.2954
5	A	215.6558	0.4138	0.2950
6	A	240.2749	0.2098	0.6514
7	A	298.0896	0.2606	2.1535
8	A	319.2289	1.0744	1.5119
9	A	358.3494	0.1803	5.3649
10	A	364.7938	0.6424	4.9536
11	A	389.0035	0.1588	11.2094
12	A	444.6790	1.2881	0.4738
13	A	463.4620	0.9277	2.6307
14	A	489.6581	1.4177	2.3653
15	A	528.5781	0.9754	32.3506
16	A	546.9346	0.5393	43.5836
17	A	582.8870	0.3626	235.6259
18	A	621.0343	1.4689	5.4196
19	A	662.5351	1.3936	2.9502
20	A	682.8388	2.2210	5.6032
21	A	793.8212	2.0182	2.0425
22	A	826.0606	0.6242	27.1340
23	A	844.2324	2.0354	67.4671
24	A	996.1879	3.1806	44.2195
25	A	1105.1121	5.5639	62.5251
26	A	1193.7801	1.5292	20.2713
27	A	1201.6885	1.1338	9.5268
28	A	1279.5290	7.9838	50.2092

29	A	1368.1488	10.7743	9.5100
30	A	1466.7831	12.0805	12.6722
31	A	1507.7208	8.6891	54.9038
32	A	1526.8307	7.7893	277.7229
33	A	1627.2049	5.1975	9.8093
34	A	1658.6377	3.3866	48.2570
35	A	1685.1052	5.8565	200.3056
36	A	2178.7853	35.2477	2.1944
37	A	3256.4487	6.8354	6.0028
38	A	3589.9182	7.9555	70.8538
39	A	3710.8287	8.9304	51.6862

molE_pbe0d

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	79.0575	0.0582	0.9975
2	A	126.4892	0.1160	4.7570
3	A	132.5095	0.1347	1.2019
4	A	185.3322	0.1867	0.5038
5	A	217.4880	0.4249	0.3827
6	A	241.4557	0.0394	241.5786
7	A	246.6823	0.2731	4.9098
8	A	299.5329	0.2482	3.5424
9	A	322.0376	1.0473	2.9076
10	A	366.9777	0.8191	5.6245
11	A	373.9077	0.5087	0.5197
12	A	453.7980	0.5869	0.4901
13	A	456.4360	0.1751	2.9711
14	A	504.1827	1.4289	0.1388
15	A	519.7999	0.9868	1.0612
16	A	541.2956	1.6342	4.6041
17	A	600.8731	0.7816	4.1531
18	A	664.9130	2.2827	0.1912
19	A	677.8373	1.4096	4.3504
20	A	690.9602	2.2095	6.6796
21	A	758.6452	3.0047	0.0583
22	A	825.1777	0.6105	32.2743
23	A	847.1962	1.9034	61.8140
24	A	995.7231	2.6621	49.1603
25	A	1128.9687	4.6154	85.2069
26	A	1169.9820	1.5640	4.6736
27	A	1196.9561	1.2753	27.3690
28	A	1296.7737	8.9312	76.6866
29	A	1366.2416	9.3266	9.3269
30	A	1405.7370	10.8432	40.5420
31	A	1518.2933	6.7870	14.7442
32	A	1548.2462	7.9556	316.5514
33	A	1632.2231	4.0610	5.9630
34	A	1658.6523	3.7974	137.1930
35	A	1696.6588	10.2656	331.4366
36	A	2357.2435	41.4214	67.6567
37	A	3253.6269	6.8222	7.5956
38	A	3632.1330	8.1339	106.8748
39	A	3759.0483	9.1947	75.1814

 molE_pbe

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	75.4147	0.0523	1.3536
2	A	120.7338	0.1052	4.6939
3	A	126.7798	0.1094	1.5485
4	A	176.1903	0.1787	0.2287
5	A	208.8713	0.3948	0.3467
6	A	235.9971	0.2144	0.0513
7	A	272.9908	0.0526	232.2068
8	A	288.7609	0.2288	3.4449
9	A	308.7818	0.8749	5.0337
10	A	352.5956	0.5122	2.5759
11	A	353.0928	0.7137	3.8711
12	A	435.8268	1.0673	0.2023
13	A	444.7886	0.1511	3.2253
14	A	482.8682	1.3094	0.2343
15	A	494.0430	0.7269	0.9707
16	A	518.8418	1.4818	5.6988
17	A	567.6689	0.6925	3.6332
18	A	627.4807	2.0506	0.0938
19	A	651.4820	1.3003	4.3663
20	A	664.2380	2.1095	6.2517
21	A	718.2990	2.8817	0.0212
22	A	776.5870	0.5315	29.4013
23	A	809.3658	1.8387	68.6550
24	A	949.4483	2.4766	46.3889
25	A	1075.2649	4.5252	76.8456
26	A	1128.0706	1.4115	8.0185
27	A	1153.4051	1.1731	30.2813
28	A	1236.3639	8.2354	69.5712
29	A	1307.6986	9.5467	15.7443
30	A	1369.9633	9.7616	27.5991
31	A	1453.0690	6.4564	17.9329
32	A	1475.9203	7.1229	274.7526
33	A	1554.1338	6.8803	17.5688
34	A	1589.5172	2.6765	83.6146
35	A	1623.1799	6.4223	319.8999
36	A	2235.5048	37.2152	60.4479
37	A	3165.1581	6.4494	6.2977
38	A	3514.4608	7.6141	88.3733
39	A	3636.5636	8.5984	63.9475

molE_rtpss

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	76.7884	0.0528	2.1667
2	A	119.1503	0.1020	4.6866
3	A	130.7154	0.0942	3.8258
4	A	177.1707	0.1840	0.2135
5	A	205.2459	0.3856	0.2645

6	A	237.2460	0.2066	0.4867
7	A	282.4912	0.2159	3.3636
8	A	305.4277	0.9556	0.9385
9	A	351.8380	0.7146	4.4401
10	A	352.6050	0.4070	5.5642
11	A	407.8763	0.1294	252.3382
12	A	428.4988	0.1579	7.1721
13	A	436.0069	0.4989	14.0537
14	A	482.2209	1.2735	1.2932
15	A	492.7302	1.0069	0.8394
16	A	521.7991	1.2497	14.6269
17	A	570.2376	0.7797	4.1005
18	A	625.8635	2.1753	0.1107
19	A	650.6720	1.3209	4.0272
20	A	666.7571	2.1682	6.8683
21	A	702.8740	3.0860	0.3218
22	A	794.9717	0.5244	28.1007
23	A	813.6315	1.9886	78.5095
24	A	954.7935	2.7284	44.9525
25	A	1077.2869	5.2238	68.8340
26	A	1151.2692	1.4603	20.2021
27	A	1175.5584	1.1692	30.4010
28	A	1239.9836	8.3666	65.5402
29	A	1312.3721	9.4884	13.2325
30	A	1375.9116	9.3659	25.1194
31	A	1464.1673	7.0445	17.5625
32	A	1485.2825	7.2036	289.0086
33	A	1571.0338	9.6866	27.3887
34	A	1619.5061	3.9378	71.6431
35	A	1646.5432	3.1017	260.7425
36	A	2249.8172	37.7029	57.3081
37	A	3194.7717	6.5713	2.7730
38	A	3502.9562	7.5680	58.4015
39	A	3619.5605	8.5057	46.0541

molE_wb97xd

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	79.1178	0.0585	0.7703
2	A	130.2476	0.1353	2.5031
3	A	132.0244	0.1348	3.9956
4	A	186.7232	0.1743	1.1154
5	A	216.0103	0.0329	244.7377
6	A	218.7510	0.3677	4.4042
7	A	247.1426	0.2352	0.0589
8	A	306.4851	0.2677	3.3982
9	A	323.1487	1.0925	2.4058
10	A	367.7599	0.8302	5.9836
11	A	376.4089	0.4653	0.6290
12	A	446.9614	0.1423	3.3253
13	A	456.9842	1.4674	0.3430
14	A	504.6757	1.4380	0.1069
15	A	520.0414	1.0842	1.1517
16	A	539.6490	1.6190	4.3146

17	A	607.3459	0.8056	3.8711
18	A	670.4956	2.4163	0.2402
19	A	680.1459	1.4851	4.3829
20	A	689.7386	2.0905	7.9576
21	A	764.4227	2.7264	0.0082
22	A	841.5543	0.6454	33.3679
23	A	843.7462	1.9640	63.8172
24	A	990.8058	2.7038	47.3053
25	A	1124.7600	5.0760	92.6338
26	A	1169.2173	1.6613	15.4638
27	A	1204.2099	1.2154	28.2982
28	A	1287.4266	9.2736	86.2303
29	A	1340.9423	7.6187	6.6230
30	A	1389.8149	10.7707	33.1413
31	A	1516.3027	7.0813	32.3236
32	A	1546.6717	8.0588	309.3437
33	A	1639.2562	4.6085	5.1170
34	A	1665.7303	3.3861	138.6921
35	A	1700.5179	9.4737	329.6088
36	A	2372.6239	41.9992	63.1016
37	A	3248.9618	6.8050	6.2628
38	A	3640.3260	8.1707	103.7914
39	A	3765.9452	9.2301	71.9242

molE_x31yp

NM#	Symm	Wavenumber	Force Const	IR Intens
1	A	78.6431	0.0575	1.0017
2	A	128.3059	0.1214	4.3081
3	A	131.4337	0.1336	1.6306
4	A	183.7062	0.1824	0.4016
5	A	215.5307	0.4124	0.4592
6	A	235.6712	0.0393	243.1959
7	A	246.5991	0.2105	0.7031
8	A	301.9462	0.2541	3.4549
9	A	318.2993	1.0575	2.6382
10	A	363.5892	0.8286	6.4759
11	A	369.2523	0.5152	0.3847
12	A	451.5594	0.1719	2.6609
13	A	453.4834	0.5670	1.0653
14	A	499.1527	1.3946	0.1304
15	A	513.8700	0.9555	1.0316
16	A	532.5962	1.5667	4.6984
17	A	596.7380	0.7616	3.8231
18	A	660.7417	2.3796	0.2734
19	A	673.6381	1.4170	5.1362
20	A	683.3509	2.1477	7.5133
21	A	759.2935	2.7520	0.0157
22	A	827.8109	0.6220	31.6351
23	A	831.1592	1.9820	69.3574
24	A	974.4208	2.6342	46.5969
25	A	1105.1592	5.1444	86.3504
26	A	1159.7585	1.6243	19.0245
27	A	1196.0210	1.2095	30.6537

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28	A	1270.5515	8.9858	74.5364
29	A	1331.5444	8.3882	6.8576
30	A	1372.8191	9.8586	32.0407
31	A	1490.6643	7.3527	38.0062
32	A	1518.2752	7.4755	296.1858
33	A	1605.5284	9.0242	26.6075
34	A	1644.6810	3.0596	75.8848
35	A	1670.7412	4.7452	339.3517
36	A	2332.5982	40.5894	65.1067
37	A	3233.8781	6.7358	6.5937
38	A	3603.2541	8.0017	105.4098
39	A	3724.1512	9.0268	70.3328

Performance of the different levels of theory. Standard deviations (std dev), intercepts (a_0), slopes (a_1) and correlation coefficients (R^2) as obtained upon least squares linear regression of the computed values of the vibrational wavenumbers vs the experimental values. N indicates the number of matching normal modes.

	APF[D]	B3LYP[D]	BLYP	CAM-B3LYP[D]	M06-2X	PBE	PBE0[D]	RevTPSS	wB97-X[D]	X3LYP	MP2
N	48	49	46	47	49	48	48	51	46	48	49
std dev / cm^{-1}	69.8	61.5	30.9	79.9	78.8	73.0	26.0	19.1	79.2	69.8	49.6
a_0 / cm^{-1}	-15.9	1.6	0.7	-15.5	-18.2	-13.8	-21.3	-11.8	-17.3	-15.9	-0.3
a_1	1.02053	1.00902	0.99341	1.02460	1.02463	1.02292	1.00646	1.00428	1.02532	1.02053	1.00112
R^2	0.99728	0.99773	0.99939	0.99679	0.99662	0.99724	0.99960	0.99974	0.99687	0.99728	0.99833

Calculated $S_n \leftarrow S_0$ ($n = 1$ to 5) excitation wavelengths (in nm) at different levels of theory.

Functional	A					B					C					D					E						
	S1-S0	S2-S0	S3-S0	S4-S0	S5-S0	S1-S0	S2-S0	S3-S0	S4-S0	S5-S0	S1-S0	S2-S0	S3-S0	S4-S0	S5-S0	S1-S0	S2-S0	S3-S0	S4-S0	S5-S0	S1-S0	S2-S0	S3-S0	S4-S0	S5-S0		
B3LYP[D]	252.29	250.14	244.45	219.76	208.94	240.39	212.37	209.97	256.80	245.50	244.73	208.90	208.02	259.61	237.10	223.08	220.88	286.47	239.31	228.60	219.37	228.77	238.92	230.03	214.83	210.71	
(TD) 6-31+G**	250.45	249.88	232.45	219.14	208.77	241.58	201.67	201.01	252.75	244.73	234.71	207.80	207.19	259.00	237.10	223.08	220.88	286.47	239.31	228.60	219.37	228.77	238.92	230.03	214.83	210.71	
(TD) 6-31++G**	254.09	249.97	245.75	219.40	209.78	258.21	243.38	241.77	214.60	211.72	258.54	246.80	245.54	210.17	208.59	201.22	258.15	238.92	224.16	219.44	288.44	240.39	238.85	243.38	215.23	210.58	
(TDA) 6-31++G**	252.24	249.38	233.63	218.80	208.19	231.87	214.09	206.05	254.51	245.59	235.74	208.48	207.83	290.84	257.53	229.80	223.84	288.44	238.46	218.72	288.44	240.39	238.85	243.38	215.23	210.58	
(TD) Aug-cc-pVDZ	254.83	253.49	246.47	222.69	210.98	259.32	247.00	242.80	216.75	213.42	259.48	250.20	246.71	212.10	211.00	203.86	260.64	239.80	227.16	220.86	290.65	241.70	241.36	244.42	217.52	212.23	
(TD) Aug-cc-pVTZ	284.44	252.93	234.32	222.09	209.37	256.09	246.57	232.56	216.26	212.57	255.36	249.29	236.38	210.17	202.35	260.00	230.70	226.80	220.16	228.64	241.28	241.28	223.53	245.72	211.79	212.58	
(TDA) Aug-cc-pVTZ	254.84	252.76	246.90	222.56	211.10	259.34	246.34	246.34	216.92	213.72	259.67	249.54	247.02	212.10	211.13	204.54	260.25	240.73	227.11	221.01	291.16	242.29	241.37	218.20	212.58	212.58	
(TD) Aug-cc-pVTZ	252.90	252.19	234.75	221.94	209.44	256.03	245.89	232.97	216.42	209.19	255.40	248.97	236.82	211.31	210.33	235.85	259.60	231.51	226.78	220.25	283.02	240.99	233.35	218.07	212.07	212.07	
BLYP	281.59	274.22	261.62	249.25	234.92	277.30	269.07	253.32	235.16	226.46	276.99	274.12	263.46	234.90	232.23	328.57	299.90	254.27	252.89	247.04	270.62	255.68	242.09	237.48	237.48	237.48	237.48
(TD) 6-31+G**	280.97	272.13	248.73	247.34	234.82	274.18	268.56	244.72	234.91	232.58	273.66	272.90	250.52	234.57	232.07	316.62	299.28	252.78	246.38	243.38	304.07	270.24	244.73	241.97	237.48	237.48	
(TD) 6-31++G**	281.21	275.88	262.59	249.23	233.77	279.30	253.53	258.42	238.09	235.65	278.72	275.23	264.20	235.85	233.12	345.95	297.20	255.88	253.11	245.95	314.44	269.01	256.97	242.00	237.89	237.89	
(TDA) 6-31++G**	280.65	273.92	248.74	248.16	233.67	276.26	271.02	245.74	237.05	245.74	251.19	235.64	232.96	238.96	232.06	296.69	252.99	245.32	244.73	306.06	268.68	246.09	241.89	237.86	237.86	237.86	
(TD) Aug-cc-pVDZ	285.46	276.71	263.32	253.53	235.08	280.80	276.00	259.23	240.45	239.35	280.52	279.18	264.88	240.05	235.33	333.56	299.32	256.95	255.58	247.43	317.00	271.43	258.20	244.53	239.07	239.07	
(TD) Aug-cc-pVTZ	284.84	274.56	253.03	248.82	234.98	278.29	274.87	246.48	240.29	238.68	279.69	275.41	251.85	239.73	235.18	321.41	298.65	255.75	246.90	246.26	308.18	271.02	247.01	244.42	238.96	238.96	
(TDA) Aug-cc-pVTZ	284.44	275.58	263.56	252.99	235.12	280.60	275.30	259.43	240.64	238.96	280.03	276.88	265.10	235.50	234.15	299.24	257.63	255.68	247.64	271.56	315.56	259.06	245.72	239.06	239.06	239.06	
(TD) Aug-cc-pVTZ	283.88	274.44	252.49	249.10	235.01	277.85	274.37	246.80	240.44	238.3	278.81	275.38	252.18	239.20	235.36	321.90	298.68	255.69	247.09	246.55	308.54	271.22	247.83	245.61	238.87	238.87	
CAM-B3LYP[D]	241.00	234.18	231.95	204.44	194.67	245.15	230.99	224.14	198.44	196.32	245.77	234.10	228.39	195.58	193.66	281.34	234.92	226.74	203.17	270.71	228.06	220.37	228.06	220.37	196.59	196.59	
(TD) 6-31+G**	238.36	231.34	223.75	203.72	192.03	241.20	223.81	222.18	197.68	188.71	241.10	227.86	225.11	193.16	190.77	271.03	234.25	218.88	204.84	202.42	262.45	220.54	219.92	196.10	193.35	193.35	
(TD) 6-31++G**	243.01	235.79	231.37	203.65	189.95	247.21	225.75	225.07	200.20	198.03	247.66	235.71	228.52	197.01	193.65	283.82	233.94	218.88	206.15	202.84	272.82	229.93	220.24	199.86	196.39	196.39	
(TDA) 6-31++G**	240.31	230.75	225.20	202.92	191.69	243.20	225.03	223.47	199.55	188.8	242.98	228.07	226.41	193.20	191.59	273.40	233.26	220.70	205.65	202.00	264.51	222.21	219.79	195.94	193.17	193.17	
(TD) Aug-cc-pVDZ	244.03	236.69	234.37	206.35	192.23	248.57	233.50	228.44	202.25	199.92	248.89	236.43	231.94	198.53	196.34	286.64	236.62	229.85	208.66	204.35	275.19	231.10	223.13	201.53	198.35	198.35	
(TD) Aug-cc-pVTZ	241.29	233.78	226.07	205.61	191.99	244.51	228.22	224.49	201.35	191.35	244.12	231.50	227.23	195.90	193.90	276.09	235.93	228.22	208.22	206.82	266.82	223.37	222.69	197.93	197.93		
(TDA) Aug-cc-pVTZ	244.07	237.20	233.73	206.40	192.46	248.64	233.87	227.79	202.34	200.26	249.12	236.85	231.29	198.86	196.36	287.32	236.25	230.79	208.39	204.49	275.72	231.98	222.78	201.93	198.61	198.61	
(TD) Aug-cc-pVTZ	241.27	233.13	226.56	205.64	192.23	244.49	227.58	224.90	201.65	191.84	244.21	230.84	226.61	195.90	194.32	276.61	235.55	222.61	207.93	203.57	267.22	224.16	222.34	198.15	193.94	193.94	
PBE0[D]	246.81	239.97	239.65	211.92	203.35	250.72	236.15	229.95	205.81	203.11	251.52	240.17	234.42	204.01	200.52	292.71	250.42	232.29	215.01	213.18	280.49	233.86	230.01	207.23	203.67	203.67	
(TD) 6-31+G**	244.92	239.21	228.33	211.24	202.43	247.43	229.70	226.35	203.33	196.92	247.31	234.01	230.38	200.29	199.40	282.46	249.78	233.78	214.68	212.46	272.57	229.62	225.62	207.03	203.40	203.40	
(TD) 6-31++G**	248.44	241.19	239.97	211.94	204.78	252.46	237.61	231.86	207.35	205.75	253.07	241.41	235.55	205.26	201.56	294.79	249.58	235.99	215.97	212.95	282.29	235.44	229.86	207.56	204.66	204.66	
(TDA) 6-31++G**	246.52	239.49	229.45	211.27	202.18	249.14	231.76	227.53	206.10	197.79	248.89	235.21	231.35	201.35	199.90	284.50	248.91	235.33	215.65	212.20	274.35	229.46	227.05	207.37	203.79	203.79	
(TD) Aug-cc-pVDZ	249.38	245.24	241.74	214.78	206.07	253.66	238.38	235.43	209.32	207.6	254.13	242.07	239.08	206.61	203.59	297.80	251.93	235.02	218.59	214.38	284.85	236.55	232.41	209.94	206.26	206.26	
(TD) Aug-cc-pVTZ	247.43	242.59	230.18	214.11	202.90	250.32	235.40	228.29	208.11	200.24	249.88	238.84	232.02	203.30	202.47	287.37	251.26	226.31	213.62	216.76	276.83	233.01	228.13	209.77	204.64	204.64	
(TDA) Aug-cc-pVTZ	249.37	242.66	241.93	214.68	206.20	253.65	238.60	234.75	209.50	207.73	254.31	242.33	238.36	206.88	203.51	298.43	251.32	235.94	218.39	214.36	285.27	237.44	231.94	210.26	206.64	206.64	
(TD) Aug-cc-pVTZ	247.34	241.76	230.58	213.99	202.88	250.21	234.64	228.65	208.10	200.21	249.89	238.06	232.42	203.22	202.39	287.82	250.63	227.13	218.09	213.54	277.13	231.54	228.93	210.09	204.67	204.67	
PBE	275.95	273.18	260.25	245.04	233.19	275.66	261.78	255.70	233.88	229.37	275.55	267.29	262.09	229.85	229.18	328.35	316.14	298.29	252.57	251.40	344.69	312.08	267.05	253.99	240.22	23	